MODELING THE ADSORPTION AND DESORPTION OF MUNITION CONSTITUENTS ON SOILS USING REVERSIBLE AND RESISTANT COMPONENTS

by

Andrew N. Miglino

A dissertation submitted to the Faculty of the University of Delaware in partial fulfillment of the requirements for the degree of Doctor of Philosophy in Civil Engineering

Spring 2015

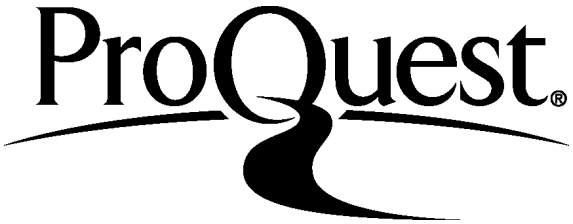
© 2015 Andrew N. Miglino
All Rights Reserved

ProQuest Number: 3718358

All rights reserved

INFORMATION TO ALL USERS
The quality of this reproduction is dependent upon the quality of the copy submitted.

In the unlikely event that the author did not send a complete manuscript
and there are missing pages, these will be noted. Also, if material had to be removed,
a note will indicate the deletion.



ProQuest 3718358

Published by ProQuest LLC (2015). Copyright of the Dissertation is held by the Author.

All rights reserved.
This work is protected against unauthorized copying under Title 17, United States Code
Microform Edition © ProQuest LLC.

ProQuest LLC.
789 East Eisenhower Parkway
P.O. Box 1346
Ann Arbor, MI 48106 - 1346

MODELING THE ADSORPTION AND DESORPTION OF MUNITION CONSTITUENTS ON SOILS USING REVERSIBLE AND RESISTANT COMPONENTS

by

Andrew N. Miglino

Approved: _____
Harry W. Shenton III, Ph.D.
Chair of the Department of Civil Engineering

Approved: _____
Babatunde Ogunnaike, Ph.D.
Dean of the College of Engineering

Approved: _____
James G. Richards, Ph.D.
Vice Provost for Graduate and Professional Education

I certify that I have read this dissertation and that in my opinion it meets the academic and professional standard required by the University as a dissertation for the degree of Doctor of Philosophy.

Signed: _____

Dominic M. Di Toro, Ph.D.
Professor in charge of dissertation

I certify that I have read this dissertation and that in my opinion it meets the academic and professional standard required by the University as a dissertation for the degree of Doctor of Philosophy.

Signed: _____

Herbert E. Allen, Ph.D.
Member of dissertation committee

I certify that I have read this dissertation and that in my opinion it meets the academic and professional standard required by the University as a dissertation for the degree of Doctor of Philosophy.

Signed: _____

Pei Chiu, Ph.D.
Member of dissertation committee

I certify that I have read this dissertation and that in my opinion it meets the academic and professional standard required by the University as a dissertation for the degree of Doctor of Philosophy.

Signed: _____

Richard Carbonaro, Ph.D.
Member of dissertation committee

ACKNOWLEDGEMENTS

Firstly, I would like to thank my advisors, Dr. Dominic Di Toro and Dr. Herbert Allen, who have guided me and taught me along the way. Without their insight and patience, very little of this would be possible.

I want to thank the rest of my committee, Dr. Pei Chiu and Dr. Richard Carbonaro. Your comments and advice has proved invaluable. Dr. Carbonaro, thanks for being a part of my academic career for many years.

I'd like to also thank my co-workers. Those of you who have shared an office with me most of all, since you've had to deal with all my mumbling. Craig, Eva, Tifany, Solmaz, Rosalina, Undine, Yasemin and Cory, thank you for hearing me out when I needed to talk about research. And thank you for sharing your experiences here in Delaware with me.

I must also thank my funding agency, the Strategic Environmental Research and Development Program (SERDP). Their funding and thirst for novel research has allowed me to learn, grow, and most of all, discover.

Finally, thank you to my wife Kimberly. You've been a voice of reason and a great sounding board. Thank you for your patience in all of this.

TABLE OF CONTENTS

LIST OF TABLES . . . . . **x**
LIST OF FIGURES . . . . . **xii**
ABSTRACT . . . . . **xv**

Chapter

1 INTRODUCTION **1**

1.1 Motivation 1

1.1.1 Models of adsorption and desorption 5
1.1.2 Experimental data 6

REFERENCES 9

2 MODELING SOIL SORPTION HYSTERESIS USING A NORMALIZED REVERSIBLE RESISTANT MODEL **12**

2.1 Background 12
2.2 Materials and methods 14
2.3 Analysis 17

2.3.1 Data exclusion 17
2.3.2 Modeling adsorption partitioning 17
2.3.3 Modeling desorption partitioning 21

2.3.3.1 Reversible model 21
2.3.3.2 Reversible resistant model 22

2.3.3.3 Multilinear model of reversible resistant partition coefficients . . . 32

2.4 Reversibility fraction . . . 37
2.5 Predictive model . . . 40
2.6 Conclusions . . . 40

REFERENCES . . . 43

3 MODELING MUNITION CONSTITUENT ADSORPTION AND DESORPTION HYSTERESIS ON SOILS USING THE SITE TRANSFORMATION MODEL . . . 48

3.1 Background . . . 48
3.2 Data and modeling procedure . . . 49

3.2.1 Isotherm determination . . . 56
3.2.2 Model parameter dependencies . . . 57

3.3 Analysis . . . 61

3.3.1 Binding constants - K_P and K_L . . . 61
3.3.2 Site transformation factor . . . 63
3.3.3 Comparing reversible resistant and site transformation models 69
3.3.4 Multilinear predictive model . . . 70

3.4 Conclusions . . . 73

REFERENCES . . . 75

4 MODELING TRANSPORT OF MUNITION CONSTITUENTS IN A SOIL COLUMN USING REVERSIBLE RESISTANT PARTITIONING . . . 78

4.1 Materials and methods . . . 79
4.2 Analysis . . . 81
4.3 Conclusions . . . 92

REFERENCES 93

5 MODELING MUNITION CONSTITUENT ADSORPTION AND DESORPTION HYSTERESIS USING DIFFUSION LIMITED TRANSPORT 95

5.1 Background 95
5.2 Data 97
5.3 Heterogeneous particle model 97
5.4 Conclusions 110

REFERENCES 111

6 CONCLUSIONS 113

Appendix

A NORMALIZED REVERSIBLE AND RESISTANT SORPTION SUPPLEMENTAL INFORMATION 116

A.1 Data treatment 116

A.1.1 Normalized aqueous and sorbed concentrations 116

A.2 Reversible model 146

A.2.1 Derivation of linear model 146
A.2.2 R code for linear fit 147
A.2.3 Reversible model parameters 150
A.2.4 Reversible model plots 155
A.2.5 Reversible model additional analysis 180

A.2.5.1 Multilinear model of reversible resistant partition coefficients 183

A.3 Reversible resistant model 184

A.3.1 Derivation of normalized reversible resistant isotherm 184

A.3.2 Derivation of normalized reversible resistant model 185
A.3.3 R code for reversible resistant fit 187
A.3.4 Reversible resistant model parameters 191

A.3.4.1 Reversible resistant model K_x 191
A.3.4.2 Reversible resistant model K_0 196

A.3.5 Reversible resistant model multilinear parameters 201
A.3.6 Reversible resistant model plots 202

B SITE TRANSFORMATION MODEL SUPPLEMENTAL INFORMATION 232

B.1 Isotherms 232
B.2 Derivation of Langmuir STM 259
B.3 Model code 262

B.3.1 Determination of dependencies 262
B.3.2 Linear/Langmuir split 269
B.3.3 STM model code 271

B.4 Model fit figures 281
B.5 STM parameters 308

B.5.1 K_P and K_L 308
B.5.2 f_{ST} 313

C TRANSPORT OF MC IN A COLUMN 314

C.1 MATLAB code 314

D DIFFUSION MODEL 320

D.1 2-layer model 320

D.1.1 Lognormal distribution of particle sizes 340

D.2 n-layer model 342

E DATA TABLES **350**

E.1 Column experiment 350
E.2 Batch experiment 353

E.2.1 Soils used 353
E.2.2 General soil properties 354
E.2.3 Trace metal analysis using USEPA 3051 356
E.2.4 25 soil sequential desorption experiment 358

LIST OF TABLES

2.1 Nominal concentrations for adsorption-desorption experiment . . 16

2.2 Multilinear partition coefficients K_{OC} 33

2.3 Multilinear partition coefficients K_{clay} 33

3.1 Dependencies of STM parameters 57

3.2 Multilinear model parameters for K_P 63

3.3 Regression coefficients for f_{ST} 66

4.1 Soils used in column analysis 81

4.2 Column model fit parameters for SSL soil 85

4.3 Multilinear derived partition coefficients for soils in column experiment 85

4.4 Reversible and resistant partition coefficients estimated for column experiment 86

4.5 Column parameters for 5 soil simulation 89

A.1 Reversible adsorption K_P 150

A.2 Reversible resistant desorption K_x 191

A.3 Reversible resistant desorption K_0 196

A.4 Multilinear parameters for reversible resistant K_x and K_0 201

B.1 STM partition coefficients 308

B.2 STM f_{ST} 313

E.1 Column experiment concentrations 351

E.2 Extracted concentrations by depth 352

E.3 Soil properties 355

E.4 Trace metal analysis 357

E.5 Concentration data for 25 soil experiment 359

LIST OF FIGURES

1.1 Hysteretic example isotherm 4

1.2 Structure of munition constituents (MC) 7

2.1 Illustration of batch sorption experiment 16

2.2 Reversible model vs observed 23

2.3 Reversible resistant model vs. observed 29

2.4 Reversible resistant Root Mean Square Error 30

2.5 Residuals for reversible and reversible resistant models 31

2.6 Reversible resistant K_x 35

2.7 Reversible resistant K_0 36

2.8 Multilinear partition coefficients for reversible resistant model K_x 37

2.9 Multilinear partition coefficients for reversible resistant model K_0 38

2.10 Reversibility fraction 39

2.11 Multilinear predicted reversible and RR sorbed concentrations . . 41

3.1 Comparison of modeled and observed sorbed concentrations for a reversible model 52

3.2 Example isotherms 53

3.3 Illustration of Site transformation model 55

3.4 Comparison of K_P determined for each MC, sorbent, and adsorption contact time. 59

3.5 Comparison of STM and observed sorbed concentrations 62

3.6 STM K_P and K_L 64

3.7 Site transformation factor 65

3.8 Regression of f_{ST} slope and intercept 67

3.9 Estimated vs. predicted f_{ST} 68

3.10 STM RMSE compared to reversible resistant model 71

3.11 Comparison of STM predicted and observed sorbed concentrations 72

3.12 Predictive site transformation model residuals 74

4.1 Breakthrough curve for column experiment 80

4.2 Modeled and observed aqueous concentrations for column experiment 84

4.3 RDX and TNT concentrations in 3m column for an 18 d (432 h) simulation 88

4.4 RDX bulk concentrations for 5 soil column simulation 90

4.5 TNT bulk concentrations for 5 soil column simulation 91

5.1 Linear residuals from the two-particle model for 5 MC 107

A.1 Normalized aqueous and sorbed concentrations 116

A.2 Reversible model fit for all sorbents and MC 155

A.3 Reversible model root mean square error 181

A.4 Reversible resistant K_P 182

A.5 Multilinear partition coefficients for reversible resistant model K_x 183

A.6 Reversible resistant model fit for all sorbents and MC 202

B.1 Isotherms for all sorbents and MC 232

B.2 STM fit for all sorbents and MC 281

ABSTRACT

The need to understand the fate of chemicals is important in performing risk assessments of chemical compounds. Munition constituents such as TNT and nitroglycerin, as well as newly developed compounds, are of significant concern due to the wide range of contamination across a variety of soil types. Currently, there are more than 15 million acres of potentially impacted soils where explosive and explosive related materials have been found in abundance. The bioavailability of these compounds and potential for transport to groundwater is controlled to a large degree by sorption onto soil.

Studies have shown both reversible and resistant (hysteretic) desorption behavior for chemicals on soils. Observations of 5 munition constituents sorbed to 25 soils and 2 reference sorbents show that a constant fraction of sorbed chemical is released during desorption. However, an analysis using a fully reversible linear partitioning model yields accurate predictions of desorption for only short adsorption contact times and only for low organic carbon containing soils. A model that accounts for incompletely reversible sorption, the reversible resistant model, improves predictive capabilities. The model′s partition coefficients can be correlated to soil properties, which allow predictions to be made for the sorption behavior of soils for which only the organic carbon and clay sized particle fraction is known.

However the dependence of the degree of hysteresis on adsorption contact time remained to be explained. Using a variable strength binding site model, the

site transformation model, shows that changes in binding strength are regular and predictable. Further, results suggest that the mechanism for hysteresis is related to soil organic carbon deformation during adsorption. To demonstrate the capabilities of the site transformation model, an a priori prediction of sorption behavior is presented. As a measure of implications for field study, a reversible resistant model is used to analyze soil column experiments. Results show the importance of accounting for hysteresis when applying bench scale results to field scale problems.

A diffusion model, employing multiple particle sizes, is developed to describe hysteresis. Results indicate the need for substantial sorbent properties for accurate modeling. An n-particle model is presented and future work is suggested.

Chapter 1

INTRODUCTION

1.1 Motivation

The need for adsorption and desorption studies arises out of the importance of determining the fate of chemicals in our environment. Studies of PAHs, PCBs, and other organic chemicals of concern have been performed previously to characterize the eventual outcome of introducing novel chemicals to soil, air and water. Chemicals can partition to multiple compartments: bulk aqueous, and interstitial aqueous solutions, and soil and sediment masses to name a few. Efforts to understand the equilibrium concentrations in these multiphase systems often use partition coefficients to describe the fate of the chemical.

The partitioning between soil and water is usually derived from a kinetic equation that quantifies the rates of adsorption to the soil and desorption from the soil:

$$\frac{dq}{dt} = k_{ads}C - k_{des}q \tag{1.1a}$$

where q is the sorbed concentration $[mg/g]$, C is the aqueous concentration $[mg/L]$, k_{ads} is the rate of adsorption $[L/mg - sec]$, and k_{des} is the rate of desorption $[1/sec]$. If the system is at steady state, then

$$\frac{dq}{dt} = 0 \tag{1.1b}$$

and Eq 1.1a becomes

$$k_{des}q = k_{ads}C \tag{1.1c}$$

and solving for the steady state sorbed concentration yields

$$q = \frac{k_{ads}}{k_{des}}C \tag{1.1d}$$

The partition coefficient, K_P [L/kg], is defined as the ratio of k_{ads} to k_{des} and describes the distribution of chemical between aqueous and sorbed phases:

$$q = K_P C \tag{1.1e}$$

The observed partition coefficient is usually soil and chemical specific. For example, a loamy soil will not necessarily behave the same as a sandy soil. To obtain a more universal partition coefficient, observed K_P for sorption to soils have been related to sorbate and sorbent specific properties, such as the mass fraction of organic carbon, f_{OC} [Karickhoff et al., 1979]

$$K_P = f_{OC}K_{OC} \tag{1.2}$$

where K_{OC} is the partition coefficient for sorption to organic carbon. In this relationship, the observed partition coefficient, K_P, is related to the organic carbon content of the sorbent, f_{OC}, by a partition coefficient describing the sorption to organic carbon, K_{OC}. In this way, a sorbent specific parameter, f_{OC} and a sorbate specific parameter, K_{OC}, are used to predict an observed partition coefficient for a sorbent-sorbate pair.

A shortcoming of equilibrium models, however, is that they assume equilibrium has been achieved. This may require long periods of contact time between sorbent and sorbate which is unlikely to be replicated in the laboratory [Steinberg et al., 1987]. Even after an apparent equilibration is observed, slow sorption processes may occur resulting in potentially large disparities between the partition coefficients obtained using equilibrium approaches [Brusseau et al., 1991].

The slow equilibration of many compounds is a frequent problem. Empirically derived models are often used to explain the behavior between initial contact and eventual equilibration [Lagergren, 1898; Ho and McKay, 1999], but these models require sorbent and sorbate specific parameters and they often yield site specific results.

An alternative to empirical slow adsorption models are models based on diffusive exchange between aqueous and sorbed compartments [Sabbah and Rebhun, 1997]. Diffusion also requires site specific parameters, however, as exchange rates are not universal and specificity to site characteristics is necessary for accurate modeling.

Given that the adsorption of chemical is potentially difficult to predict universally, it should not be surprising that predicting desorption is also fraught with problems. A major problem is the observation of hysteresis. Hysteresis occurs when adsorption and desorption partitioning are not consistent in magnitude [Karickhoff and Morris, 1985]. This is most easily observed using isotherm plots, where the sorbed concentration is plotted against the aqueous concentration, Figure 1.1.

Adsorption followed by sequential desorptions are used to analyze this problem. Adsorption is allowed to occur for a period of time and then repeated desorption steps are performed with a regular interval between each, indicated by subscripts $D1$ and $D2$ in Figure 1.1. Experimentally, this involves the replacement of the aqueous

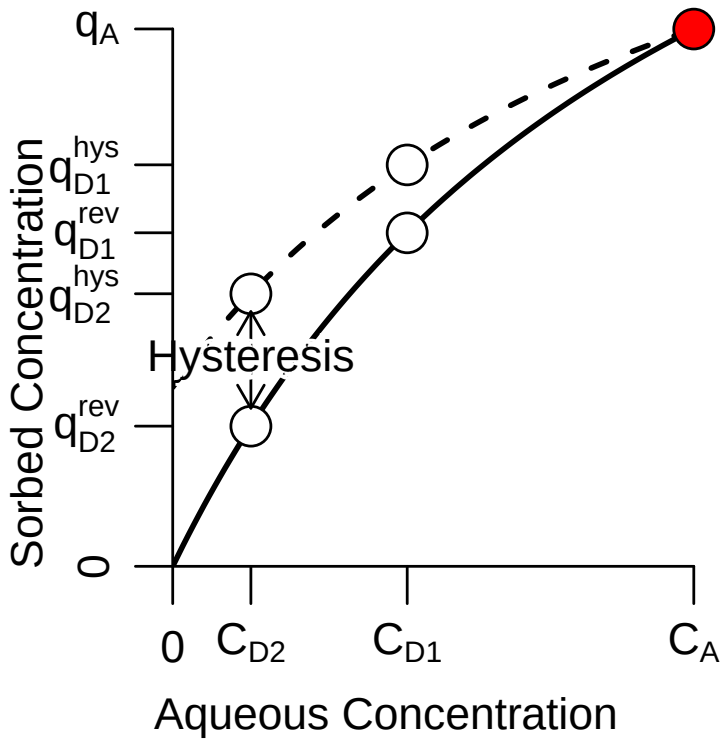


Figure 1.1: An example of an isotherm showing hysteretic behavior. Sorbed concentration, q. versus aqueous concentration, C. The subscripts A, $D1$, and $D2$ refer to a sequence of adsorption, and two sequential desorptions. Solid line shows adsorption behavior while the dashed line shows desorption behavior for the sorbent-sorbate pair. Data are synthetic.

phase to allow the chemical to reach a new apparent equilibrium. During this sequence, chemical is repeatedly depleted from the sorbed phase, and an analysis of the desorption isotherm can be made.

The discrepancy between the two lines in Figure 1.1 can be attributed to a difference in behavior depending on whether the system is adsorbing or desorbing. This behavior has been observed for many chemical types, including pesticides, PCBs, PAHs, [Pignatello and Xing, 1996] and other organic compounds [Kan et al., 1998]. Efforts to model hysteresis can be grouped into three major groups.

1.1.1 Models of adsorption and desorption

The first group of models treats adsorption and desorption similarly in that both are described by partitioning, as in Eq 1.1e or a variant thereof, and a transport processes, often diffusion [Wu and Gschwend, 1988]. The observed hysteresis is the result of the slow desorption of chemical from interior binding sites followed by diffusion into the bulk aqueous compartment [van Beinum et al., 2006]. The assumption is that the material is reversibly sorbed, but the experiment did not wait long enough to observe a true equilibrium [Sabbah et al., 2005].

The second group suggests, similarly to the first group, that there are fast rates of adsorption that account for the observed apparent equilibrium during adsorption and slower reversible or irreversible sorption rates that account for the hysteretic fraction observed during desorption [Cornelissen et al., 1997]. Reasons for irreversibility include crystallization of the sorbate, multiple sorption sites with differing rates of sorption, or a loss of the sorbate via mineralization [Limousin et al., 2007]. Most of these models employ an empirical relationship such as a fast and slow first order rate, Eq 1.3

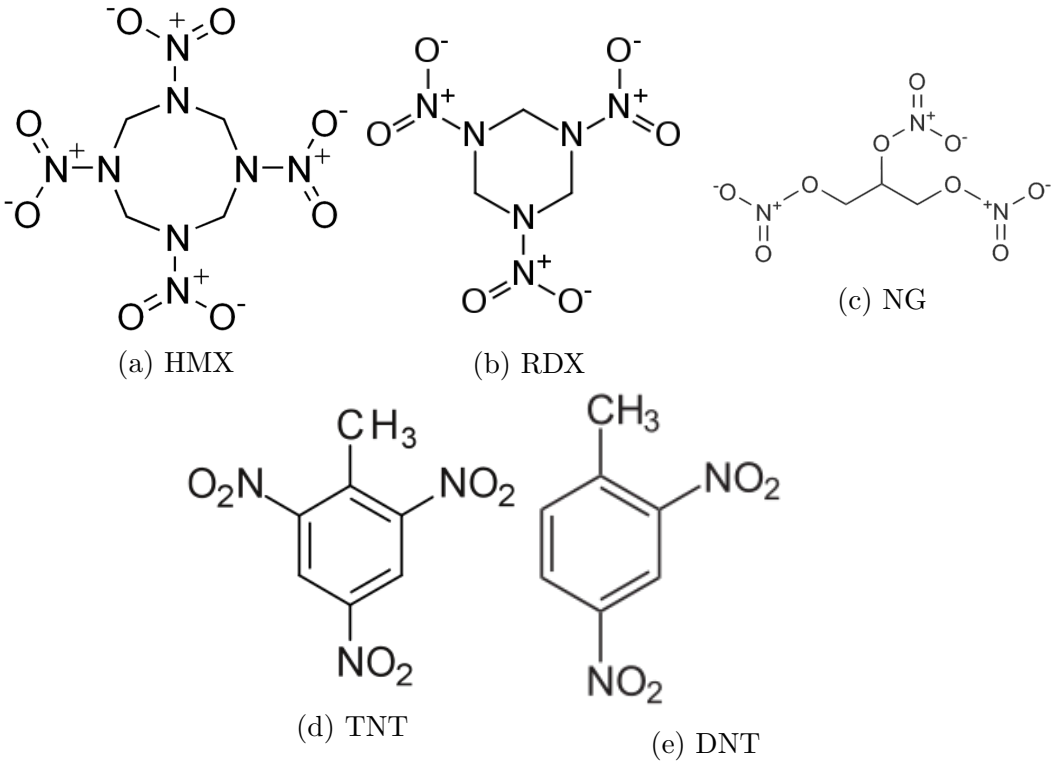
$$\frac{q(t)}{q(0)} = \phi_{fast} e^{-k_{fast} t} + (1 - \phi_{fast}) e^{-k_{slow} t} \tag{1.3}$$

where $q(t)$ is a sorbed concentration at time t, ϕ_{fast} is the fraction of chemical associated with fast desorption, and k_{fast} and k_{slow} are first order rate constants for the *fast* and *slow* desorption processes, respectively. As with the diffusion models of the first group, however, it is difficult to develop universal models or relationships that can be used at multiple locations for multiple chemicals [Birdwell et al., 2007].

The final group is based on the idea that there is a fundamental difference between adsorption and desorption. To describe desorption partitioning, the adsorption partition coefficient cannot be used. Instead, a separate isotherm, describing the desorption behavior is used. Though there are many fewer of these models, they have been applied to multiple sorbents and sorbates with some success [Di Toro and Horzempa, 1982; Di Toro et al., 1985; Di Toro, 2013]. Moreover, there is evidence to suggest that the equilibration process itself brings about fundamental changes to the sorbent, allowing for a change in binding site strength as a function of adsorption [Sander and Pignatello, 2005; Sander et al., 2006]. Much like the K_{OC} models, the adsorption and desorption partition coefficients can be related to sorbent and sorbate properties [Gonzalez Forero, 2013].

1.1.2 Experimental data

The development of meaningful relationships between hysteresis and sorbent and sorbate properties requires a large data set with multiple sorbents and sorbates that employs varying adsorption and desorption times. The present work uses the data generated as part of the SERDP ER-1688 research project [Allen et al., 2015]. Five munition constituents (MCs), RDX, HMX, NG, TNT and 2,4-DNT, illustrated in Figure 1.2, were used in all experiments as the sorbates. These munitions are nitro-substituted aliphatics, aromatics and nitroamines and their partition coefficients are likely to be different resulting in differring adsorption and desorption behaviors. Each



(a) HMX (b) RDX (c) NG

(d) TNT (e) DNT

Figure 1.2: Structure of munition constituents (MC) (a) octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine (HMX) (b) 1,3,5-trinitroperhydro-1,3,5-triazine (RDX) (c) 1,2,3-trinitroxypropane (NG) (d) 2,4,6-trinitrotoluene (TNT) (e) 2,4-dinitrotoluene (DNT).

sorbate was amended to 25 soil sorbents and 2 reference sorbents. The soils were selected to represent the variations found in field conditions as well as both high and low organic carbon and fraction clay size particles.

Using this large data set, several key topics are addressed in this dissertation:

- Determining the extent of hysteresis using both equilibrium and transport models,
- Understanding the effect of contact time between sorbent and sorbate, and
- Developing correlations and models to aid in prediction of adsorption and desorption partitioning

This dissertation comprises five chapters, each analyzing sorption data using a different modeling framework. Chapter 2 compares reversible and reversible resistant partitioning models to examine the extent of hysteresis. Using these partitioning models relationships of sorbent and sorbate properties are found. In addition it is shown that model incorporating adsorption contact time is necessary to fully describe resistant desorption.

In Chapter 3 the data are analyzed using a site transformation model in which resistance to desorption is related to sorbent and sorbate properties. Results of this model shows a relationship between the transformation of binding sites with adsorption contact time which suggests a possible mechanistic interpretation for MC hysteresis. Chapter 4 and 5 explore modeling the time dependence of adsorption and desorption as a transport processes both with and without resistant partitioning. Chapter 6 provides a summary of findings and a description of suggested future work.

Bibliography

Allen, H. E., Di Toro, D. M., Kuo, D. T. F., Gonzalez Forero, R., Michelson, R., Michelson, K., Miglino, A., Checkai, R. T., Kuperman, R. G., Simini, M., and Hawari, J. (2015). Improving understanding of the fate and transport of munitions constituents to enhance sustainability of operational ranges. Technical report, University of Delaware. SERDP Project ER-1688.

Birdwell, J., Cook, R. L., and Thibodeaux, L. J. (2007). Desorption kinetics of hydrophobic organic chemicals from sediment to water: A review of data and models. *Environmental Toxicology and Chemistry*, 26(3):424–434.

Brusseau, M., Jessup, R., and Rao, P. (1991). Nonequilibrium sorption of organic-chemicals - elucidation of rate-limiting processes. *Environmental Science & Technology*, 25(1):134–142.

Cornelissen, G., Rigterink, H., Vrind, B. A., tenHulscher, T. E. M., Ferdinandy, M. M. A., and vanNoort, P. C. M. (1997). Two-stage desorption kinetics and in situ partitioning of hexachlorobenzene and dichlorobenzenes in a contaminated sediment. *Chemosphere*, 35(10):2405–2416.

Di Toro, D. M. (2013). Site transformation model of adsorption-desorption hysteresis. *Abstracts of Papers of the American Chemical Society*, 245.

Di Toro, D. M. and Horzempa, L. M. (1982). Reversible and resistant components of PCB adsorption desorption - isotherms. *Environmental Science & Technology*, 16(9):594–602.

Di Toro, D. M., Jeris, J. S., and Ciarcia, D. (1985). Diffusion and partitioning of hexachlorobiphenyl in sediments. *Environmental Science & Technology*, 19(12):1169–1176.

Gonzalez Forero, R. (2013). *Factors Controlling the Reversible and Resistant Adsorption and Desorption of Munitions Constituents on Soils*. PhD dissertation. University of Delaware.

Ho, Y. S. and McKay, G. (1999). Pseudo-second order model for sorption processes. *Process Biochemistry*, 34(5):451–465.

Kan, A. T., Fu, G., Hunter, M., Chen, W., Ward, C. H., and Tomson, M. B. (1998). Irreversible sorption of neutral hydrocarbons to sediments: Experimental observations and model predictions. *Environmental Science & Technology*, 32(7):892–902.

Karickhoff, S., Brown, D., and Scott, T. (1979). Sorption of hydrophobic pollutants on natural sediments. *Water Research*, 13(3):241–248.

Karickhoff, S. W. and Morris, K. R. (1985). Sorption dynamics of hydrophobic pollutants in sediment suspensions. *Environmental Toxicology and Chemistry*, 4(4):469–479.

Lagergren, S. (1898). Zur theorie der sogenannten adsorption gelster stoffe. *Kungliga Svenska Vetenskapsakademiens. Handlingar*, 24(4):1–39.

Limousin, G., Gaudet, J. P., Charlet, L., Szenknect, S., Barths, V., and Krimissa, M. (2007). Sorption isotherms: A review on physical bases, modeling and measurement. *Applied Geochemistry*, 22(2):249–275.

Pignatello, J. J. and Xing, B. (1996). Mechanisms of slow sorption of organic chemicals to natural particles. *Environmental Science & Technology*, 30(1):1–11.

Sabbah, I., Ball, W. P., Young, D. F., and Bouwer, E. J. (2005). Misinterpretations in the modeling of contaminant desorption from environmental solids when equilibrium conditions are not fully understood. *Environmental Engineering Science*, 22(3):350–366.

Sabbah, I. and Rebhun, M. (1997). Adsorption-desorption of trichlorophenol in water-soil systems. *Water Environment Research*, 69(5):1032–1038.

Sander, M., Lu, Y. F., and Pignatello, J. J. (2006). Conditioning-annealing studies of natural organic matter solids linking irreversible sorption to irreversible structural expansion. *Environmental Science & Technology*, 40(1):170–178.

Sander, M. and Pignatello, J. J. (2005). An isotope exchange technique to assess mechanisms of sorption hysteresis applied to naphthalene in kerogenous organic matter. *Environmental Science & Technology*, 39(19):7476–7484.

Steinberg, S. M., Pignatello, J. J., and Sawhney, B. L. (1987). Persistence of 1,2-dibromoethane in soils: Entrapment in intraparticle micropores. *Environmental Science & Technology*, 21:1201–1208.

van Beinum, W., Beulke, S., and Brown, C. D. (2006). Pesticide sorption and desorption by lignin described by an intraparticle diffusion model. *Environmental Science & Technology*, 40(2):494–500.

Wu, S. and Gschwend, P. M. (1988). Numerical modeling of sorption kinetics of organic compounds to soil and sediment particles. *Water Resources Research*, 24:1373–1383.

Chapter 2

MODELING SOIL SORPTION HYSTERESIS USING A NORMALIZED REVERSIBLE RESISTANT MODEL

2.1 Background

Munition constituents (MC) such as HMX, RDX, nitroglycerin (NG), TNT and 2,4-DNT, are a potential source of contamination in firing ranges due to incompletely detonated rounds or residue from routine use. Soil contamination is estimated to affect at least 15 million acres at a cleanup cost of 15 - 140 billion dollars for U.S. Army ranges alone [U.S. Government Accountability Office, 2004]. Due to weak sorption, MC are available for desorption and eventual transport to surface and ground water. As a result, understanding sorption behavior for these chemicals is of utmost concern, since determining the partitioning behavior is a vital component of fate and risk analysis. Without accurate partitioning analysis, modeling cannot accurately portray the transport of these materials.

Standard methods for modeling partitioning between phases assume that the system is at equilibrium after both adsorption and desorption. These equilibrium relationships are defined by a partition coefficient which describes the relationship between the bulk and sorbed components. A futher assumption of these models is that there is no difference between the values of desorption and adsorption partition coefficients [Karickhoff et al., 1979]. However, the determination of accurate partition coefficients for long sorption times is frequently difficult because of discrepancies between the degree or rate of adsorption and desorption [Karickhoff and Morris,

1985]. This discrepancy between the degree of adsorption and desorption is often referred to as hysteresis [Pignatello and Xing, 1996].

There are three major groups of hysteretic models currently in use. The first suggest that the systems do not reach a true equilibrium, even for long sorption times (i.e. months to years) [Young and Ball, 1999] due to slow transport phenomena such as intra-particle diffusion [Altfelder et al., 2000; Brusseau et al., 1991; Farrell et al., 1999; Kan et al., 1998; van Beinum et al., 2006; Wu and Gschwend, 1986; Yang et al., 2008; Culver et al., 1997]. In these cases, slow diffusive processes cause a gradual uptake and release that is not symmetric with respect to adsorption and desorption since the magnitude of transport is determined by chemical concentration gradients. Diffusive processes can take many years to reach a true equilibrium state [Sabbah et al., 2005]. In addition, these models may require site specific parameters, some of which are difficult to determine prior to study, e.g. diffusion rates, sorbent particle sizes and chemistry of the system, which limits the applicability of these models to new sites.

A second group apply differing kinetic rates to adsorption and desorption. These empirical solutions typically use a two-compartment model [Chen and Nyman, 2005; Cornelissen et al., 1997] that proposes two different sorption sites with different kinetic rate constants, one fast and one slow. There is often no relationship to sorbent and sorbate properties, limiting the use of these models for new sites. Attempts have been made to correlate the first order rates derived by the two-compartment model to an apparent diffusion rate [Birdwell et al., 2007], although results are inconsistent. Other models relating first order kinetics to multiple binding sites have been employed [Ho and McKay, 1998; Huang et al., 1998; Xue et al., 1995]. The models rely on at least a single rate constant for each binding site and sorbate pair. Since no strong correlation has been observed between these rates and

sorbent/sorbate properties it is not possible to apply these models to new situations without site specific experimentation.

The third group assumes adsorption and desorption behavior is described by two sets of isotherms, one for the reversibly sorbed fraction and another for the fraction that is resistant or potentially irreversibly sorbed. Although many models exist that use separate isotherms for adsorption and desorption [Huang and Weber, 1997], few describe both adsorption and desorption using a single isotherm that uses a reversible component and a hysteretic component. Models of this category include the reversible resistant (RR) [Di Toro and Horzempa, 1982] and site transformation models (STM) [Di Toro, 2013]. The RR model retains a portion of the adsorbed concentration as irreversibly bound using reversible and resistant partition coefficients. The STM extends on this idea by allowing for the transformation of weakly binding sites to strongly binding sites. Hysteresis is caused by the strongly bound adsorbates not desorbing under aqueous concentrations used for desorption.

In this chapter the reversible and reversible/resistant model is applied to model 5 munition constituent's sorption onto 25 soils and 2 reference sorbents with varying properties in order to observe a range of reversible and hysteretic behaviors. The application of a reversible partitioning model is used to show the extent of hysteresis. The RR model is used to investigate the influence of sorbent properties and contact time as well as to suggest to the mechanistic basis for this behavior.

2.2 Materials and methods

Batch sorption experiments were conducted by R. Gonzalez [Gonzalez Forero, 2013] using 1:1 (5 g: 5 mL) soil to solution ratios in 12 mL centrifuge tubes. Two reference sorbents and 25 soils were hydrated for 5 days prior to the addition of MC in a solution containing 0.01 M calcium chloride ($CaCl_2$) and 0.01 M sodium azide (NaN_3)

which was added as a biological inhibitor. This solution was amended with an MC mixture consisting of octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine (HMX), 1,3,5-trinitroperhydro-1,3,5-triazine (RDX), 1,2,3-trinitroxypropane (NG), 2,4,6-trinitrotoluene (TNT) and 2,4-dinitrotoluene (DNT). Five sets of MC concentrations (Table 2.1) were used in the experiment. *AL1* contained all munitions at a relatively low concentration. *AL2* was a replicate of *AL1* and was used as an analytical and experimental check. *AH1*, with all munitions at a relatively high concentration, was used to examine the linearity of sorption. It had been observed in preliminary experiments that a degradation byproduct of TNT eluted at the same time as DNT during HPLC analysis. To isolate the behavior of TNT and DNT two special cases were used. *DH1* contained all munitions except TNT at the *AH1* concentration. *TH1* contained only TNT at the AH1 concentration.

The procedure for adsorption and subsequent sequential desorptions is shown in Figure 2.1. Samples were equilibrated (step 0) for 2, 48, 240, or 720 hours by rotation in an end-over-end shaker at 10 rpm after which the tubes were centrifuged for 30 min at 3000 rpm ($750g$) and sampled. Supernatant was discarded and replaced with 5 mL of solution containing 0.01 M $CaCl_2$ and 0.01 M NaN_3. The samples were re-equilibrated for 1 h (step 1) by rotating at 10 rpm in the end-over-end shaker. Previous studies had shown that one hour was sufficient to achieve an apparent steady state condition during desorption processes [Gonzalez Forero, 2013]. This procedure of sampling, discarding the supernatant and re-equilibrating with a clean solution was repeated for a total of 4 desorptions (steps 1 through 4). Finally, in order to complete the mass balance, samples were extracted with 5 mL of acetonitrile and rotated at 10 rpm in the end-over-end shaker for 1 hour. The tubes were centrifuged for 30 min at 3000 rpm ($750g$) and supernatant was sampled. To recover all sorbed material, the extraction was performed three times. Each sequence of adsorption,

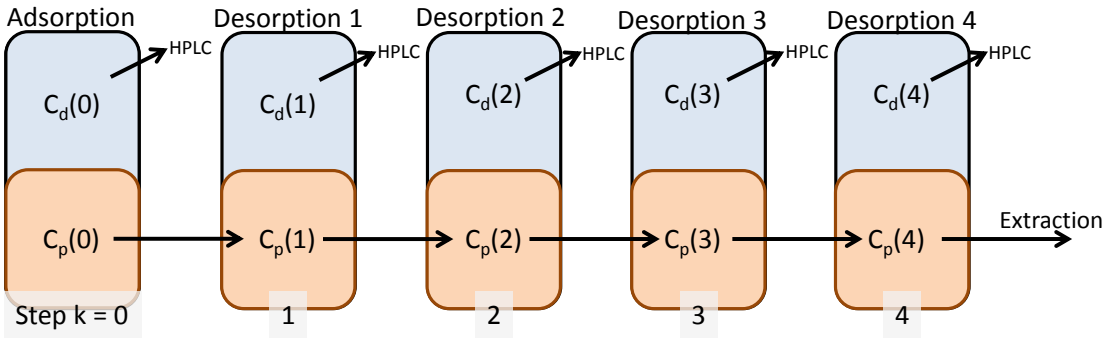


Figure 2.1: An illustration of the batch sorption experiment. Arrows leaving the aqueous phase indicate removal and anlysis via HPLC. Soil remains in the sample until extraction after step 4.

Table 2.1: Nominal concentrations $[mg/L]$ for the five MC groups employed in the adsorption-desorption experiment.

	Concentration				
Group	HMX	RDX	NG	TNT	DNT
AL1	0.75	3	3	3	10
AL2	0.75	3	3	3	10
AH1	1.5	10	10	10	20
DH1	1.5	10	10	0	20
TH1	0	0	0	10	0

desorption, extraction samples were analyzed in an Agilent 1200 Series HPLC with a Zorbax SB-C18 reverse phase column at a wavelength of 214 nm. The flow rate used was 2 mL min^{-1} for a methanol:water gradient of 30:70 percent to 65:35 percent from 0 to 2.8 min, and 65:35 percent to 30:70 percent from 2.8 to 3.2 min. The data are included as Appendix E.2.4.

Soil characteristics were determined by the Plant and Soil Science Department at University of Delaware. Soil weight fraction organic carbon, f_{OC}, ranged between 0.067% and 18.2%. The particle size distribution was determined by the Bouyoucos [Bouyoucos, 1962] method. The clay size fraction, f_{clay}, was comprised of

particles $< 2\mu m$ and ranged between 4.02% and 86%. The reference sorbents were kaolinite (70.3% clay and 0.043% organic carbon (OC)) purchased from the Clay Minerals Society and Pahokee peat (11.4% clay and 28.1% OC) purchased from the International Humic Substances Society. A complete listing of soil characteristics is included in Appendix E.2.1, E.2.2, and E.2.3

2.3 Analysis

2.3.1 Data exclusion

Samples for which the sorbent matrix material in the aqueous or extracted phase interfered with quantification of MC peaks in the HPLC analysis were excluded. In addition, sequences that contained incomplete or missing samples precluding the calculation of a mass balance were removed from further analysis. Further, for several soils the 2 and 720 h sorptions were not performed due to time constraints.

Degradation was observed for NG, TNT, and DNT despite the presence of sodium azide, NaN_3, to inhibit biota. This degradation could have been abiotic [Comfort et al., 1995]. As a screening criteria, if the mass loss exceeded 20% of the initial mass the data were excluded from further analysis. The mass recovered from the two hour data set was used as the initial total mass since degradation would have been minimal in this set. If two hour data were unavailable, the two day (48 h) data was used as initial mass. After these criteria was applied, the remaining data, comprising 6,640 observations, were used in the modeling.

2.3.2 Modeling adsorption partitioning

Data were composed of an adsorption followed by 4 sequential desorptions. Due to observed hysteresis, a separate analysis of the adsorption and desorption

behavior were conducted. Linear isotherms were used to relate the sorbed concentration, q, to the aqueous concentration, C, using the partition coefficient, K_P:

$$q = K_P C \tag{2.1}$$

During adsorption the MC partitions between the bulk aqueous (dissolved) and the bulk particulate (sorbed). The fractionation of the MC into the phases is quantified by the fraction dissolved, f_d, and fraction particulate, f_p, parameters:

$$C_d = f_d C_{tot} \tag{2.2}$$

$$C_p = f_p C_{tot} \tag{2.3}$$

where C_p is the particulate-bound concentration, and C_{tot} is the total concentration.

The fractions of the MC in each phase is related to the partition coefficient by the following equations [Schwarzenbach et al., 2002]:

$$f_d = \frac{1}{1 + mK_p} \tag{2.4}$$

$$f_p = \frac{mK_p}{1 + mK_p} = 1 - f_d \tag{2.5}$$

where f_d is the fraction dissolved $[unitless]$, f_p is the fraction particulate $[unitless]$, K_p is the partition coefficient, $[L\ water/kg\ soil]$, and m is the soil-water ratio, $[kg\ soil/L\ water]$.

Using this sorption model, the sequence of observed aqueous concentrations can be modeled as follows. At adsorption (step 0), the aqueous concentration is the

fraction dissolved multiplied by the initial total concentration, $C_{tot}(0)$:

$$C_d(0) = f_d C_{tot}(0) \tag{2.6}$$

In the experiment under analysis (illustrated in Figure 2.1), the aqueous portion was then removed and analyzed to determine $C_d(0)$. The aqueous phase was then replaced with clean (MC-free) liquid, allowing for desorption from the particulate phase. The total concentration for the first desorption, step 1, is the fraction particulate of the total concentration for the adsorption step:

$$C_{tot}(1) = f_p C_{tot}(0) \tag{2.7}$$

The corresponding dissolved concentration that results is given by

$$C_d(1) = f_d C_{tot}(1) \tag{2.8a}$$

which can be expressed as

$$= f_d f_p C_{tot}(0) \tag{2.8b}$$

and using Eq 2.5 yields

$$= f_d(1 - f_d) C_{tot}(0) \tag{2.8c}$$

Following this sequence, for k desorption steps, the dissolved concentration is

$$C_d(k) = f_d(1 - f_d)^k C_{tot}(0) \tag{2.9}$$

Therefore, for a reversible adsorption-desorption model, the sequence of dissolved concentrations depends on two parameters, the fraction dissolved, f_d, and the initial

concentration, $C_{tot}(0)$.

Since Eq 2.9 is linear with respect to $C_{tot}(0)$, the aqueous concentration can be normalized allowing for a simultaneous analysis of all data set in Table 2.1 that have different initial concentrations. This is accomplished by dividing the observed concentration by the the initial concentration:

$$C_d^N(k) = \frac{C_d(k)}{C_{tot}(0)} \tag{2.10}$$

where the normalized concentration is denoted by the superscript N. Substituting Eq 2.9 into Eq 2.10 yields

$$C_d^N(k) = f_d(1-f_d)^k \tag{2.11}$$

Eq 2.11 is the reversible model used to analyzed the adsorption and sequential desorption aqueous concentration data. The normalized sorbed concentration is given by

$$q_T^N(k) = {}^1/_m(1-f_d)^{(k+1)} \tag{2.12}$$

The reversible partitioning model, Eq 2.11, was fit to only the adsorption data to derive an adsorption partition coefficient. Fitting was performed by minimizing the root mean square errors (RMSE) between normalized observed (obs) and modeled (mod) aqueous concentrations:

$$RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n}\left(log_{10}C_{d,Obs,i}^N(k) - log_{10}C_{d,Mod,i}^N(k)\right)^2} \tag{2.13}$$

where n is the number of adsorption concentrations and $k = 0$ to restrict the fitting

to adsorption data only. The partition coefficients (K_P) were estimated[1] for each sorbent, munition, and adsorption duration using R statistical software and the *nls* package [R Core Team, 2014]. Estimated partition coefficients are listed in Appendix A.2.3.

2.3.3 Modeling desorption partitioning

2.3.3.1 Reversible model

Desorption concentrations were predicted using the reversible model, Eq 2.11, and the estimated adsorption partition coefficients (listed in Appendix A.2.5). Adsorption partition coefficients were used since the reversible model treats adsorption and desorption identically. The reversible model predicts that the aqueous concentrations should exhibit linear behavior when plotted on a log-linear scale. This is demonstrated by taking the log of both sides of Eq 2.11:

$$log_{10}C_d^N(k) = log_{10}\left(f_d\left(1-f_d\right)^k\right) \tag{2.14a}$$

and separating terms on the right hand side

$$log_{10}C_d^N(k) = log_{10}f_d + log_{10}\left(1-f_d\right)^k \tag{2.14b}$$

which yields

$$log_{10}C_d^N(k) = log_{10}f_d + (k)log_{10}\left(1-f_d\right) \tag{2.14c}$$

Eq 2.14c is linear in k with slope $log_{10}(1-f_d)$ and intercept $log_{10}f_d$.

[1] Code provided in Appendix A.2.2

The results[2] are shown in Figure 2.2 which compares the predicted and observed normalized aqueous concentrations for two soils. Normalized concentrations are shown versus the experimental step: adsorption, desorption 1, desorption 2, desorption 3 and desorption 4 (A, 1, 2, 3, 4 respectively). From the plot it is evident that the model systematically over predicts desorption. This is most evident in the 720 h data for DNT where the model overpredicts the aqueous concentration by an order of magnitude. In addition, the discrepancy between observed and predicted aqueous concentrations increases as the adsorption contact time increases. This over prediction is due the reversible model allowing too much chemical to desorb. As a result, the degree to which the model overpredicts the aqueous concentration is an indication of the extent of hysteresis. These results indicate the need to include hysteresis in the modeling framework for these sorbents and sorbates.

2.3.3.2 Reversible resistant model

To model hysteretic sorption, the reversible resistant (RR) model was used [Di Toro and Horzempa, 1982]. This model has previously been used to explain hysteretic sorption of PCBs and other chemicals [Di Toro, 1985]. The RR model uses linear partition coefficients to describe the total sorbed concentration, $q_T\,[g/kg]$, as the sum of the reversibly bound, q_x, and the resistantly bound, q_0, concentrations. Each of these components is defined by a partition coefficient, $K_x\,[L/kg]$ and $K_0\,[L/kg]$ respectively. The derivation below follows [Di Toro, 2013].

At adsorption, the component sorbed concentrations are equal to the aqueous

[2] Full set of comparisons is shown in Appendix A.2.4

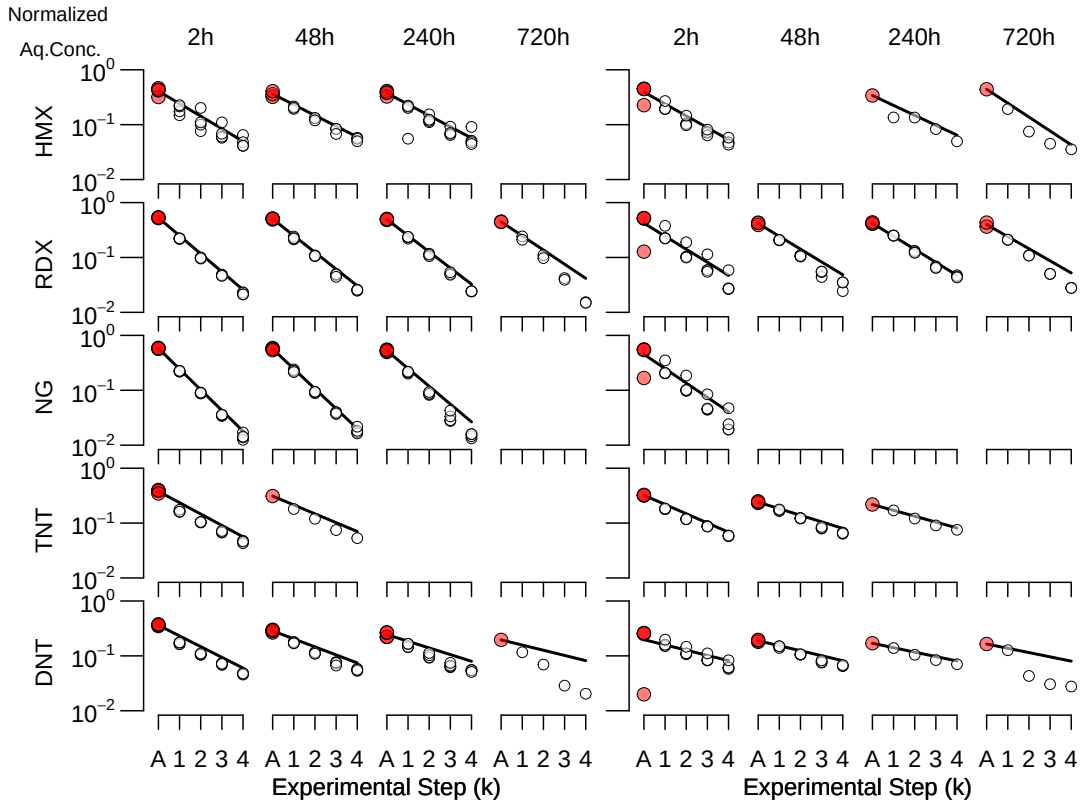


Figure 2.2: Comparison of reversible model (lines) with observed data (points) for Matapeake (left) and Houthalein (right) soils. Concentrations are normalized to the initial concentration $\left[\frac{mg/L}{mg/L}\right]$. Filled circles indicate adsorption concentrations. Hollow circles indicate desorption concentrations. 2h, 48h, 240h, and 720h refer to the duration of the adsorption contact time. A, 1, 2, 3, 4 refer to the adsorption and the four desorption steps ($k = 0, 1, 2, 3, 4$ in Eq 2.11). For the Houthalein 2 h adsorption duration, several data were not replicated by the other data sets. These data were not excluded by the mass balance criteria and are shown as the orange circles.

concentrations multiplied by the respective partition coefficient, Eqs 2.15 and 2.16.

$$q_{x,Ads} = K_x C_{d,Ads} \tag{2.15}$$

$$q_{0,Ads} = K_0 C_{d,Ads} \tag{2.16}$$

where $C_{d,Ads}$ is the aqueous concentration during the adsorption step $[mg/L]$, $q_{x,Ads}$ is the reversibly sorbed concentration $[mg/g]$, and $q_{0,Ads}$ is the resistant sorbed concentration $[mg/g]$. The total sorbed concentration, $q_T\,[g/kg]$, is the sum of these two components:

$$q_{T,Ads} = K_x C_{d,Ads} + K_0 C_{d,Ads} \tag{2.17a}$$

This equation can be rewritten as the sum of the reversible and resistant partition coefficients times the aqueous concentration,

$$q_{T,Ads} = (K_x + K_0)\, C_{d,Ads} \tag{2.17b}$$

By defining the adsorption partition coefficient, $K_P\ [L/kg]$, as the sum of K_x and K_0, the adsorption isotherm is derived:

$$q_{T,Ads} = K_P C_{d,Ads} \tag{2.17c}$$

The adsorption isotherm is defined by slope K_P and the intercept is at the origin.

During subsequent desorptions, however, the resistantly bound portion remains fixed at $q_{0,Ads}$ determined at the adsorption concentration (Eq 2.16),

$$q_{0,Des} = q_{0,Ads} = K_0 C_{d,Ads} \tag{2.18}$$

where $q_{0,Des}$ is the resistant component concentration $[mg/g]$. At desorption, the reversible component remains proportional to the aqueous concentration

$$q_{x,Des} = K_x C_{d,Des} \tag{2.19}$$

The total adsorbed concentration is

$$q_{T,Des} = q_{x,Des} + q_{0,Des} \tag{2.20}$$

Therefore, desorption occurs along an isotherm defined by slope K_x and intercept $K_0 C_{d,Ads}$.

$$q_{T,Des} = K_x C_{d,Des} + K_0 C_{d,Ads} \tag{2.21}$$

Thus, the RR model portrays hysteresis as the result of a resistantly bound concentration, $K_0 C_{Ads}$, that does not desorb at the aqueous concentration at each of the desorption steps.

For a data analysis comparable to Eq 2.11, a normalized version of the RR model is required. The derivation is presented in Appendix A.3.1 and the result is

$$q^N_{T,Ads} = m\left(K_x + K_0\right) C^N_{d,Ads} \tag{2.22}$$

$$q^N_{T,Des} = mK_x C^N_{d,Des} + mK_0 C^N_{d,Des} \tag{2.23}$$

where q^N_T is the total sorbed concentration normalized to the initial concentration

$$q^N_T = \frac{mq_T}{C_{tot}(0)} \tag{2.24}$$

where m is the soil-water ratio $[g/mL]$, and N denotes a normalized concentration.

The equations used to describe partitioning for consecutive desorptions using the RR model can be normalized in the same way as the reversible model (Appendix A.3.2). The result is that only the reversibly bound normalized concentration, $(1 - f_0)$, desorbs:

$$C_d^N(k) = (1 - f_0)\, f_x\, (1 - f_x)^k \tag{2.25}$$

where $C_d^N(k)$ is the normalized aqueous concentration for experimental step k, f_0 is the fraction of the initial concentration bound to resistant sites:

$$f_0 = \frac{mK_0}{1 + mK_x + mK_0} \tag{2.26}$$

and f_x is the aqueous phase fraction of the reversibly bound concentration:

$$f_x = \frac{1}{1 + mK_x} \tag{2.27}$$

The normalized sorbed concentration is given by

$$q_T^N = {}^1\!/_m \left((1 - f_0)(1 - f_x)^{(k+1)} + f_0\right) \tag{2.28}$$

Eq 2.25 is the reversible resistant model used for analysis. In comparison to the reversible model, Eq 2.11, the RR model is identical, with the exception of the adjustment to the initial concentration, $(1 - f_0)$. As a result, the RR model also exhibits log-linear behavior:

$$log_{10} C_d^N(k) = log_{10}\,(1 - f_0) + log_{10} f_x + (k) log_{10}\,(1 - f_x) \tag{2.29}$$

The reversible-resistant model was applied to the data allowing for time dependent reversible, K_x, and resistant, K_0, partition coefficients. The fit of these parameters was performed in R[3] using the *nls* non-linear least squares package [R Core Team, 2014]. Sorbed concentrations were required to properly fit the resistant component. The normalized sorbed concentration for step k was computed by summing the normalized aqueous concentrations for steps k through 4 and the extracted mass, normalized to the initial mass :

$$q^N_{T,Obs}(k) = \sum_{i=k}^{4} C^N_d(i) + \frac{M_{ext}}{C_{tot}(0)V(0)} \tag{2.30}$$

The sum of squared residuals (ssq) between observed and modeled aqueous and sorbed concentrations were minimized to estimate the partition coefficients. In order to properly weigh the adsorption and desorption data, the adsorption residual was given a weight of 4 relative to a unity weight for the four consecutive desorptions.

$$ssq = \sum_{\substack{0\leq k\leq 4\\ 1\leq i\leq 5}} W(k)\left[\left(log_{10}C^N_{d,Obs,i}(k) - log_{10}C^N_{d,Mod,i}(k)\right)^2 + \left(log_{10}q^N_{T,Obs,i}(k) - log_{10}q^N_{T,Mod,i}(k)\right)^2\right] \tag{2.31}$$

where k is the experimental step, i denotes the experimental concentration group as described in Table 2.1, and $W(k)$ is the weighting function: for $k = 0$, $W = 4$ and for $k > 0$, $W = 1$. The estimated partition coefficients, K_x and K_0 are shown in Appendices A.3.4.1 and A.3.4.2. Application of the RR model to the data shows good agreement with observed concentration[4]. Figure 2.3 presents the results for

[3] Code provided in Appendix A.3.3

[4] Full set of comparisons are shown in Appendix A.3.6

all MC and two soils. The RR model accurately predicts the aqueous concentration for each sorption time, indicating that time dependent partition coefficients with a resistant component is sufficient to describe the observed concentrations.

To gauge the improvement obtained by using the RR model, a comparison of the reversible and RR models was conducted. RMSE were calculated for each MC, soil and sorption time and compared in Figure 2.4. Throughout the range of f_{OC} the RR model is an improvement over the reversible model. For several soils, the improvement is dramatic (e.g. RDX on Aberdeen BTi soil (BT) and DNT on Lewis Core (LCO) soil). NG shows less improvement per soil which is attributed to variability within the 720 h data set. As is shown in Figure 2.4B, the RR model decreases RMSE for the 2, 48 and 240 h adsorption contact time for NG, indicating an overall improvement to the fit.

Residuals from the reversible and RR model fits of C_d^N were compared to illustrate of the importance of including a hysteretic fraction. From the model results, shown previously in Figures 2.2 and 2.3, it was expected that the RR model would show improvement for higher f_{OC} soils. Residuals of the aqueous concentration are shown as a function of sorbent in Figure 2.5. It is apparent that for all MC there is bias in the reversible model residuals. Predicted aqueous concentrations are always greater than observed, indicated by the negative residual. Over-prediction of aqueous concentrations is due to the lack of resistant sorption, as is evidenced by the RR residuals where there is no bias. Aqueous concentrations are accurately portrayed by the RR model because a portion of the chemical is unable to participate in desorption.

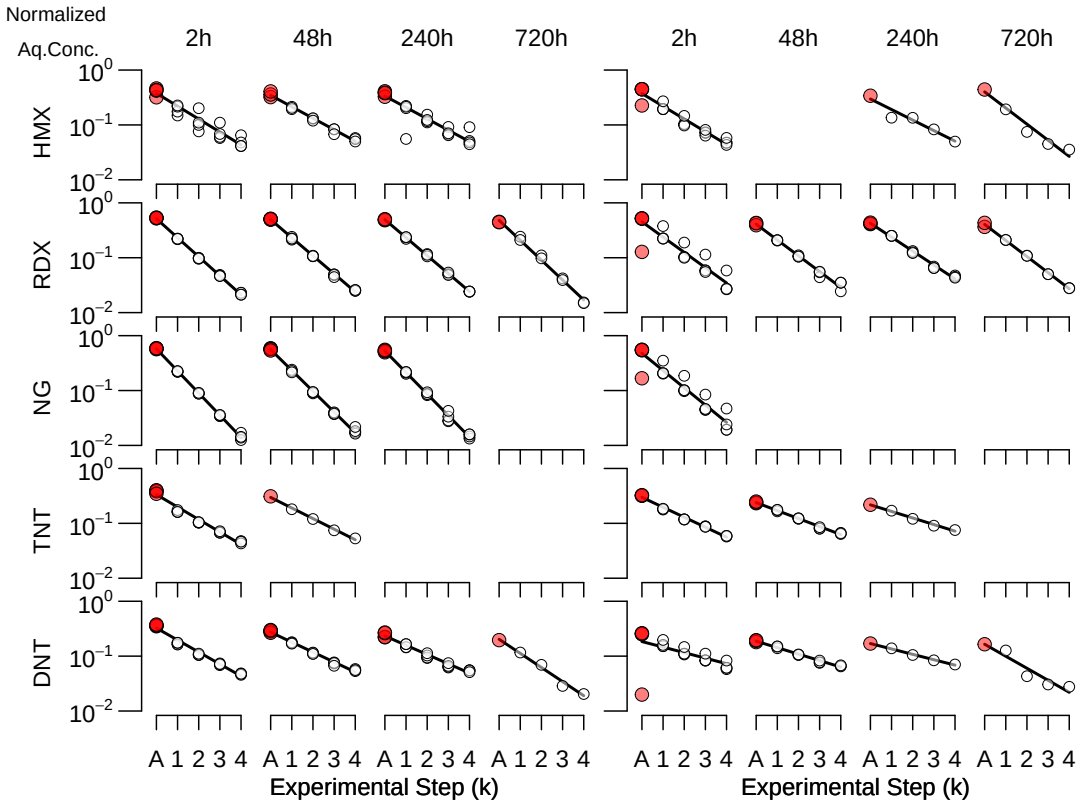


Figure 2.3: Comparison of RR model (lines) with observed data (points) for Matapeake (left) and Houthalein (right) soils. Concentrations are normalized to the initial concentration $\left[\frac{mg/L}{mg/L}\right]$. Filled circles indicate adsorption point. Hollow circles indicate desorption points. 2h, 48h, 240h, and 720h refer to the duration of the adsorption step. A, 1, 2, 3, 4 refer to the adsorption and the four desorption steps. ($k = 0, 1, 2, 3, 4$ in Eq 2.25). For the Houthalein 2 h adsorption duration, several data were not replicated by the other data sets. These data were not excluded by the mass balance criteria and are shown as the orange circles.

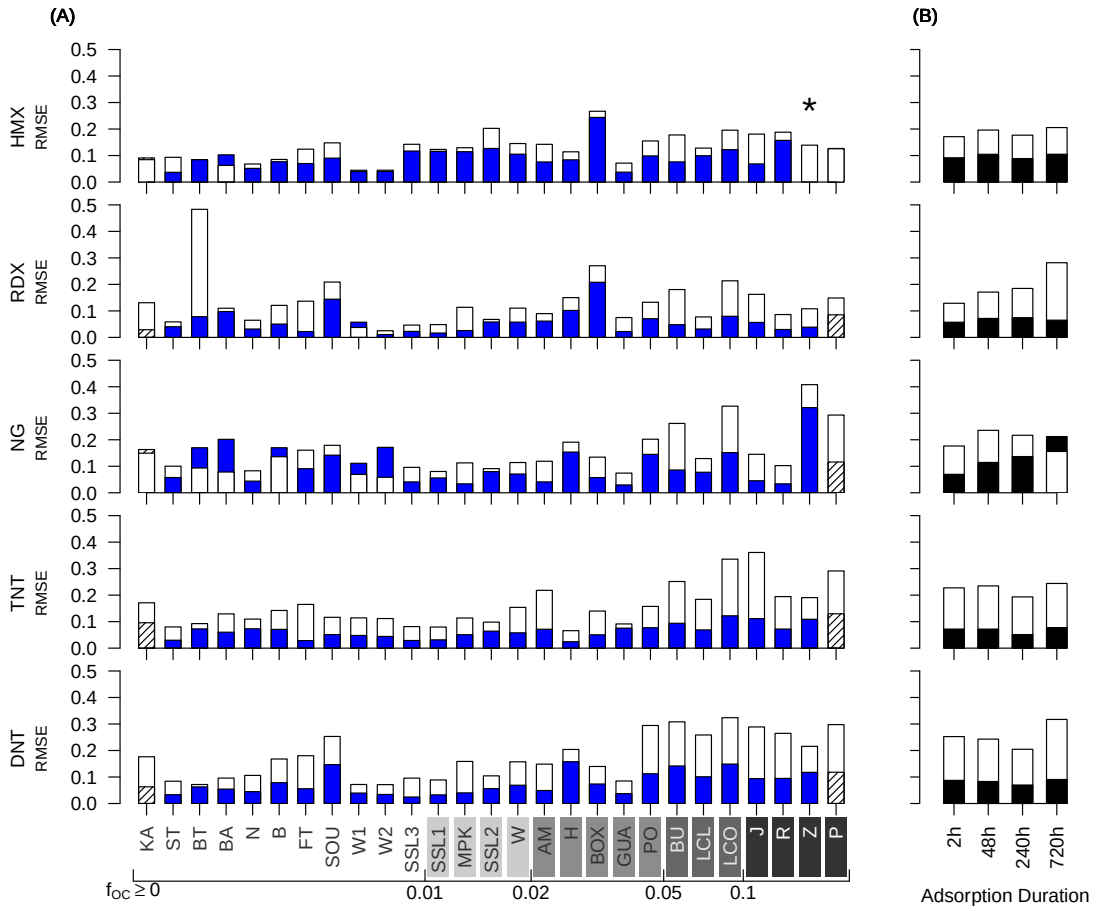


Figure 2.4: RMSE, Eq 2.13, for RR model predicted aqueous concentrations, C_{aq}^{N}, compared to reversible model aqueous concentrations. (A) RMSE determined for each soil (B) RMSE determined for each adsorption contact time. Filled bars indicate RR determined RMSE. Hollow bars indicate reversible model RMSE. Hashed bars indicate reference sorbents.$*$ indicates a soil with either the reversible or RR RMSE value missing.

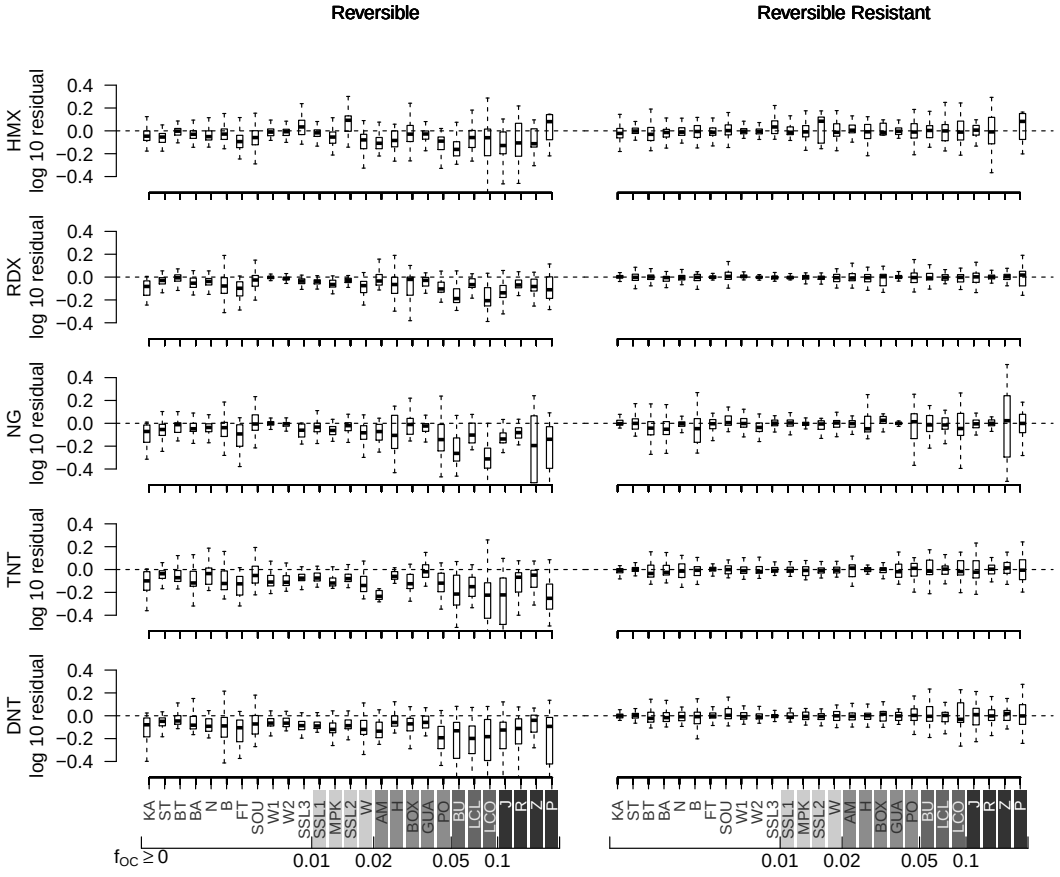


Figure 2.5: Comparison of log_{10} residuals (log_{10}observed $-$ log_{10}predicted) for reversible and RR model aqueous concentrations as determined by the respective model. Bias shows the over-prediction of linear derived aqueous concentrations due to lack of resistant sorption. Outliers have been omitted for clarity.

2.3.3.3 Multilinear model of reversible resistant partition coefficients

Since the model predicts the observed concentrations well, an investigation of the RR model partition coefficients was conducted. The partition coefficients, listed in Table 2.2 and Table 2.3, were analyzed by using multilinear models [Gonzalez Forero, 2013]. The multilinear models decompose a partition coefficient into multi-site partitioning to the sorbent matrix using sorbent specific partition coefficients. In this analysis, the sorbent properties were organic carbon (OC) content and clay sized particle fractions:

$$K_x(i,j) = f_{OC}(i)K_{OC,x}(j) + f_{clay}(i)K_{clay,x}(j) \tag{2.32}$$

$$K_0(i,j) = f_{OC}(i)K_{OC,0}(j) + f_{clay}(i)K_{clay,0}(j) \tag{2.33}$$

where $K_{OC,x}(j)$ and $K_{OC,0}(j)$ are the reversible and resistant partition coefficients associated with MC j binding to OC, $K_{clay,x}(j)$ and $K_{clay,0}(j)$ are the reversible and resistant partition coefficients associated with MC j binding to clay sized particles, $f_{OC}(i)$ is the OC mass fraction of sorbent i $[g\ OC/g\ sorbent]$, and $f_{clay}(i)$ is the clay sized particle mass fraction of sorbent i $[g\ clay/g\ sorbent]$,. Sorbent specific partition coefficients $K_{OC,x}$, $K_{OC,0}$, $K_{clay,x}$, and $K_{clay,0}$ are shown in Tables 2.2 and 2.3. It has been previously observed by Gonzalez that using these two sites is sufficient to accurately model the adsorption partition coefficient.

Figure 2.6 is a plot of K_x vs. f_{OC} for each MC (rows) and each adsorption contact time (columns) on log-log axes. The partition coefficients are shown as points with error bars of one standard error. The two reference sorbents are shown as squares. The multilinear model is shown as the solid red line. To evaluate the

Table 2.2: Multilinear class partition coefficient K_{OC} $[L/kg]$ for K_x and K_0

	MC	K_{OC}^{2h}	K_{OC}^{48h}	K_{OC}^{240h}	K_{OC}^{720h}
K_x	HMX	3.81e+01	5.45e+01	4.79e+01	5.23e+01
	RDX	2.26e+01	2.89e+01	3.18e+01	2.88e+01
	NG	1.71e+01	2.33e+01	2.94e+01	6.22e+01
	TNT	3.37e+01	6.56e+01	8.50e+01	5.46e+01
	DNT	4.58e+01	7.50e+01	9.51e+01	3.69e+01
K_0	HMX	1.03e+01	1.71e+01	2.64e+01	2.48e+01
	RDX	5.22e+00	7.61e+00	1.07e+01	1.14e+01
	NG	4.64e+00	8.19e+00	1.85e+01	1.19e+01
	TNT	3.45e+01	6.62e+01	8.82e+01	7.45e+01
	DNT	4.09e+01	8.73e+01	1.19e+02	8.63e+01

Table 2.3: Multilinear class partition coefficient K_{clay} $[L/kg]$ for K_x and K_0

	MC	K_{clay}^{2h}	K_{clay}^{48h}	K_{clay}^{240h}	K_{clay}^{720h}
K_x	HMX	4.67e+00	4.06e+00	3.79e+00	3.52e+00
	RDX	2.72e+00	2.54e+00	2.46e+00	2.53e+00
	NG	1.88e+00	1.78e+00	2.04e+00	2.12e+00
	TNT	4.28e+00	4.15e+00	4.29e+00	4.35e+00
	DNT	3.85e+00	3.55e+00	3.23e+00	3.49e+00
K_0	HMX	2.45e-01	2.36e-01	6.74e-01	3.06e-01
	RDX	1.02e-01	1.54e-01	2.50e-01	2.70e-01
	NG	7.73e-02	1.12e-01	2.59e-01	3.40e-01
	TNT	2.40e-01	4.55e-01	1.01e+00	5.06e-01
	DNT	1.59e-01	2.12e-01	4.17e-01	2.80e-01

contribution of clay size particles, models with only a single sorption site, OC:

$$K_x(i,j) = f_{OC}(i)K_{OC,x}(j) \tag{2.34}$$

$$K_0(i,j) = f_{OC}(i)K_{OC,0}(j) \tag{2.35}$$

are shown as the dashed red lines in Figures 2.6 and 2.7.

Multilinear predicted K_x for $f_{OC} > 0.01$ are approximately linear with respect to f_{OC}, as shown by the similarity to a K_{OC} only regression (dashed red line). Below $f_{OC} = 0.01$, deviation from a linear relationship with f_{OC} is seen. This non-linearity is due to the increasing importance of binding to the clay size particle fraction as f_{OC} decreases.

The multilinear estimated $K_{OC,x}$ and $K_{clay,x}$ (Figure 2.8) $K_{OC,x}$ and $K_{clay,x}$ are constant with respect to adsorption duration for all MC with the exception of NG. This suggests that there is no change in the reversible component as the duration of adsorption increases.

Resistant partition coefficients show less deviation from a K_{OC} model (Eq 2.35) than K_x, Figure 2.7. This is seen especially for TNT and DNT. K_0 for these MC are linear with respect to f_{OC} for f_{OC} values $> 10^{-3}$. However, unlike K_x, the magnitude of K_0 appears to increase as adsorption contact time increases. This indicates an increase in resistant sorption as contact time increases.

The OC and clay partition coefficients, $K_{OC,x}$ and $K_{OC,0}$, (Figure 2.9) support the observation that hysteresis increases as f_{OC} and adsorption duration increase. $K_{clay,0}$ for TNT and DNT partition coefficients s correlated almost exclusively to binding to organic carbon, as shown by the similarity of the multilinear model in Figure 2.7 to a $K_{OC,0}$ model (Eq A.12). This strongly suggests that organic matter is the site of resistant sorption, lending support to polymer expansion and other OC

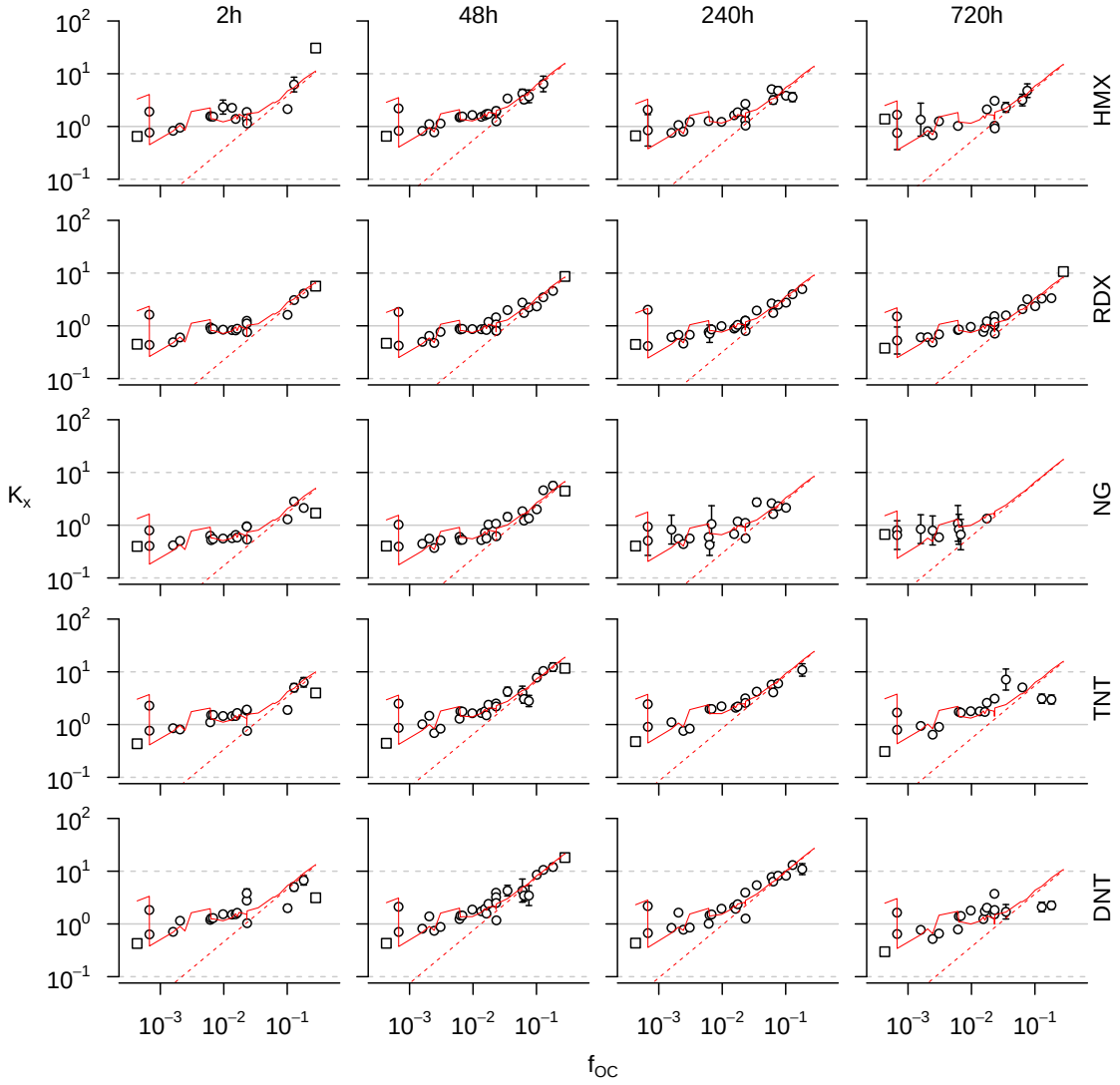


Figure 2.6: Reversible partition coefficients, K_x, [L/kg] from RR model for soils are shown by mean (point) ± std. error (error bars) if the standard error is greater than the symbol. Solid red line shows K_x predicted by the two-site multilinear regression (Eq A.13). Dashed red line shows K_x predicted by Eq 2.34. Square points indicate reference sorbents not used in the multilinear regression.

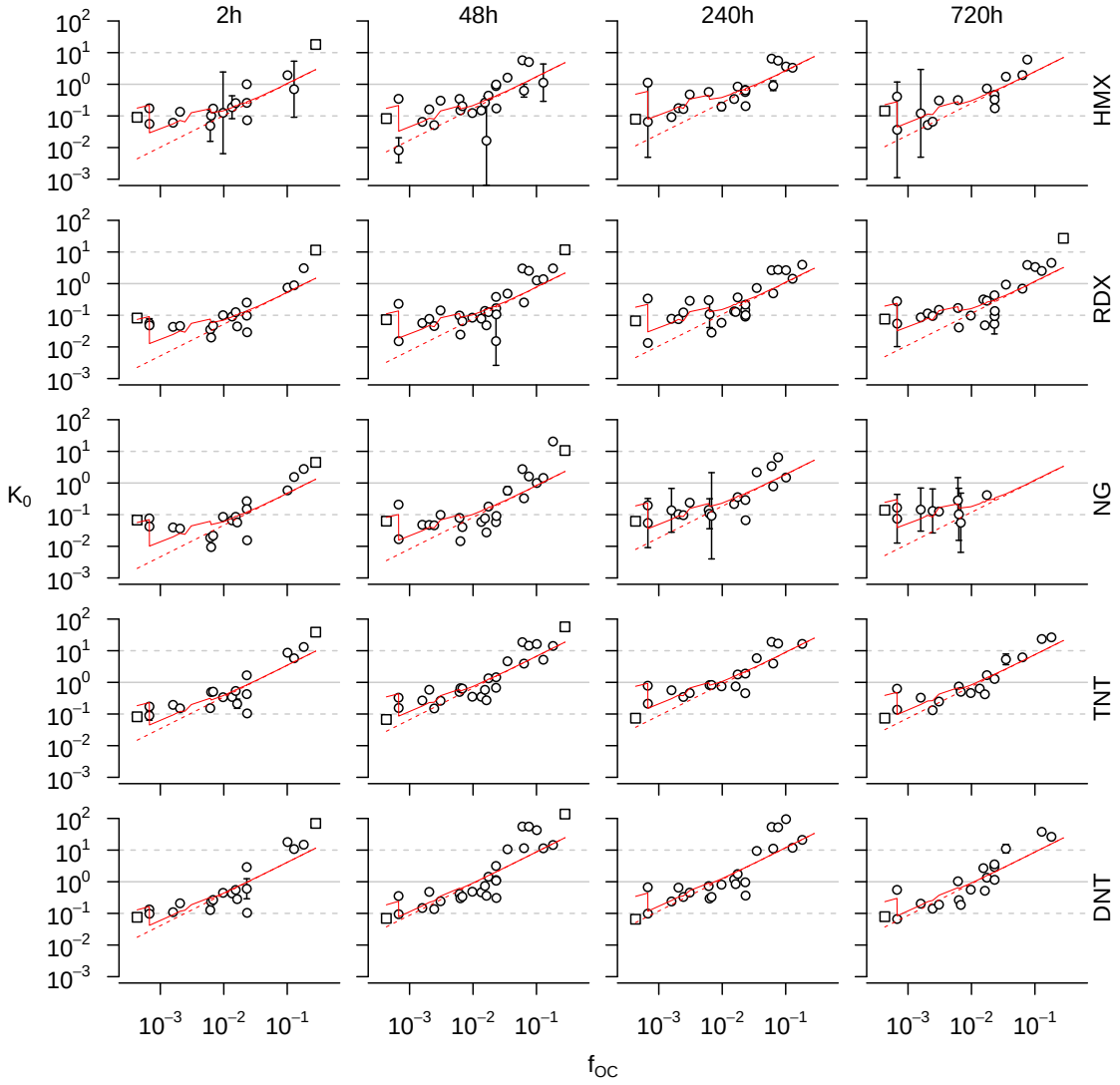


Figure 2.7: Resistant partition coefficients, K_0, [L/kg] from RR model for soils are shown by mean (point) ± std. error (error bars) if the standard error is greater than the symbol. Solid red line shows K_0 predicted by the two-site multilinear regression (Eq A.14). Dashed red line shows K_0 predicted by Eq 2.35. Square points indicate reference sorbents not used in the multilinear regression.

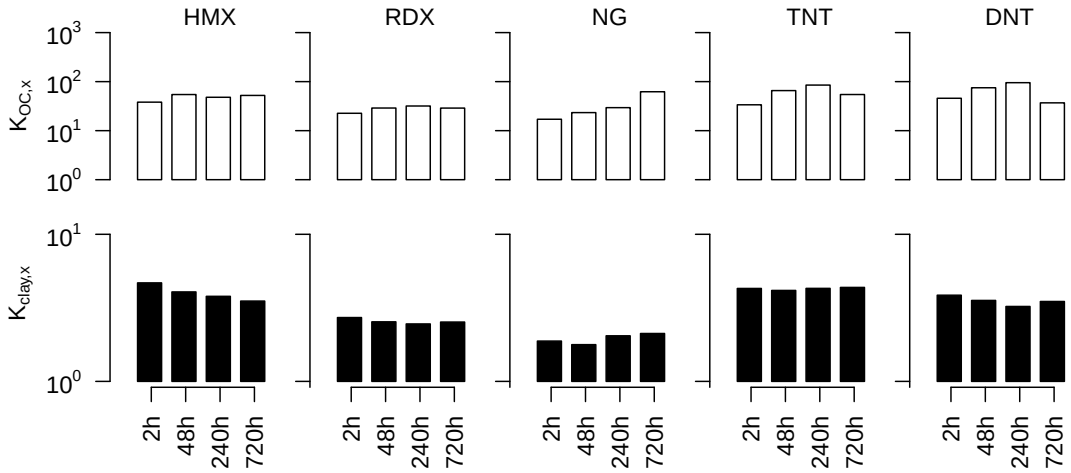


Figure 2.8: Multilinear component partition coefficients, $K_{OC,x}$ and $K_{clay,x}$ [L/kg], for the reversible partition coefficients, K_x, versus adsorption contact time. Hollow bars show $K_{OC,x}(j)$, filled bars show $K_{clay,x}(j)$

modification theories [Chilom and Rice, 2005; Sander et al., 2006; Weber Jr. et al., 1998]. In addition, $K_{OC,0}$ shows a dependence with sorption time. This suggests that the resistantly bound component increases with increasing adsorption contact time.

2.4 Reversibility fraction

To better understand the extent of partitioning due to resistant sorption, the fraction of K_p associated with reversible sorption was calculated:

$$RF = \frac{K_x(i,j)}{K_x(i,j) + K_0(i,j)} = \frac{K_x(i,j)}{K_P(i,j)} \tag{2.36}$$

where RF is the reversibility fraction. $RF \simeq 1$ indicates complete reversibility, while decreasing values indicate increasing hysteresis. RF values are plotted vs. f_{OC} for each soil and adsorption contact time in Figure 2.10. Highly reversible munitions, such as HMX and RDX, display little change in RF with either adsorption contact

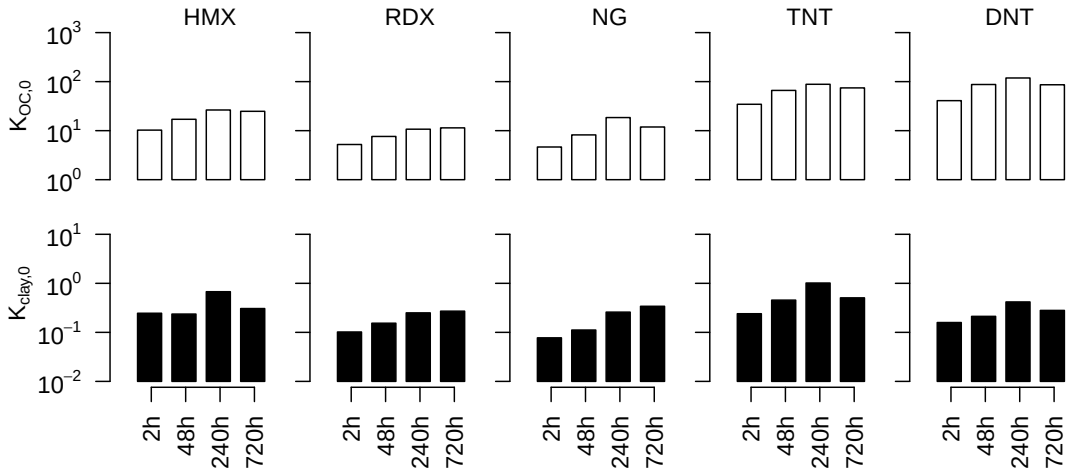


Figure 2.9: Multilinear component partition coefficients, $K_{OC,0}$ and $K_{clay,0}$ [L/kg], for the resistant partition coefficients, K_0, versus adsorption contact time. Hollow bars show $K_{OC,0}(j)$, filled bars show $K_{clay,0}(j)$

time or soil, whereas MC with larger resistant component sorption, such as TNT and DNT, show significant changes indicating that not only do high f_{OC} soils display greater hysteresis, but as adsorption contact time increases a larger fraction of soils show hysteretic behavior.

The results of the RF suggest an increase in resistant binding with respect to sorption time and f_{OC} is responsible for the observed increase in hysteretic behavior. The RR model has no mechanistic or empirical explanation for the time dependency. Therefore, development of a model that incorporates this change in binding strength as a function of the adsorption contact time and sorbent properties can further explain observed hysteresis. The site transformation model [Di Toro, 2013] will be used to model this phenomena as part of Chapter 3.

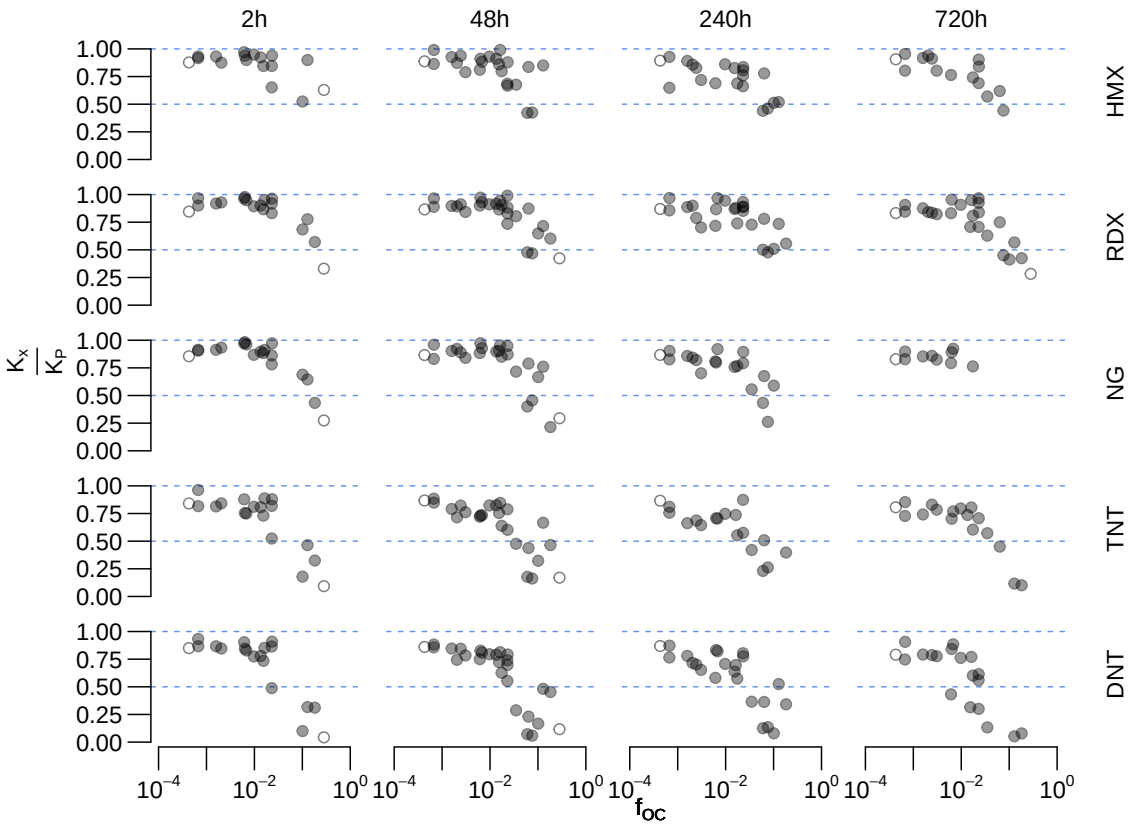


Figure 2.10: Reversibility fraction, $\frac{K_x}{K_P}$, for RR model. Points are the ratio of the reversible partition coefficient, K_x to the total partition coefficient, K_P. Filled points are soils, hollow points are reference sorbents. 2h, 48h, 240h, and 720h refer to the adsorption contact time.

2.5 Predictive model

The reversible model (Eq 2.14c) requires two sorbate parameters (K_{OC} and K_{clay}) and two sorbent parameters (f_{OC} and f_{clay}) to estimate aqueous and sorbed normalized concentrations. However, the RR model (Eq 2.25) requires four sorbate parameters for each adsorption duration ($K_{OC,x}$, $K_{clay,x}$, $K_{OC,0}$ and $K_{clay,0}$) and the same sorbent parameters to estimate aqueous and sorbed normalized concentrations due to the inclusion of hysteresis. To measure the predictive capabilities of the two models, a comparison was made using the multilinear predicted partition coefficients (Tables 2.2 and 2.3).

The log_{10} residuals for normalized aqueous concentrations are shown for each sorbent and MC in Figure 2.11. The reversible model shows negative biasing for many soils due to the reversible model not incorporating resistant sorption. When compared to the RR model, this bias is corrected. Both models show large residuals for low and high f_{OC} soils. As shown in Figure 2.5, the RR model should predict significantly more accurate concentrations given precise partition coefficients. The error for multilinear predicted partition coefficients is large in some cases, especially at very low and high f_{OC} (Figs A.4, 2.6, and 2.7). Increased accuracy in multilinear predictions are expected to show greater improvement when using the RR model.

2.6 Conclusions

From the analysis provided above, a reversible approach to MC sorption can accurately predict behavior for low f_{OC} soils and short adsorption times. As f_{OC} increases, however, a model incorporating hysteresis is required. The reversible resistant model is valid across the range of observed f_{OC} for both fully reversible and highly resistant cases at the cost of an additional fitting parameter.

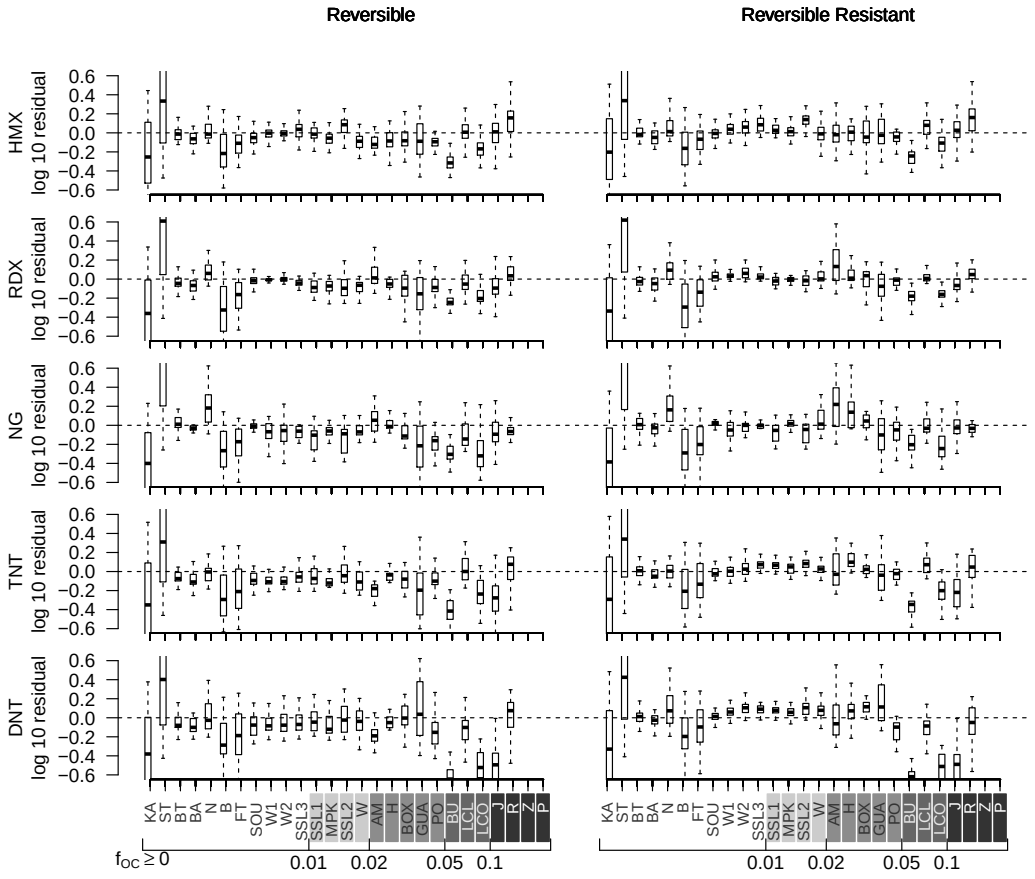


Figure 2.11: log_{10} residuals (log_{10}observed − log_{10}predicted) of normalized aqueous concentrations for each sorbent and MC for reversible (Eq 2.14c) and RR models (Eq 2.25) using multilinear predicted partition coefficients (Tables 2.2 and 2.3). Shading indicates increasing f_{OC}

A reversibility fraction shows how hystereic behavior changes across multiple soils and sorption times. The time dependent nature of the resistant partition coefficient suggests that a kinetic processes is occurring, while the relationship to f_{OC} strongly points to a change in organic matter sorption behavior, through changing binding strength or deformation of the polymeric structure of OC. However, other theories such as slow diffusive transport from interior OC sites are not excluded. Further investigation is needed to understand the effect of sorption duration, however from the analysis provided, a positive correlation to binding strength is expected.

In the next chapter, an analysis of the relationship between resistance and adsorption contact time is performed using a model that directly includes changing binding site strength.

REFERENCES

Altfelder, S., Streck, T., and Richter, J. (2000). Nonsingular sorption of organic compounds in soil: The role of slow kinetics. *Journal of Environmental Quality*, 29(3):917–925.

Birdwell, J., Cook, R. L., and Thibodeaux, L. J. (2007). Desorption kinetics of hydrophobic organic chemicals from sediment to water: A review of data and models. *Environmental Toxicology and Chemistry*, 26(3):424–434.

Bouyoucos, G. (1962). Hydrometer method improved for making particle size analysis of soils. *Agronomy Journal*, (54):464–465.

Brusseau, M., Jessup, R., and Rao, P. (1991). Nonequilibrium sorption of organic-chemicals - elucidation of rate-limiting processes. *Environmental Science & Technology*, 25(1):134–142.

Chen, S. H. and Nyman, M. C. (2005). Slow desorption behavior of one highly resistant aromatic amine in Lake Macatawa, Michigan, USA, sediment. *Environmental Toxicology and Chemistry*, 24(12):3020–3029.

Chilom, G. and Rice, J. A. (2005). Glass transition and crystallite melting in natural organic matter. *Organic Geochemistry*, 36(10):1339–1346.

Comfort, S. D., Shea, P. J., Hundal, L. S., Li, Z., Woodbury, B. L., Martin, J. L., and Powers, W. L. (1995). TNT transport and fate in contaminated soil. *Journal of Environment Quality*, 24(6):1174.

Cornelissen, G., Rigterink, H., Vrind, B. A., tenHulscher, T. E. M., Ferdinandy, M. M. A., and vanNoort, P. C. M. (1997). Two-stage desorption kinetics and

in situ partitioning of hexachlorobenzene and dichlorobenzenes in a contaminated sediment. *Chemosphere*, 35(10):2405–2416.

Culver, T. B., Hallisey, S. P., Sahoo, D., Deitsch, J. J., and Smith, J. A. (1997). Modeling the desorption of organic contaminants from long-term contaminated soil using distributed mass transfer rates. *Environmental Science & Technology*, 31(6):1581–1588.

Di Toro, D. M. (1985). A particle interaction-model of reversible organic-chemical sorption. *Chemosphere*, 14(10):1503–1538.

Di Toro, D. M. (2013). Site transformation model of adsorption-desorption hysteresis. *Abstracts of Papers of the American Chemical Society*, 245.

Di Toro, D. M. and Horzempa, L. M. (1982). Reversible and resistant components of PCB adsorption desorption - isotherms. *Environmental Science & Technology*, 16(9):594–602.

Farrell, J., Grassian, D., and Jones, M. (1999). Investigation of mechanisms contributing to slow desorption of hydrophobic organic compounds from mineral solids. *Environmental Science & Technology*, 33(8):1237–1243.

Gonzalez Forero, R. (2013). *Factors Controlling the Reversible and Resistant Adsorption and Desorption of Munitions Constituents on Soils*. PhD dissertation. University of Delaware.

Ho, Y. S. and McKay, G. (1998). A comparison of chemisorption kinetic models applied to pollutant removal on various sorbents. *Process Safety and Environmental Protection*, 76(4):332–340.

Huang, W. L. and Weber, W. J. (1997). A distributed reactivity model for sorption by soils and sediments .10. relationships between desorption, hysteresis, and the chemical characteristics of organic domains. *Environmental Science & Technology*, 31(9):2562–2569.

Huang, W. L., Yu, H., and Weber, W. J. (1998). Hysteresis in the sorption and desorption of hydrophobic organic contaminants by soils and sediments - 1. a comparative analysis of experimental protocols. *Journal of Contaminant Hydrology*, 31(1-2):129–148.

Kan, A. T., Fu, G., Hunter, M., Chen, W., Ward, C. H., and Tomson, M. B. (1998). Irreversible sorption of neutral hydrocarbons to sediments: Experimental observations and model predictions. *Environmental Science & Technology*, 32(7):892–902.

Karickhoff, S. W., Brown, D. S., and Scott, T. A. (1979). Sorption of hydrophobic pollutants on natural sediments. *Water Research*, 13(3):241–248.

Karickhoff, S. W. and Morris, K. R. (1985). Sorption dynamics of hydrophobic pollutants in sediment suspensions. *Environmental Toxicology and Chemistry*, 4(4):469–479.

U.S. Government Accountability Office (2004). DOD operational ranges: More reliable cleanup cost estimates and a proactive approach to identifying contamination are neded.

Pignatello, J. J. and Xing, B. (1996). Mechanisms of slow sorption of organic chemicals to natural particles. *Environmental Science & Technology*, 30(1):1–11.

R Core Team (2014). *R: A Language and Environment for Statistical Computing*. R Foundation for Statistical Computing, Vienna, Austria.

Sabbah, I., Ball, W. P., Young, D. F., and Bouwer, E. J. (2005). Misinterpretations in the modeling of contaminant desorption from environmental solids when equilibrium conditions are not fully understood. *Environmental Engineering Science*, 22(3):350–366.

Sander, M., Lu, Y. F., and Pignatello, J. J. (2006). Conditioning-annealing studies of natural organic matter solids linking irreversible sorption to irreversible structural expansion. *Environmental Science & Technology*, 40(1):170–178.

Schwarzenbach, R. P., Gschwend, P. M., and Imboden, D. M. (2002). *Environmental Organic Chemistry*. John Wiley & Sons, Inc, Hoboken, NJ, USA.

van Beinum, W., Beulke, S., and Brown, C. D. (2006). Pesticide sorption and desorption by lignin described by an intraparticle diffusion model. *Environmental Science & Technology*, 40(2):494–500.

Weber Jr., W. J., Huang, W., and Yu, H. (1998). Hysteresis in the sorption and desorption of hydrophobic organic contaminants by soils and sediments: 2. effects of soil organic matter heterogeneity. *Journal of Contaminant Hydrology*, 31(12):149–165.

Wu, S. C. and Gschwend, P. M. (1986). Sorption kinetics of hydrophobic organic-compounds to natural sediments and soils. *Environmental Science & Technology*, 20(7):717–725.

Xue, S. K., Iskandar, I. K., and Selim, H. M. (1995). Adsorption-desorption of 2,4,6-trinitrotoluene and hexahydro-1,3,5-trinitro-1,3,5-triazine in soils. *Soil Science*, 160(5):317–327.

Yang, W., Duan, L., Zhang, N., Zhang, C., Shipley, H. J., Kan, A. T., Tomson, M. B., and Chen, W. (2008). Resistant desorption of hydrophobic organic contaminants in typical Chinese soils: Implications for long-term fate and soil quality standards. *Environmental Toxicology and Chemistry*, 27(1):235–242.

Young, D. F. and Ball, W. P. (1999). Two-region linear/nonlinear sorption modeling: Batch and column experiments. *Environmental Toxicology and Chemistry*, 18(8):1686–1693.

Chapter 3

MODELING MUNITION CONSTITUENT ADSORPTION AND DESORPTION HYSTERESIS ON SOILS USING THE SITE TRANSFORMATION MODEL

3.1 Background

In Chapter 2, it was shown that hysteresis was observed for 5 munition constituents sorbed onto 25 soils. Resistance to desorption increased as a function of f_{OC}. In addition, as the duration of adsorption contact time increased, more soils exhibited resistant behavior. This relationship of contact time to hysteresis has been noted previously for chlorophenols [Palomo and Bhandari, 2006], herbicides [Lesan and Bhandari, 2003] and PAHs [Wang et al., 2012], but has not been satisfactorily explained.

This effect is shown by the behavior of the reversible fraction which is the fraction of the total partition coefficient associated with reversible sorption, Figure 2.10. It showed that as contact time increases, the degree of resistant sorption increases. A possible mechanism is an increase in the binding strength of the sorbent. Work performed by Sander [Sander and Pignatello, 2005, 2009], Chilom [Chilom and Rice, 2005], and Lu [Lu and Pignatello, 2002] suggest that a transition in organic carbon binding strength, through pore filling or polymeric rearrangement, may explain the observed resistance to desorption exhibited by many chemicals. These changes may not only physically change the sorbate, but may allow access to different binding sites with different sorption energies [Gebremariam et al., 2012; Huang et al., 1998; Kan

et al., 1998]. Hysteresis is due to a strongly bound portion which does not desorb under observed solute conditions. These processes are not necessarily instantaneous, suggesting kinetics may also be involved [Sander et al., 2006].

Although there are several sorption models that describe adsorption or desorption behavior, few explain the transition between the two processes. A recently developed model, the Site Transformation Model (STM) [Di Toro, 2013], is based on the idea that sites change binding strength as a function of adsorption concentration, resulting in hysteresis. Moreover, the model can be applied to both linear and Langmuir isotherms, enabling modeling of nonlinear sorption. In this work, the STM is applied to a data set of 5 munition constituents and 25 soils during adsorption and sequential desorptions to determine sorbent-model correlations as well as develop predictive tools for the model parameters. Moreover, a relationship between hysteretic behavior, adsorption contact time, and sorbent organic carbon content is made that allows for characterization of hysteresis for new soils.

3.2 Data and modeling procedure

The data analyzed in this chapter were used in the previous chapter. It is comprised of batch sorption experiments for 5 munition constituents (MC), octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine (HMX), 1,3,5-trinitroperhydro-1,3,5-triazine (RDX), 1,2,3-trinitroxypropane (NG), 2,4,6-trinitrotoluene (TNT) and 2,4-dinitrotoluene (DNT). These MC were sorbed to 25 soils and 2 reference sorbents for 4 adsorption contact times (2, 48, 240, and 720 h). Soils varied in organic carbon (f_{OC}) from 0.067% to 18.2% and clay size fraction (f_{clay}) from 4.02% to 84.0%. The reference sorbates were a high f_{OC} (28.1%), low f_{clay} (11.4%) sorbent and a high f_{clay} (70.3%), low f_{OC} (0.043%) sorbent. Soil properties were determined by the Plant and Soil Science Department at University of Delaware. Clay size fraction was measured by the

Bouyoucos method [Bouyoucos, 1962]. Sorbent properties are listed in Appendix E.2.2. Observations were made of the aqueous concentration after adsorption and after 4 sequential desorptions spaced 1 h apart. An extractions was used to complete the mass balance. A screening criteria requiring 80% mass recovery was used, as degradation was not accounted for in modeling. The experiment resulted in 6,640 aqueous concentration observations and an equal number of sorbed concentrations.

A previous study of these MC and sorbents showed that correctly modeling hysteresis is a necessity in accurately describing sorbed concentrations during desorption. We showed that a reversible model, using the adsorption partition coefficient, could not predict aqueous or sorbed concentrations during desorption. The reversible model is:

$$q = K_P C \tag{3.1}$$

where q is the sorbed concentration for [g/mg], K_P is the adsorption partition coefficient [L/kg] fit to the sorbed adsorption concentration, and C is the aqueous concentration [mg/L]. The reversible model used a partition coefficient estimated for each MC, sorbent and adsorption duration. A comparison between observed and modeled sorbed concentrations is shown as Figure 3.1. Data are shown as hexagons, with the shade of the hexagon indicating the number of observed-modeled pairs. A 1:1 line (solid red) shows that modeled sorbed concentrations are biased low indicating that the reversible model underpredicts sorbed concentrations. This is due to the inability of the reversible model to incorporate hysteresis since it treats adsorption and desorption using the same isotherm. As a result, a model that applied hysteresis is necessary to model the behavior of MC on soil. The reversible model under predicts sorbed concentrations since it does not include hysteresis. Therefore,

a model that includes hysteresis was used to explain the observed behavior.

The adsorption and desorption data are modeled using the site transformation model (STM) [Di Toro, 2013]. Figure 3.2 shows aqueous concentration plotted vs. sorbed concentration for all MC (rows) and all adsorption times (columns) on Matapeake soil[1]. Adsorption concentrations are shown as the filled red points and desorption concentrations are shown as the hollow points. HMX, RDX, and NG show linear adsorption and desorption, as illustrated by the connected straight lines. TNT and DNT, however, show deviation from linearity. These isotherms appear to show curvature. A Langmuir STM was therefore proposed to model the observed behavior.

The STM is formulated using a general isotherm model. For application to these data, the isotherm model used is the Langmuir isotherm. The Langmuir isotherm is typically defined as:

$$q = \frac{q_T K_L C}{1 + K_L C} \tag{3.2}$$

where q is the mass of sorbent per unit mass sorbate $[mg/kg]$. K_L is the Langmuir constant $[L/mg]$, q_T is the maximum site density $[mg/kg\,soil]$, and C is the aqueous concentration of the sorbate $[mg/L]$. The STM equations are (derivation is provided in Appendix B.2):

$$q_A = \frac{q_T K_L C_A}{1 + K_L C_A} + f_{ST} \frac{q_T K_L C_A}{1 + K_L C_A} \tag{3.3a}$$

$$q_D = \frac{q_T K_L C_D}{1 + K_L C_D} + f_{ST} \frac{q_T K_L C_A}{1 + K_L C_A} \tag{3.3b}$$

[1] A full set of isotherms is contained in Appendix B.1

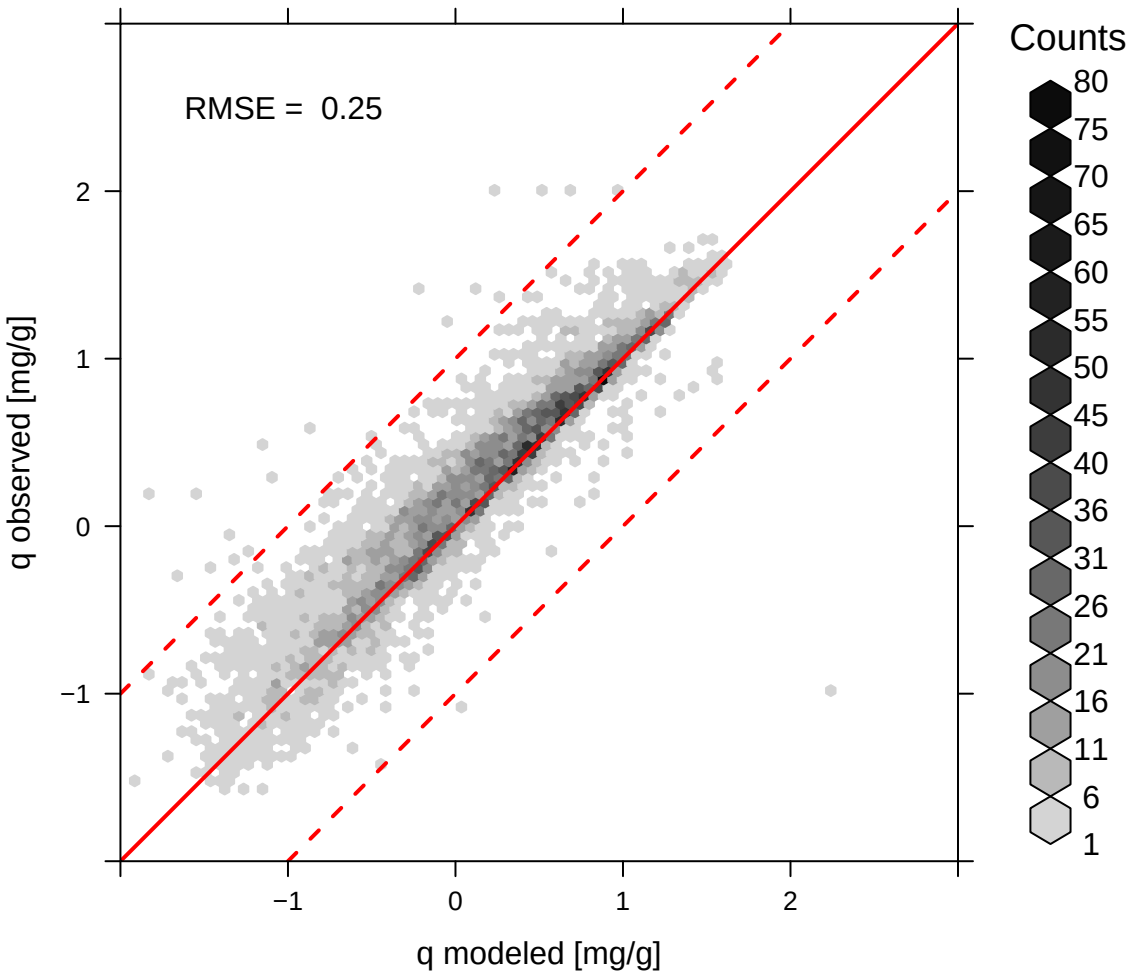


Figure 3.1: Comparison of modeled and observed sorbed concentrations for a reversible model (fit to the adsorption point). Data is grouped into hexagons, the shading of which indicates the number of data. The red solid line indicates unity, dashed lines are spaced at 1 log unit from unity.

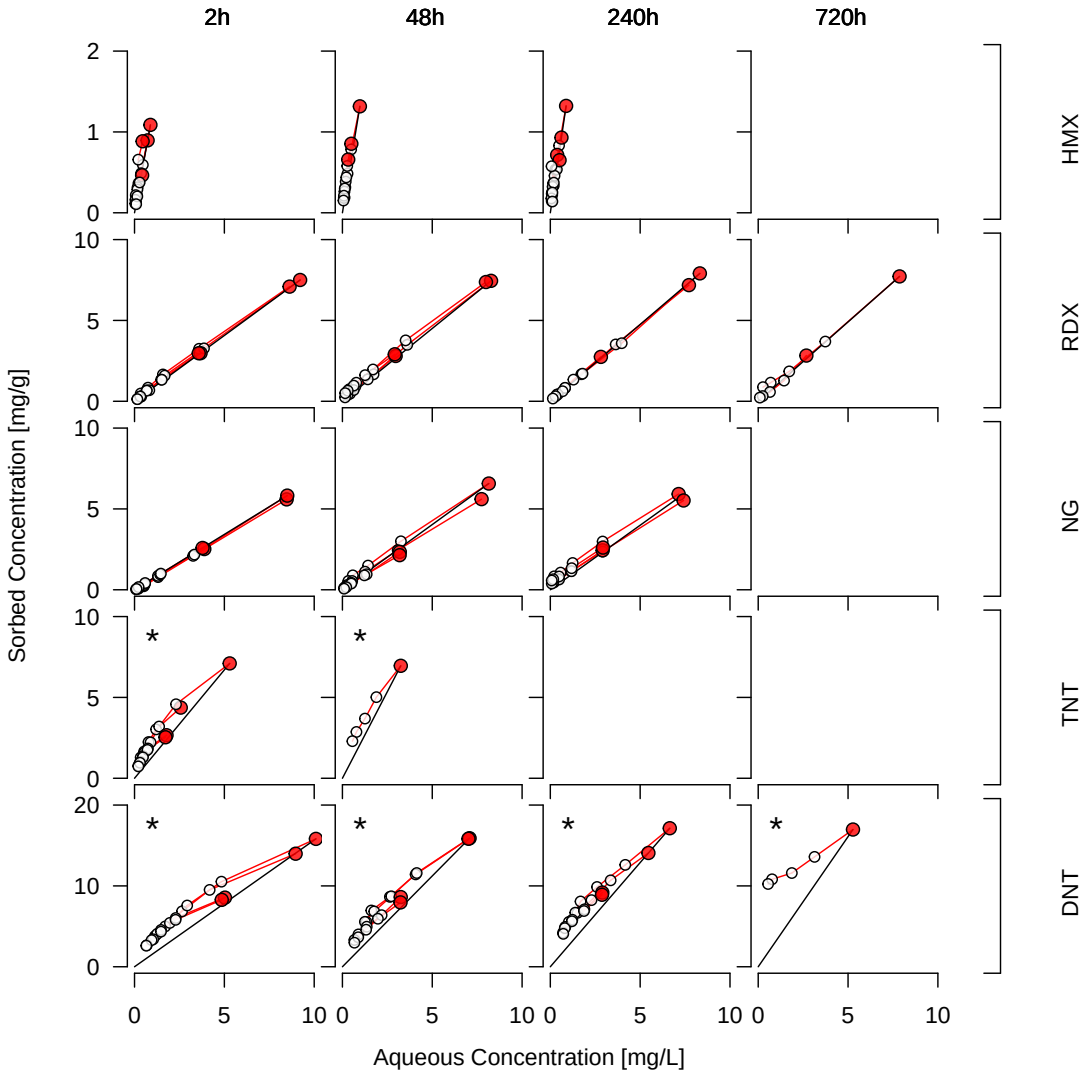


Figure 3.2: Linear and Langmuir isotherms for MC on Matapeake (MPK) soil. Lines show relationship between observations. Red points are concentrations after adsorption, hollow points are sequential desorption concentrations.

where q_A is the concentration of chemical sorbed on the particles $[mg/kg\,soil]$ after adsorption contact time, q_D is the concentration of chemical sorbed on the particles $[mg/kg\,soil]$ after a single desorption, f_{ST} is the site transformation factor described below $[unitless]$, C_A is the aqueous concentration after adsorption contact time $[mg/L]$ and C_D is the aqueous concentration after a single desorption $[mg/L]$.

The adsorption isotherm, Eq 3.3a is the sum of two Langmuir isotherms. The first term quantifies sorption to weakly sorbing sites. The second quantifies sorption to strong sites. The quantity of strong sites is determined by the magnitude of the site transformation factor, f_{ST}. For adsorption, both terms are a function of C_A, the aqueous concentration. However, for the desorption isotherm, Eq 3.3b, only the first term is a function of the aqueous concentration at desorption, C_D. The second term, defining the resistant component, is fixed at the aqueous adsorption concentration, C_A.

This behavior is illustrated in Figure 3.3 which shows sorbed and aqueous concentrations for an example system. During adsorption, the sorbed concentration follows the black line in Figure 3.3A, the adsorption isotherm (Eq 3.3a). During desorption, the sorbed concentration follows the red line in Figure 3.3A, the desorption isotherm (Eq 3.3b). Only the weak sites show depletion, the dashed blue line in Figure 3.3B. In contrast, the strong sorbing sites, the dashed red line in Figure 3.3B, remain constant. The net result of the differing behavior between strongly and weakly sorbing sites is the total sorbed curve during desorption, as illustrated in Figure 3.3A. This differing behavior is the cause of hysteresis.

In addition to Langmuir behavior, many soils exhibited linear partitioning. The linear isotherm is a special case of the Langmuir isotherm for which $K_L C \ll 1$.

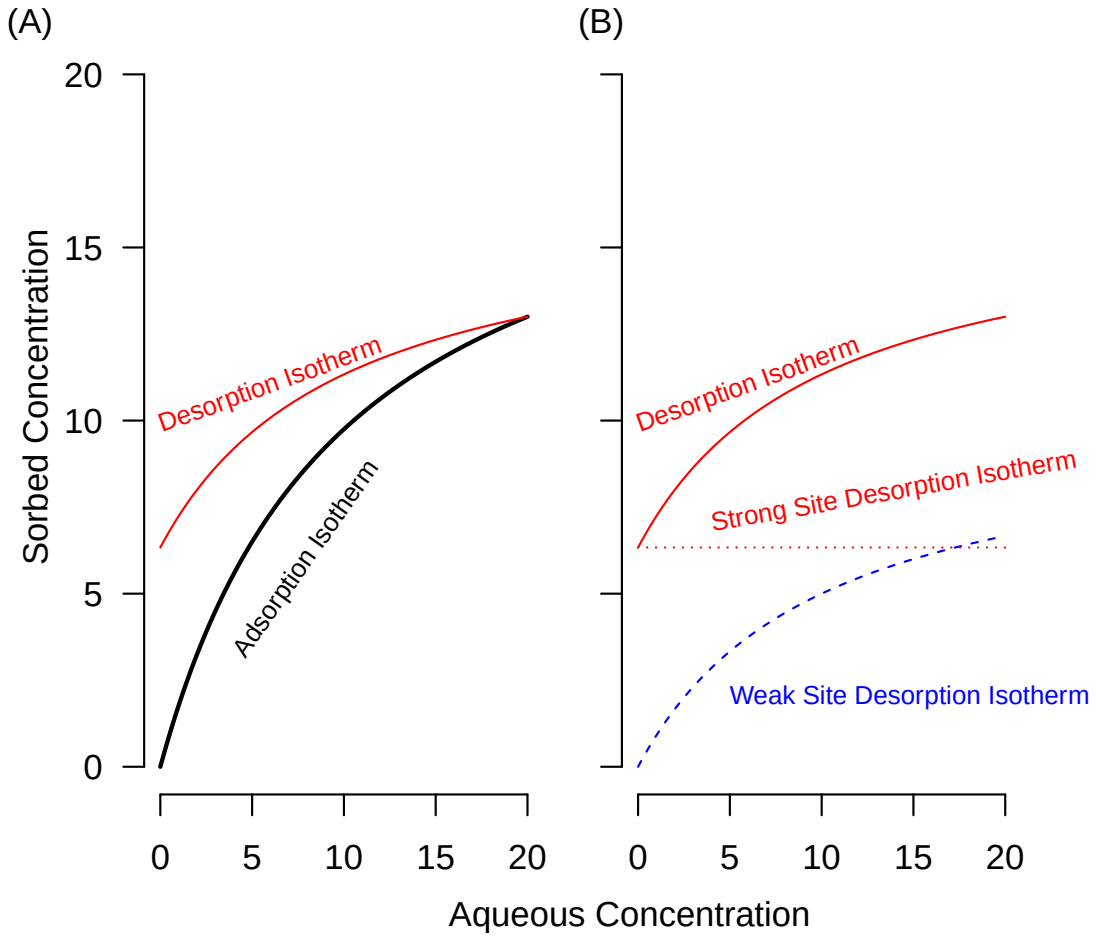


Figure 3.3: Illustration of STM. (A) Behavior during adsorption (black) and desorption (red). The discrepancy between the lines (hysteresis) is evident from the individual sorbed components (B). Strong sites (red) during desorption remain fixed, weak sites (blue) follow Langmuir behavior.

The STM equations reduce to:

$$q_A = q_T K_L C_A + f_{ST} q_T K_L C_A \tag{3.4a}$$

$$q_D = q_T K_L C_D + f_{ST} q_T K_L C_A \tag{3.4b}$$

In the linear case, the parameters q_T and K_L cannot be independently determined. Therefore, the product was fit as a single parameter, K_P:

$$q_A = K_P C_A + f_{ST} K_P C_A \tag{3.5a}$$

$$q_D = K_P C_D + f_{ST} K_P C_A \tag{3.5b}$$

The method employed to determine which STM formulation, Eqs 3.3 or 3.5, would be applied for each data set is described in the following section.

3.2.1 Isotherm determination

If the Langmuir equations (Eqs 3.3) are applied to linear adsorption and desorption data, q_T and K_L cannot be determined independently since they occur as the product $q_T K_L$ in Eqs 3.5. Fitting a large K_L is offset by fitting a small q_T and vice versa. This is a useful observation since it allows each set of data to be separated into either linear or Langmuir isotherms without introducing potential biases from a visual separation.

Initially a data set is fit using the Langmuir STM (Eq 3.3). Fitting was performed using R statistical software and the *optim* method [R Core Team, 2014] to minimize the root mean square error (RMSE) of sorbed concentrations[2]. RMSE

[2] Code provided in Appendix B.3.2

Table 3.1: Possible STM parameter dependencies

Parameter	Initial Dependencies	Final Dependencies
K_P	M[1], S[2], T[3]	M, S
K_L	M, S, T	M, S
f_{ST}	M, S, T	S, T

[1] Dependency on munition constituent
[2] Dependency on sorbent
[3] Dependency on adsorption contact time

was calculated using Eq 3.6.

$$RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n}\left(log_{10}q_{i,obs} - log_{10}q_{i,model}\right)^2} \tag{3.6}$$

where n is the total number of observations in the data set, $q_{i,obs}$ and $q_{i,mod}$ are the sorbed concentrations, subscripts *obs* and *model* indicate observed or modeled values, respectively.

After fitting, the correlation coefficient between q_T and K_L was determined from the inverse of the Hessian matrix. If the correlation coefficient exceeded 0.90, the linear STM model (Eqs 3.5) was used, otherwise a Langmuir STM model (Eqs 3.3) was used. The threshold of 0.90 was chosen because using lower values resulted in a sharp increase in soils with clear Langmuir behavior being described as linear. Values above 0.90 were not used because this caused an increasing number of sorbent-sorbate pairs to be fit by Langmuir isotherms which leads to to significant estimation error in K_L.

3.2.2 Model parameter dependencies

It was necessary to determine the dependency of model parameters on sorbate and sorbent properties. The possible parameterizations are shown in Table 3.1. The

first test attempted to determine if K_P and K_L for each MC and sorbent were statistically different for each adsorption duration. A model with sorbent, sorbate, and adsorption contact time dependence in K_P and K_L was applied to each data set. Figure 3.4 shows estimated K_P for each MC, sorbent and asdorption contact time. The estimated K_P's were tested[3] using a paired t-test [Walpole et al., 2007] against a null hypothesis that there was no difference between K_P for different adsorption contact times, t_{ads}. At an $\alpha = 0.05$ it would be expected that 5% of the test would result in rejection of the null hypothesis by chance. Therefore, a Bonferroni correction [Dunn, 1961] was applied to the value of α. For conducting N tests, the correct level of significance is α/N. At this level of significance the null hypothesis was rejected for 7.5% of the 509 tests performed. Rejections of the null hypothesis predominantly corresponded to K_P estimated for high f_{OC} soils, but the rejection did not occur in a regular manner. TNT and DNT exhibit the greatest number of rejections of the null hypothesis. The expected behavior would be that K_P increases as adsorption contact time increases or remains constant. Figure 3.4 shows that several data sets show decreasing, or inconsistent changes in K_P. Thus, it was concluded that K_P and K_L were not changing with t_{ads}, hence the exclusion of an adsorption time dependency for K_P in Table 3.1.

[3] Code provided in Appendix B.3.1

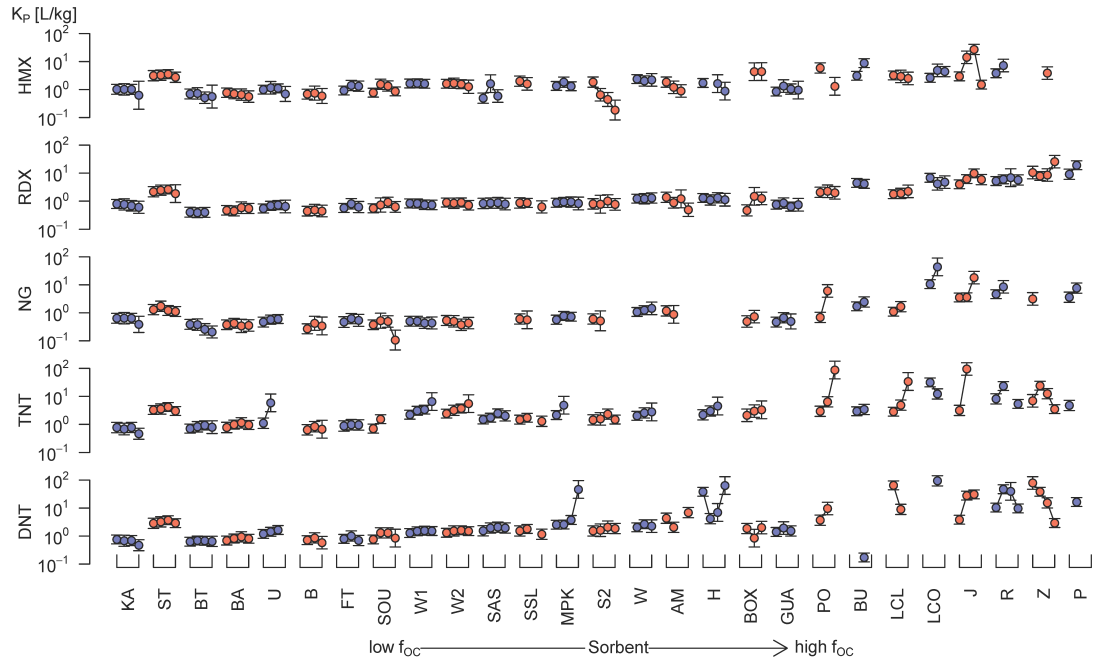


Figure 3.4: Comparison of K_P (mean $\pm$ std. error) determined for each MC (row) versus sorbent (ordered low to high f_{OC}). Adsorption contact time increases for each data set from left to right. Color alternates between sorbents. Connective line shows values related by data set.

The site transformation factor determines the extent of the conversion of weak sites to strong sites. It has previously been hypothesized that polymeric rearrangement of the sorbent is independent of sorbate [Lu and Pignatello, 2002; Weber et al., 1992]. This suggests that the site transformation factor may be independent of the sorbate, in this case the MC. Based on this suggestion, f_{ST} determined for each sorbent, sorbate, and adsorption duration were compared. The null hypothesis for this test was that there was no difference between MC specific f_{ST} for a sorbent/adsorption duration pairs. The test alpha value, $\alpha = 0.05$ was corrected using the Bonferroni method. A total of 474 tests were performed, none of which resulted in a rejection of the null hypothesis. Therefore, it was concluded that f_{ST} was not changing with respect to MC.

These tests on K_P and f_{ST} yielded parameters dependent on the variables, shown below:

$$K_P = f(M, S) \tag{3.7a}$$

$$K_L = f(M, S) \tag{3.7b}$$

$$f_{ST} = f(S, T) \tag{3.7c}$$

where M is a dependence on sorbate (munition constituent), S is a dependence on soil or reference sorbent, and T is dependence on the adsorption contact time. This parameterization of the model will be used for all further analysis of the data (Table 3.1).

3.3 Analysis

With parameter dependencies and isotherm choices resolved, the appropriate model parameter could be estimated. Data sets were grouped by sorbent and adsorption contact time for analysis. R and the *optim* method [R Core Team, 2014] were used for estimating the parameters by minimizing the RMSE (Eq 3.6) of sorbed concentrations[4]. The observed and modeled sorbed concentrations are shown for all MC and sorbents in Figure 3.5. The plot shows data grouped by the number of data points in a hexagonal region, with the number in the region indicated by the shade of the hexagon. The figure shows that observed and modeled values are in good agreement, as evident by the proximity of the majority of comparisons to the 1:1 line and the unbiased distribution thereof. Therefore, an analysis of estimated model parameters was conducted.

3.3.1 Binding constants - K_P and K_L

In the previous chapter, a multilinear model was used to correlate sorbent parameters with estimated partition coefficients. The multilinear model is:

$$K_P(i,j) = f_{OC}(i)K_{OC}(j) + f_{clay}(i)K_{clay}(j) \tag{3.8}$$

where $f_{OC}(i)$ and $f_{clay}(i)$ are the fractions, $[g/g]$, organic carbon and clay size particles, respectively, for sorbate i, and $K_{OC}(j)$ and $K_{clay}(j)$ are the site specific partition coefficients $[L/kg]$, for MC j. The estimated site specific partition coefficients are listed in Table 3.2. To contrast the multilinear model, a single site f_{OC} model was

[4] Code provided in Appendix B.3.3

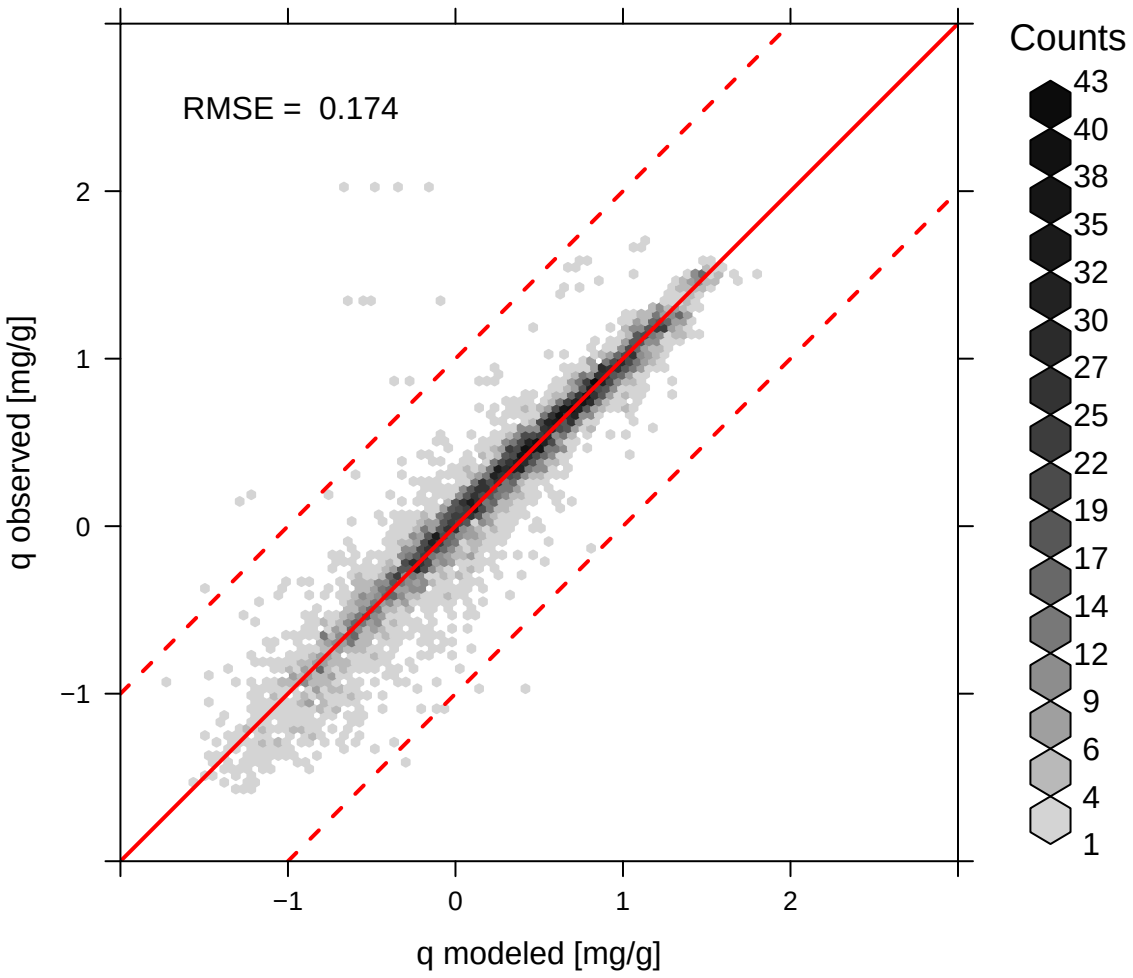


Figure 3.5: Comparison of STM predicted using estimated parameters and observed sorbed concentrations. Data is grouped into hexagons, the shading of which indicates the number of data. The red solid line indicates unity, dashed lines are spaced at 1 log unit from unity.

Table 3.2: Multilinear model parameters for K_P [L/kg] (Eq 3.2)

MC	$log_{10}K_{OC}$	$log_{10}K_{clay}$
HMX	1.74(±0.0480)	0.596(±0.0512)
RDX	1.37(±0.0508)	0.315(±0.0506)
NG	1.47(±0.0782)	0.118(±0.102)
TNT	2.07(±0.0823)	0.789(±0.102)
DNT	2.39(±0.0883)	0.470(±0.207)

also used:

$$K_P(i,j) = f_{OC}(i)K_{OC}(j) \tag{3.9}$$

The single site model (dashed red line) shows good agreement with STM estimated partition coefficients for $f_{OC} > 0.1$ for HMX and RDX, and $f_{OC} > 0.01$ for NG, TNT and DNT (Figure 3.6). For soils above these thresholds, the dominant sorption site is organic carbon. Below these threshold values, deviation from a linear relationship is seen. This deviation is well predicted by the multilinear model (solid red line). The observed threshold for non-linear behavior, $f_{OC} < 10^{-2}$ corresponds to a value where $f_{OC}K_{OC}$ is approximately equal to K_{clay}, suggesting that below this threshold binding to clay size particle sites are the dominant sites for sorption. The derivation of the multilinear model used soils that exhibited no Langmuir behavior. Therefore, an analysis of K_L using the multilinear model could not be performed.

3.3.2 Site transformation factor

Linear and Langmuir partition constants are well researched and used frequently in engineering practices. The site transformation factor, f_{ST}, is novel, however, and an investigation of its sorbent and sorbate relationships was conducted. The behavior was expected to be similar to the previously described Reversibility

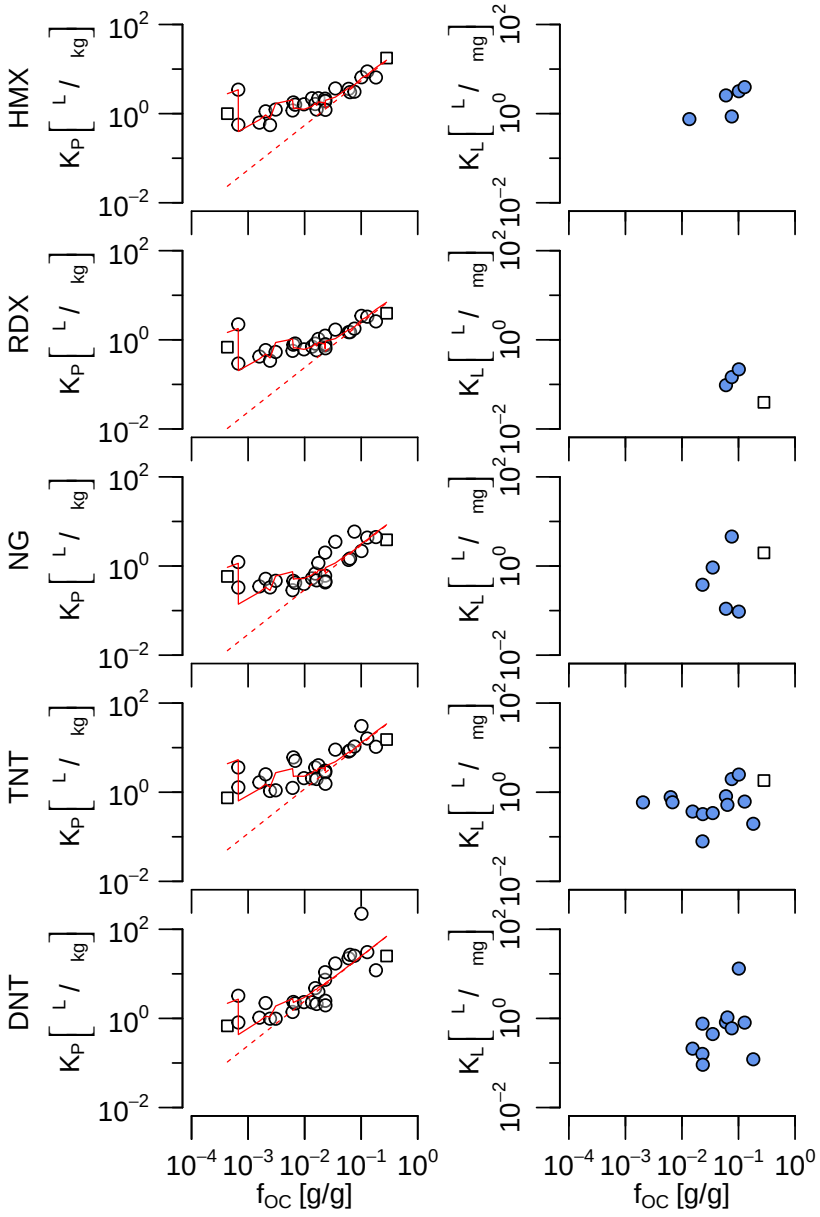


Figure 3.6: Partition coefficients, K_P, and Langmuir constants, K_L, estimated by STM (points). Solid red line shows K_P as predicted by the two-site multilinear regression, Eq 3.8. Dashed red line shows K_P predicted by a K_{OC} only model, Eq 3.9. Squares indicate reference sorbents not used in the multilinear regression.

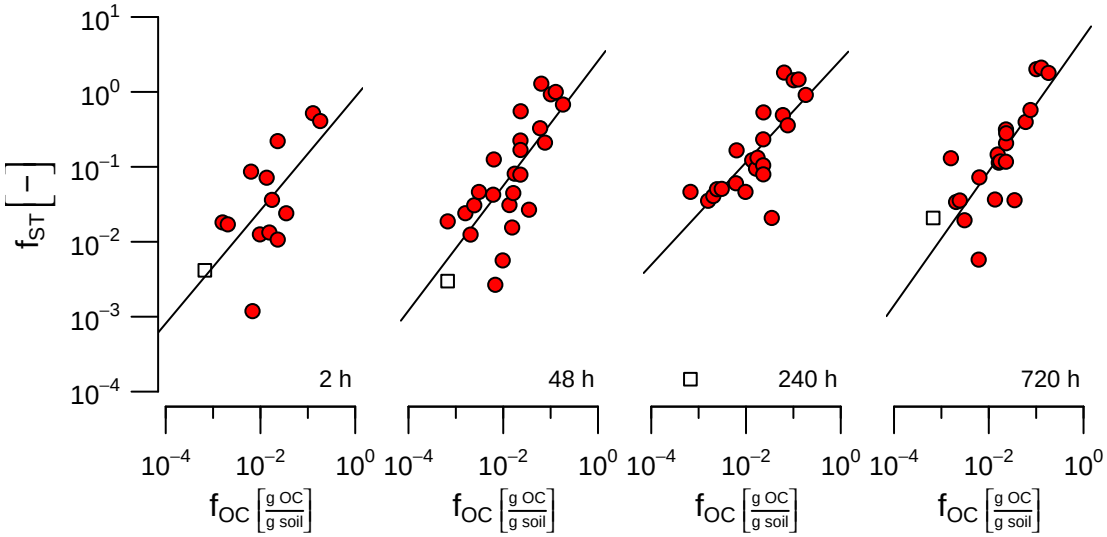


Figure 3.7: Estimated f_{ST} for each adsorption duration. Points are soils, squares are reference sorbents not used in the log-log regression. Line indicates log-log regression. Parameters listed in Table 3.3

Fraction (Eq 2.36) which shows that soils with higher f_{OC} display greater hysteresis and that hysteresis is also a function of adsorption contact time (Figure 2.10). A plot of f_{ST} vs. fraction organic carbon, Figure 3.7, shows the relationship of the site transformation factor to f_{OC}. It is clear that the transformation factor is directly related to soil f_{OC} content, and that an increase in f_{OC} corresponds to a proportional increase in f_{ST}:

$$log_{10} f_{ST} = m_{ST} log_{10} f_{OC} + b_{ST} \tag{3.10}$$

where m_{ST} and b_{ST} are the slope and intercept of the regression.

The four f_{ST} regressions were visually similar. The slope and intercept of a log-log regression for each contact time showed that the slopes were similar, while the intercepts increased as adsorption contact time increased (Table 3.3). The slopes

Table 3.3: Coefficients for regression on f_{ST} for 2, 48, 240, and 720h adsorption durations (Eq 3.10)

t_{ads}	m_{ST}	b_{ST}	R^2
2h	0.778 ($\pm$0.248)	0.0851 ($\pm$0.485)	0.457
48h	0.864 ($\pm$0.153)	0.573 ($\pm$0.304)	0.581
240h	0.709 ($\pm$0.109)	0.560 ($\pm$0.218)	0.665
720h	0.892 ($\pm$0.146)	0.837 ($\pm$0.281)	0.664

and intercepts from are plotted against log_{10} (t_{ads}) to develop a model for the time dependence of the transformation, Figure 3.8.

To develop a model for f_{ST}, regressions on m_{ST} and b_{ST} were developed. The regression of the slope parameter,

$$m_{ST} = 0.0189\,(\pm 0.0513)\,log_{10}t_{ads} + 0.777\,(\pm 0.105) \tag{3.11}$$

yields a constant value ($p = 0.749$). The intercept regression, however,

$$b_{ST} = 0.270\,(\pm 0.0549)\,log_{10}t_{ads} + 0.0256\,(\pm 0.112) \tag{3.12}$$

shows dependence in time ($p = 0.0388$), but no statistically significant intercept ($p = 0.839$). Using these results a regression model for f_{ST} is fit to the data in Figure 3.8.

$$log_{10}f_{ST} = 0.820\,(\pm 0.0487)\;log_{10}\,(f_{OC}) + 0.280\,(\pm 0.0466)\;log_{10}\,(t_{ads}) \tag{3.13}$$

The model for f_{ST}, Eq 3.13, is applicable over the range of f_{OC} observed ($0.0043 \leq f_{OC} \leq 0.281$) and adsorption contact times ($2h \leq t_{ads} \leq 720h$). A plot of the regression predicted f_{ST} vs. STM estimated f_{ST} is presented in Figure 3.9. The regression

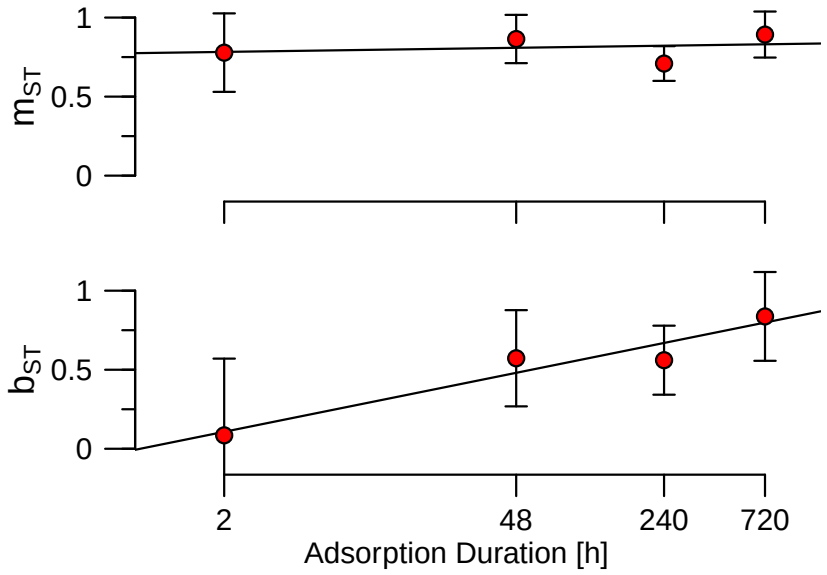


Figure 3.8: f_{ST} regression estimated slope,m_{ST}, and intercept, b_{ST}.

(Eq 3.13) shows good agreement between estimated and predicted f_{ST} values. Reference sorbents were not used in the development of the regression, but show agreement with predicted values, with the exception of the 720h low f_{OC} sorbent.

The f_{ST} regression, Eq 3.13, indicates that the organic carbon content of the sorbent determines the extent of reversibility. This strongly suggests that organic matter is site responsible for hysteresis in soil. Further, it supports the hypothesis that physical deformation is sorbate independent. Secondly, the strong dependence on adsorption contact time (t_{ads}) shows that a kinetic component may be the transformation of binding site strength. Chemical hysteresis has been suggested in other works as a function of organic carbon and contamination age, i.e. duration of adsorption [Nam et al., 1998].

There is a limitation to the empirical model of f_{ST} (Eq 3.13). It cannot be

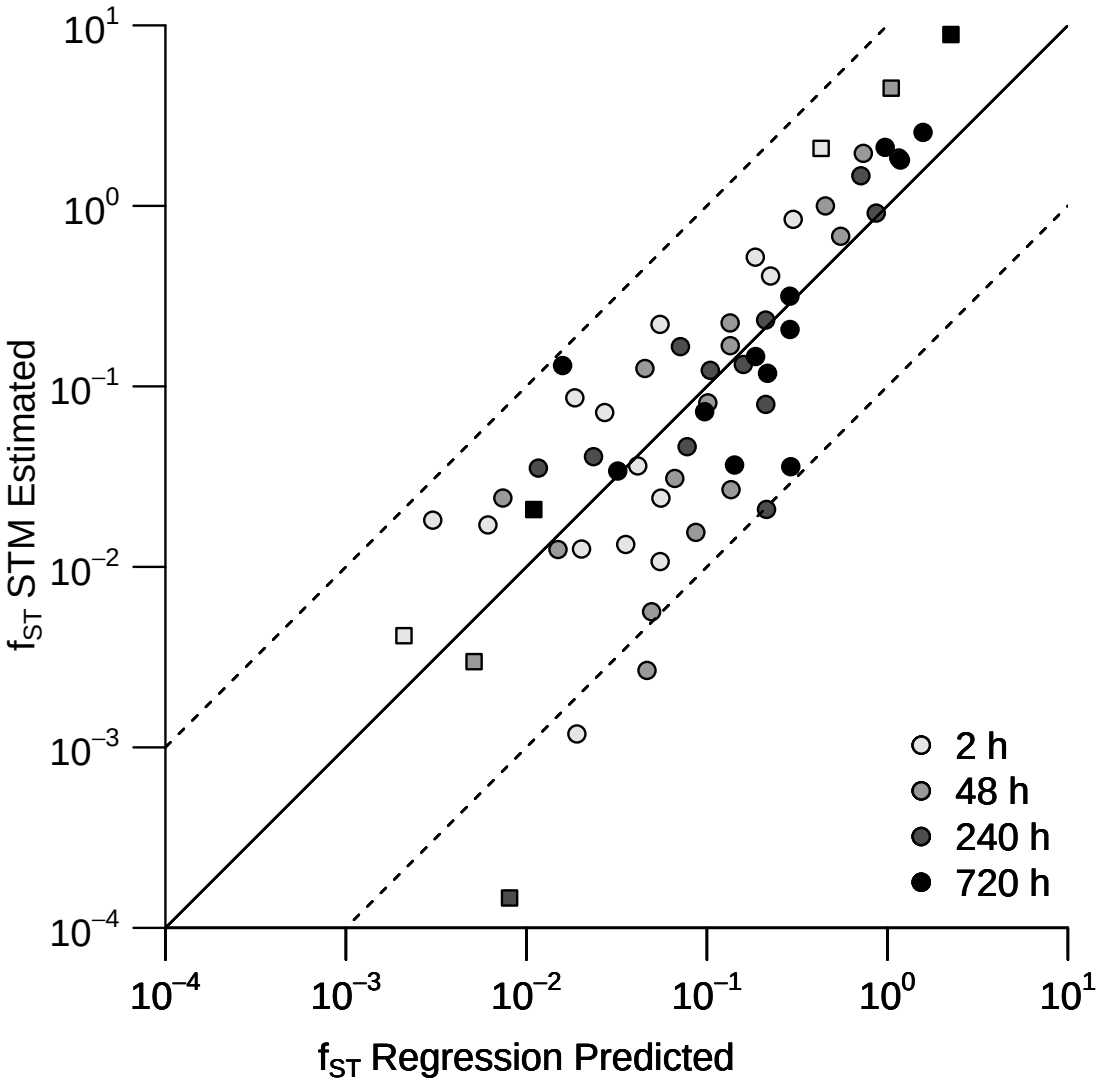


Figure 3.9: STM estimated f_{ST} vs. regression predicted (Eq 3.13) f_{ST}. Points are soils, squares are reference sorbents. Darker shading indicates increased adsorption contact time. Solid line indicates a unity comparison. Dashed lines indicate factors of 10.

determined if there is a maximum f_{ST} as time increases, but since the transformation factor cannot increase indefinitely, it must have a maximum value. Establishing the appropriate dependence will require further investigation.

3.3.3 Comparing reversible resistant and site transformation models

Understanding the time dependent behavior of hysteresis is vital to accurate assessment of sorption. In Chapter 2 the reversible resistant (RR) model was used to describe the data. In the RR model, the time component was not treated explicitly. Rather each adsorption contact time used a different partition coefficient. In contrast, the STM uses only a single partition coefficient for each MC and soil. The time dependence is found only in the site transformation factor, f_{ST} (Eq 3.13). Therefore the STM can predict both adsorption and desorption hysteretic behavior using only f_{OC} and the adsorption contact time, t_{ads}.

To compare these two models, the RMSE (Eq 3.6) were calculated for both the RR (Eq 2.28) and STM (Eqs 3.3 and 3.5). Both models used estimated parameters (Appendix A.3.4.1 an A.3.4.2 for RR partition coefficients, Appendix B.5 for STM parameters) to compare a best case scenario. The log_{10} ratios of RMSE_{RR} and RMSE_{STM} for each MC and sorbent are shown in Figure 3.10A. The grey shaded bars correspond to soils for which Langmuir isotherms are used. Positive values indicate reduced RMSE when the STM is applied. In comparison to the RR model the STM is more accurate at predicting sorbed concentrations, as shown by the number of positive RMSE reductions. This is especially true for the higher f_{OC} sorbents which show dramatic improvement for the STM as f_{OC} increases. Several soils showed no improvement, predominantly for RDX which showed greater RMSE_{STM} for the middle third of f_{OC} soils. The RMSE_{STM} for RDX on these soils was an average of 31.4% greater than the corresponding RMSE_{RR} , however for soils with $f_{OC} > 0.03$

predictions improved by an average of 72%. For TNT the improvement was greater. Average improvement for sorbents with $f_{OC} > 0.03$ was 76%.

When comparing the RMSE for different adsorption contact times, error decreases in each case, Figure 3.10B, indicating that the single time dependent parameter, f_{ST} is sufficient to describe hysteretic behavior independent of sorbent properties.

3.3.4 Multilinear predictive model

The RR model requires four sorbate parameters ($K_{OC,x}, K_{OC,0}, K_{clay,x}K_{clay,0}$) and two sorbent parameters (f_{OC} and f_{clay}) to predict sorbed concentrations. These parameters are adsorption contact time specific and no relationship has been found between them. In contrast, the STM requires two sorbate parameters (K_{OC}, K_{clay}), two sorbent parameters (f_{OC}, f_{clay}), and the adsorption contact time (t_{ads}) to estimate sorbed concentrations. As a measure of the predictive capabilities of the STM, the multilinear model, Eq 3.8, and f_{ST} regression, Eq 3.13, were added to the STM.

$$\begin{aligned} q_A(i,j) = &\left(f_{OC}(i)K_{OC}(j) + f_{Clay}(i)K_{Clay}(j)\right) C_A(i,j) \\ &+ f_{ST}(i)\left(f_{OC}(i)K_{OC}(j) + f_{Clay}(i)K_{Clay}(j)\right) C_A(i,j) \end{aligned} \tag{3.14a}$$

$$\begin{aligned} q_D(i,j) = &\left(f_{OC}(i)K_{OC}(j) + f_{Clay}(i)K_{Clay}(j)\right) C_D(i,j) \\ &+ f_{ST}(i)\left(f_{OC}(i)K_{OC}(j) + f_{Clay}(i)K_{Clay}(j)\right) C_D(i,j) \end{aligned} \tag{3.14b}$$

where i and j refer to sorbent i and sorbate j respectively and f_{ST} is given by Eq 3.13. As there was no suitable method for predicting K_L, the Langmuir data sets were not included. A comparison of observed and modeled sorbed concentrations is shown as Figure 3.11. The figure shows that the data is well represented by the modeled values. No apparent bias is observed. Further, the RMSE (Eq 3.6) is low, RMSE = 0.283. This value is a small increase to the fit model RMSE of 0.186.

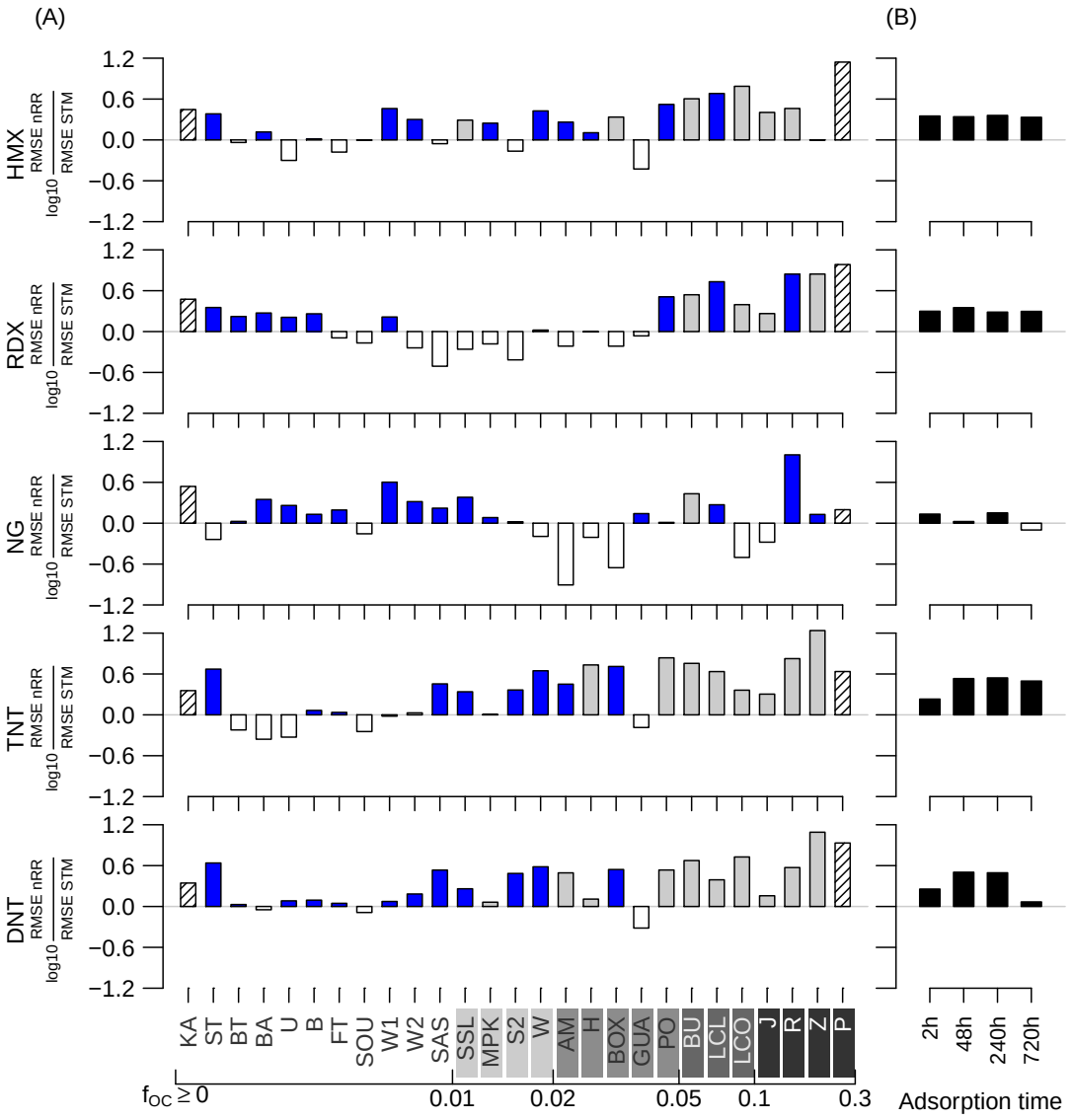


Figure 3.10: log_{10} ratio of RMSE, RR:STM, for predicted sorbed concentrations. (A) RMSE calculated for each sorbent. (B) RMSE for each adsorption duration. Bars are colored for positive values and hollow for negative values. Filled bars are soils. Hashed bars are reference sorbents. Grey shaded bars correspond to soils for which Langmuir isotherms are used. Axis shading indicates increasing f_{OC}.

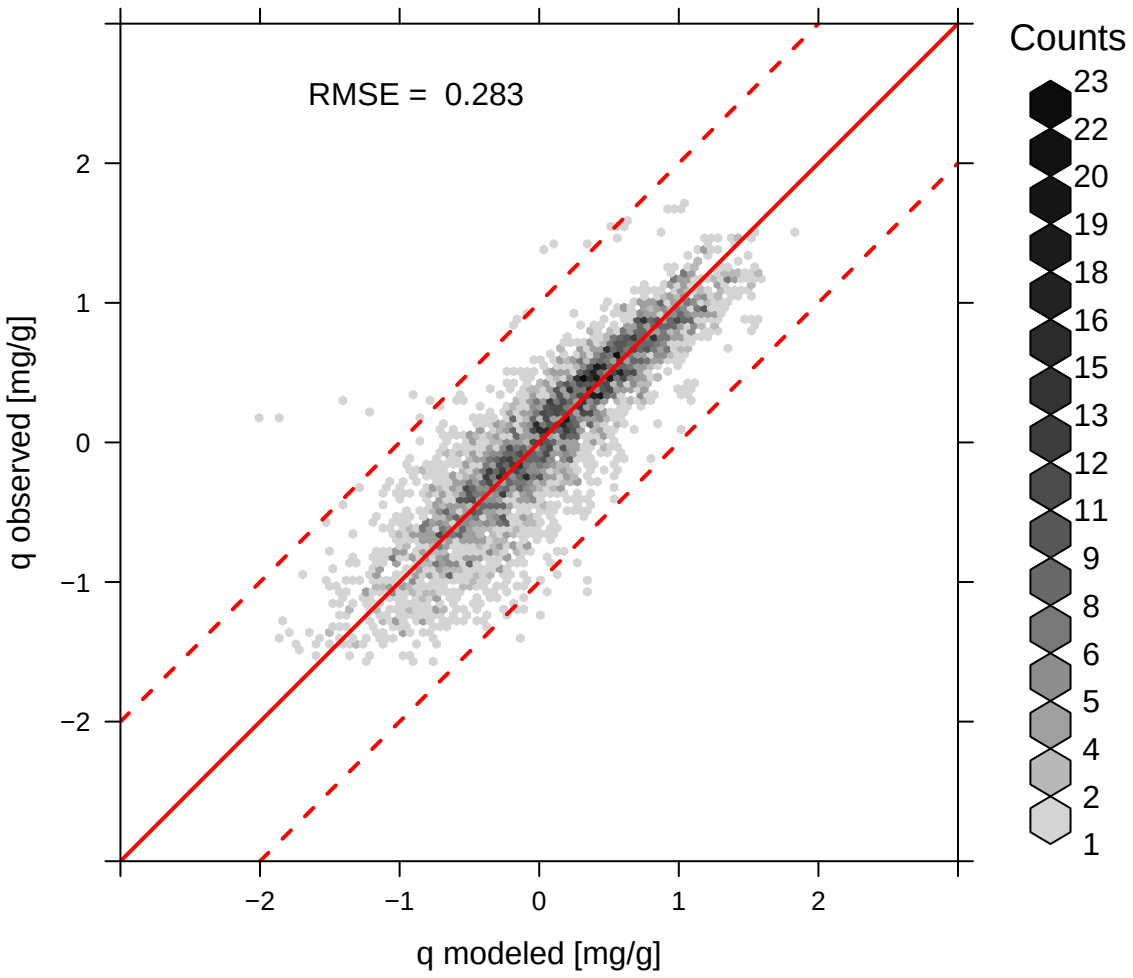


Figure 3.11: Comparison of STM predicted using predicted parameters and observed sorbed concentrations. Data is grouped into hexagons, the shading of which indicates the number of data. The red solid line indicates unity, dashed lines are spaced at 1 log unit from unity.

To determine if there are sorbent specific biases, residuals were calculated between observed and predicted sorbed concentrations, Figure 3.12. Linear data is well described by the multilinear model, with most data within a factor of 2. It is difficult to determine if the model predicts well for high f_{OC} sorbents since most data were fit using Langmuir isotherms. However, HMX, RDX, and NG show several data sets that are in close agreement with predictions.

3.4 Conclusions

The STM incorporates binding strength changes and can reproduce the observed hysteretic sorption. In comparison to other models, the STM requires only one time dependent parameter, the site transformation factor, f_{ST}, significantly reducing the number of parameters that need to be estimated. Moreover, the relationship to f_{OC} and length of adsorption contact time makes physical sense within the framework of glassy/rubbery soil organic carbon sorption wherein the sorbent matrix is deformed by the adsorption process. This induces a change in the binding properties of the sorbent through a change in binding site strength, a physical change in the sorbent, or other processes. An implication of this observation is that short adsorption contact times and/or low f_{OC} sorbents lead to highly reversible systems, regardless of the sorbate. This observed sorbate independence supports the hypotheses posed by other researchers and is further evidence for a sorbent transformation process. The new parameter, f_{ST}, requires further analysis to determine if it is bounded, since the current data suggests a log-linear trend in relation to the duration of adsorption.

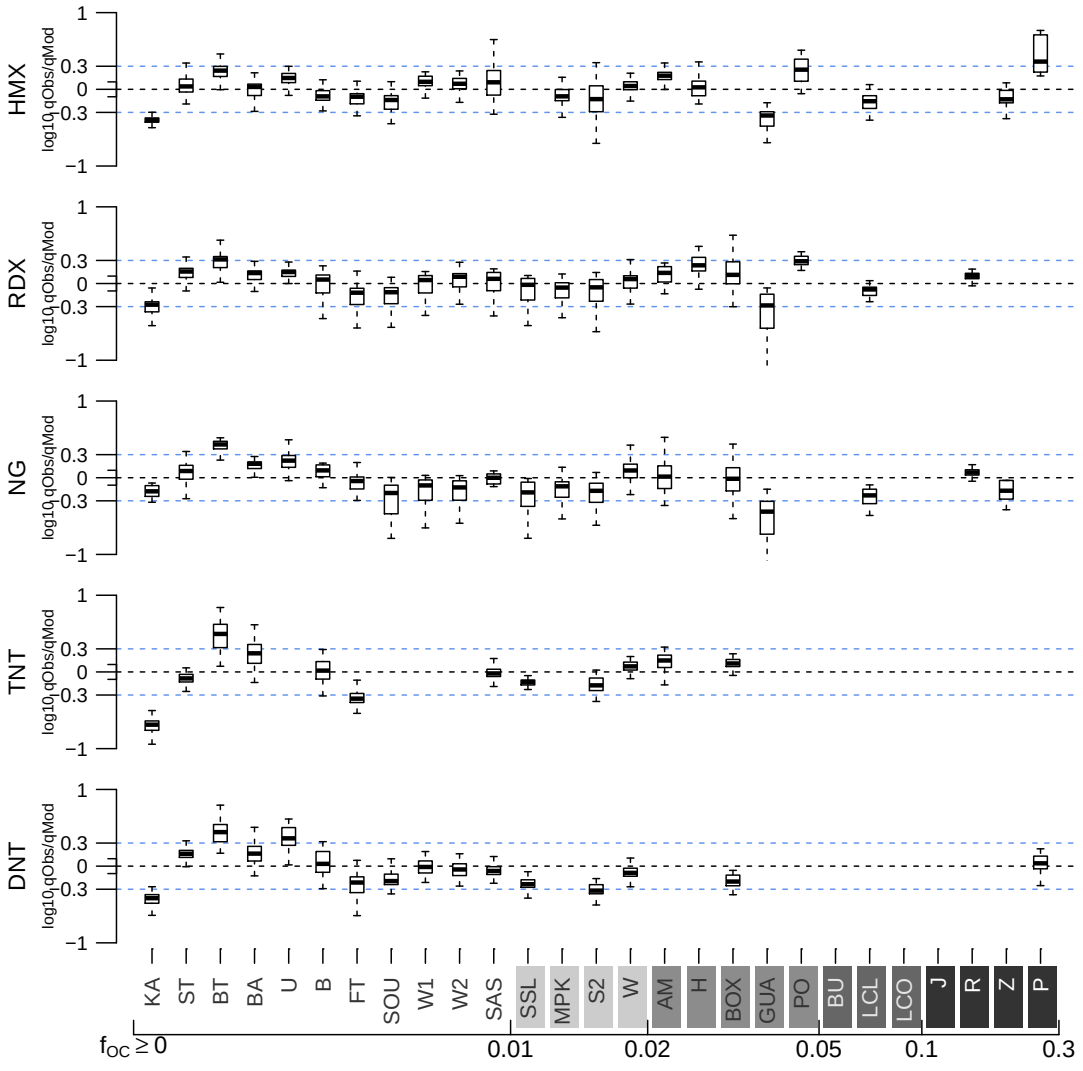


Figure 3.12: Linear prediction of sorbed concentrations for each MC and sorbent using Eqs 3.14a - 3.14b and 3.13. Langmuir data was not included. Axis shading indicates increasing f_{OC}.

REFERENCES

Bouyoucos, G. (1962). Hydrometer method improved for making particle size analysis of soils. *Agronomy Journal*, (54):464–465.

Chilom, G. and Rice, J. A. (2005). Glass transition and crystallite melting in natural organic matter. *Organic Geochemistry*, 36(10):1339–1346.

Di Toro, D. M. (2013). Site transformation model of adsorption-desorption hysteresis. *Abstracts of Papers of the American Chemical Society*, 245.

Dunn, O. J. (1961). Multiple comparisons among means. *Journal of the American Statistical Association*, 56(293):52–64.

Gebremariam, S. Y., Beutel, M. W., Flury, M., Harsh, J. B., and Yonge, D. R. (2012). Nonsingular adsorption/desorption of chlorpyrifos in soils and sediments: Experimental results and modeling. *Environmental Science & Technology*, 46(2):869–75.

Huang, W. L., Yu, H., and Weber, W. J. (1998). Hysteresis in the sorption and desorption of hydrophobic organic contaminants by soils and sediments - 1. a comparative analysis of experimental protocols. *Journal of Contaminant Hydrology*, 31(1-2):129–148.

Kan, A. T., Fu, G., Hunter, M., Chen, W., Ward, C. H., and Tomson, M. B. (1998). Irreversible sorption of neutral hydrocarbons to sediments: Experimental observations and model predictions. *Environmental Science & Technology*, 32(7):892–902.

Lesan, H. and Bhandari, A. (2003). Atrazine sorption on surface soils: Time-dependent phase distribution and apparent desorption hysteresis. *Water Research*, 37(7):1644–1654.

Lu, Y. F. and Pignatello, J. J. (2002). Demonstration of the "conditioning effect" in soil organic matter in support of a pore deformation mechanism for sorption hysteresis. *Environmental Science & Technology*, 36(21):4553–4561.

Nam, K., Chung, N., and Alexander, M. (1998). Relationship between organic matter content of soil and the sequestration of phenanthrene. *Environmental Science & Technology*, 32(23):3785–3788.

Palomo, M. and Bhandari, A. (2006). Impact of aging on the formation of bound residues after peroxidase-mediated treatment of 2,4-DCP contaminated soils. *Environmental Science & Technology*, 40(10):3402–3408.

R Core Team (2014). *R: A Language and Environment for Statistical Computing*. R Foundation for Statistical Computing, Vienna, Austria.

Sander, M., Lu, Y. F., and Pignatello, J. J. (2006). Conditioning-annealing studies of natural organic matter solids linking irreversible sorption to irreversible structural expansion. *Environmental Science and Technology*, 40(1):170–178.

Sander, M. and Pignatello, J. J. (2005). An isotope exchange technique to assess mechanisms of sorption hysteresis applied to naphthalene in kerogenous organic matter. *Environmental Science & Technology*, 39(19):7476–7484.

Sander, M. and Pignatello, J. J. (2009). Sorption irreversibility of 1,4-dichlorobenzene in two natural organic matter-rich geosorbents. *Environmental Toxicology & Chemistry*, 28(3):447–457.

Walpole, R. E., Myers, R. H., Myers, S. L., and Ye, K. (2007). *Probability and Statistics for Engineers and Scientists*. Pearson Prentice Hall.

Wang, Z., Chen, S., Xu, Y., and Tang, J. (2012). Aging effects on sorption-desorption behaviors of PAHs in different natural organic matters. *Journal of Colloid and Interface Science*, 382(1):117–122.

Weber, W., McGinley, P., and Katz, L. (1992). A distributed reactivity model for sorption by soils and sediments. 1. conceptual basis and equilibrium assessments. *Environmental Science & Technology*, 26:1955–1962.

Chapter 4

MODELING TRANSPORT OF MUNITION CONSTITUENTS IN A SOIL COLUMN USING REVERSIBLE RESISTANT PARTITIONING

In the preceding chapters, it has been shown that hysteretic sorption is an important component of sorption in batch systems. Field sites, however, are not batch systems. Column studies are frequently used to portray the transport of chemical in a soil profile. To date, there has been little study of munition constituent sorption in column studies. Research has shown that the sorption of RDX and TNT retards the elution of these MC from soil columns [Dontsova et al., 2006]. Further, it has been previously seen that the breakthrough of RDX from a column occurs significantly sooner than for TNT [Sharma et al., 2013]. Chappell et. al. [Chappell et al., 2011] has shown that partition coefficients for TNT frequently over-predict transport of chemical through soil columns. Unrecoverable chemical has been previously found in MC column studies [Comfort et al., 1995], but reversible and resistant partitioning has not been implemented in column studies, despite the potential for such a partitioning model to explain observed discrepancies between influent and recovered concentrations.

Due to the lack of literature, an analysis of the sorption of two munition constituents (MC) was undertaken. RDX and TNT vary greatly in their batch study behavior. RDX shows little hysteresis, whereas TNT shows significant hysteresis as well as degradation. Application of the reversible resistant model [Di Toro and

Horzempa, 1982] is expected to show the importance of hysteretic sorption when column transport studies are performed.

4.1 Materials and methods

The data used for this analysis was obtained as part of a SERDP project, ER-1688. A concise description of the experiment is contained here, the full methodology details can be found in [Allen et al., 2015]. The experiment consisted of a borosilicate column, 10 cm x 2.2 cm in diameter packed with 45.43 g Sassafras Sandy Loam (SSL) soil with 0.7 cm glass wool as a spacer. Selected soil properties are shown in Table 4.1. A solution of 0.005 M $CaNO_3$ and 0.01 M NaN_3 was added at a rate of 0.2 mL/min for 32 h. The influent was then changed to a solution composed of 10 mg/L Cl, as a tracer, 5.5 mg/L RDX, 9 mg/L TNT, 0.005 M $CaNO_3$ and 0.01M NaN_3. This solution was added at a rate of 0.2 mL/min for 24 h. After this period, the solution was returned to the 0.005 M $CaNO_3$ and 0.01 M NaN_3 solution for an additional 24 h. Effluent was sampled every 30 min and was analyzed for Cl, RDX, and TNT. At the end of the experiment, the soil in the column was extracted every 2 cm using acetonitrile. Samples were analyzed using an Agilent 1200 Series HPLC with a Zorbax SB-C18 reverse phase column at a wavelength of 214 nm. The flow rate used was 2 mL/min for a methanol:water gradient of 30:70 percent to 65:35 percent from 0 to 2.8 min, and 65:35 percent to 30:70 percent from 2.8 to 3.2 min.

Breakthrough curves for TNT, RDX, and chloride are shown in Figure 4.1. RDX was advectively retarded when compared to chloride, however, the breakthrough curves were similar, with RDX eventually reaching 100% of the influent concentration at approximately 10 h. TNT, however, showed significant retardation. Concentrations do not reach inflow concentrations even after 24 h.

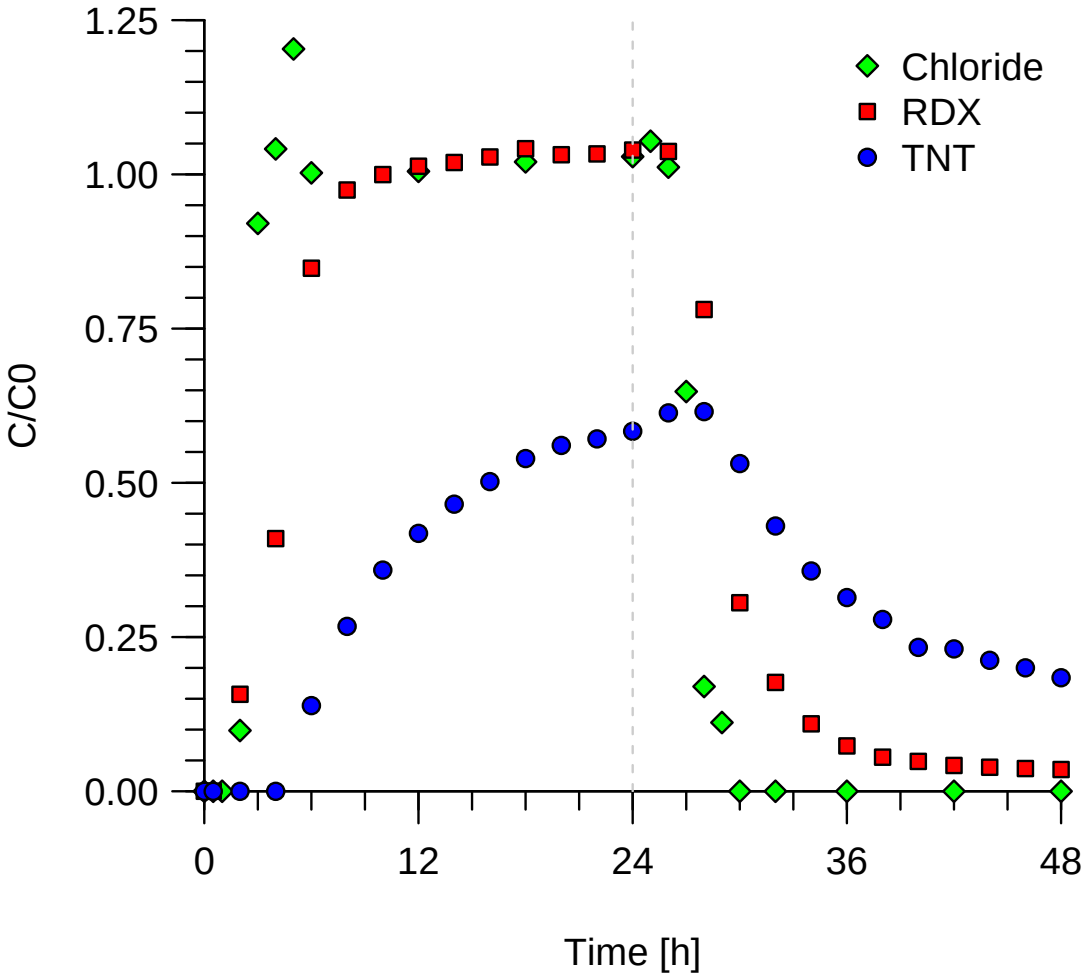


Figure 4.1: Break-through curves for RDX, TNT, and chloride (tracer). Vertical line at 24 h indicates switchover to solution containing no MC or chloride.

Table 4.1: Soils used in this analysis. * indicates the soil used for column experiments

Soil	TOC	Sand	Silt	Clay
	[%]	[%]	[%]	[%]
SSL*	1.33	55	28	18
Aberdeen BT	0.07	83.8	7.1	9.1
Souli	0.61	42.4	14.4	43.2
Houthalein	2.31	85.9	10.1	4
Rhydtalog	12.83	43.8	43.7	12.5
Zedveld	18.23	45.8	32.5	21.7

4.2 Analysis

An advective-diffusive model was used to model the transport of chemical within the column. The modeled column was composed of 200 segments ($\Delta x = 0.05$ cm) of equal size to mitigate the effects of numerical dispersion. For the diffusion coefficient, the model used a single value for all three species.

Partitioning was controlled using the reversible resistant (RR) Model [Di Toro and Horzempa, 1982]. This model has has not been applied to column studies previously. The RR model is defined as:

$$C_{tot} = C_d + mq_x + mq_0 \tag{4.1}$$

$$= C_d + C_x + C_0 \tag{4.2}$$

$$C_x = mK_xC_d \tag{4.3}$$

$$C_0 = mK_0C_d \tag{4.4}$$

where C_{tot} is the total bulk concentration $[mg/L]$, C_d is the aqueous phase concentration $[mg/L]$, m is the soil-water ratio $[kg/L]$, q_x and q_0 are the reversibly and resistantly sorbed concentrations per unit sorbent, respectively $[mg/kg]$, C_x and C_0 are the bulk concentrations of the reversibly and resistantly sorbed concentrations

per unit sorbent, respectively $[mg/L]$, and K_x and K_0 are the partition coefficients for the reversible and resistant components, respectively $[L/kg]$. Bulk concentrations were used to simplify the modeling.

The RR model describes partitioning by allowing sorption to two sorbent sites: a reversible site that is always in equilibrium with the aqueous phase, and a resistant site that that is in equilibrium only while adsorbing. The model defines hysteresis as a lack of desorption from the resistant sites. Each site is defined by a partition coefficient, K_x for reversible sites and K_0 for resistant sites. The corresponding sorbed concentration is q_x or q_0 for reversible and resistant concentrations, respectively.

The resulting advection-diffusion model, Eqs 4.5 - 4.7, depends on whether the sorbent is adsorbing or desorbing, i.e. adding to or depleting from the sorbed phase:

$$V_i \frac{dC_{tot,i}}{dt} = QC_{d,i-1} - QCd, i + \frac{DA}{l}\left(C_{d,i-1} - C_{d,i}\right) + \frac{DA}{l}\left(C_{d,i+1} - C_{d,i}\right) - k_r C_{d,i} V_i \tag{4.5}$$

$$C_{d,i} = \begin{cases} \dfrac{C_{tot,i}}{1 + mK_x + mK_0} & \text{During adsorption} \quad (4.6a) \\ \dfrac{C_{tot,i} - C_{0,i}}{1 + mK_x} & \text{During desorption} \quad (4.6b) \end{cases}$$

$$C_{0,i} = mK_0 C_{a,i} \tag{4.7}$$

where V_i, is the volume of layer i $[L^3]$, $C_{tot,i}$ is the total concentration in layer i $[mg/L]$, Q is the volumetric flow rate of the aqueous phase $[L^3/min]$, $C_{d,i}$ is the dissolved concentration for layer i $[mg/L]$, D is the effective diffusion coefficient

$[cm^2/min]$, A is the interfacial area between layers $[cm^2]$, l is the diffusive length $[cm]$, and k_r is a first order degradation rate $[1/min]$, K_x is the reversible partition coefficent $[L/kg]$, K_0 is the resistant partition coefficient $[L/kg]$, m is the soil-water ratio $[kg/L]$, C_0 is the resistant concentration in bulk units $[mg/L]$, and C_a is the concentration in the aqueous phase during adsorption $[mg/L]$.

Model estimated parameters were, D, K_x^{RDX}, K_0^{RDX}, k_r^{RDX}, K_x^{TNT}, K_0^{TNT}, k_r^{TNT}. Chloride was assumed to only be in the dissolved phase, $K_x = K_0 = 10^{-9}$ where 10^{-9} was used as a lower limit due to simplify the model requirements. Variables were fit by Matlab using a pattern search algorithm that minimized the linear sum of squares between observed and modeled aqueous concentrations, Eq 4.8:

$$ssq = \sum_{j=1}^{3} \sum_{k=1}^{n} \left(C_{d,k,obs}(j) - C_{d,k,mod}(j) \right)^2 \tag{4.8}$$

where n is the number of observations, $C_{d,k}(j)$ is the k observation of an aqueous concentration for chemical j, and the subscripts *obs* and *mod* refer to observed and modeled concentrations, respectively.

Figure 4.2 shows the dissolved, sorbed, and total concentrations for the advection-diffusion model after application to the data. For all three chemicals, the dissolved concentration is well predicted. Chloride and RDX show no resistant component, while TNT shows the presence of a small amount of resistance. It should be noted that although there is little difference between the reversible/resistant model dissolved concentration and the completely reversible case for TNT, the optimization did converge to a non-zero resistant partition coefficient. This suggests that hysteretic processes are occurring within the column. The lack of a hysteretic component for RDX is not unexpected as the batch studies did not show resistant sorption

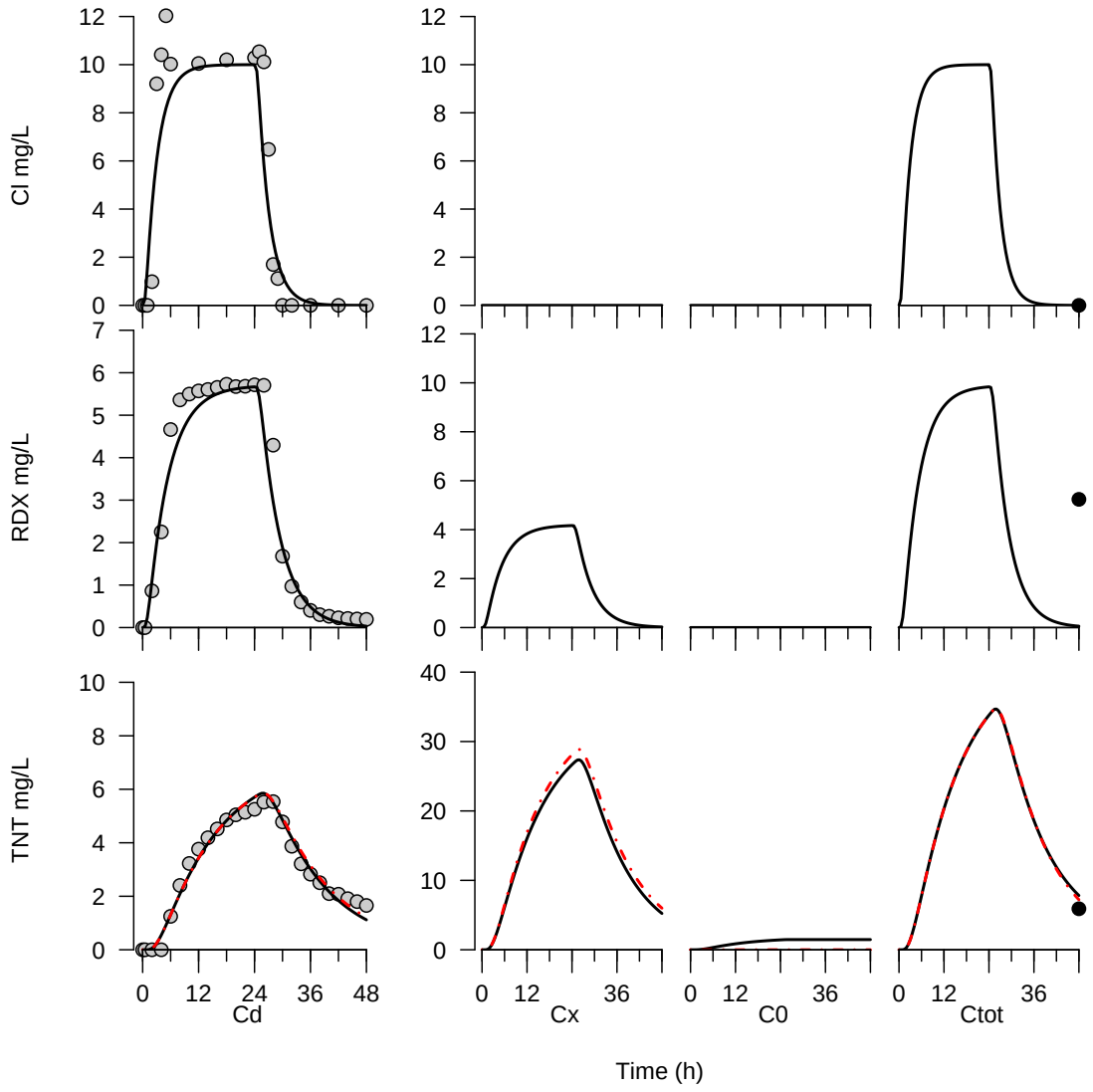


Figure 4.2: Advection-diffusion model prediction. Black lines use reversible/resistant partitioning. Red line shows a reversible model ($K_0 = 0$). Points on C_d plots are observed concentrations. Points in C_{tot} plots are the extracted concentrations.

Table 4.2: Parameters estimated by Matlab pattern search algorithm.

		Species		
		Cl	RDX	TNT
D	$[cm^2/d]$	344	344	344
K_x	$[L/kg]$	1×10^{-9} *	0.0703	4.68
K_0	$[L/kg]$	1×10^{-9} *	1×10^{-9} *	0.250
k_r	$[d^{-1}]$	0.00	8.64×10^{-8}	1.90

* Lower limit value

Table 4.3: Multilinear component partition coefficients [L/kg].

	$K_{OC,x}$	$K_{OC,0}$	$K_{clay,x}$	$K_{clay,0}$
RDX	28.9	7.61	2.54	0.154
TNT	65.6	66.2	4.15	0.455

for SSL soil. Model estimated parameters are shown in Table 4.2.

To check the validity of the model optimized parameters, the previously developed multilinear model [Gonzalez Forero, 2013] was used. This model decomposes the total partition coefficient into sorbent matrix specific parameters. Gonzalez used both 2 and 3 site parameterizations of the model and found little improvement over an organic carbon fraction (f_{OC}) and clay size fraction (f_{clay}) model:

$$K_x = f_{OC}K_{OC,x} + f_{clay}K_{clay,x} \tag{4.9}$$

$$K_0 = f_{OC}K_{OC,0} + f_{clay}K_{clay,0} \tag{4.10}$$

The multilinear derived partition coefficients, as well as sorbent matrix partition coefficients, are shown in Table 4.3.

Advection-diffusion model estimated K_x^{RDX} compare favorably to multilinear model derived values, shown in Table 4.3, however, predicted K_0 from each model

Table 4.4: Reversible and resistant partition coefficients [L/kg] determined by the multilinear model.* indicates the soil used in this experiment.

		Soil					
		SSL*	BT	SOU	H	R	Z
RDX	K_x	0.843	5.83	1.24	4.03	0.77	0.250
	K_0	0.129	1.42	0.113	0.996	0.183	0.0191
TNT	K_x	1.62	12.9	2.19	8.93	1.68	0.422
	K_0	0.965	12.2	0.601	8.55	1.54	0.0859

are markedly different. The pattern optimized partition coefficient for RDX is effectively zero but the multilinear resistant partition coefficient is $\gg 0$ ($K_0^{RDX} = 0.129$). Due to this discrepancy, it was hypothesized that the pattern fit optimized value was merely an artifact of a small resistant component. To test the validity of this hypothesis, a sensitivity analysis was performed. It was found that a value of $K_0^{RDX} = 0.0316$ showed an increase in the resistant sorption without significantly affecting the observed aqueous concentrations. This sensitivity limit (SL) value is much closer to a multilinear (ML) model predicted partition coefficient ($K_{ML,0}^{RDX} = 0.129$, $K_{SL,0}^{RDX} = 0.0316$).

Extractions had been performed on the column to determine the sorbed phase chemical after a flushing period. Extracted TNT was found at an average concentration of 2.39 ± 0.248 $\mu g/g$ *wet soil*. The advective-diffusive model predicts a concentration of 2.91 $\mu g/g$ *wet soil* indicating that the modeled and observed concentrations are similar. RDX, however, was extracted at a concentration of 0.722 ± 0.0644 $\mu g/g$ *wet soil* for the top 6 cm of the column and 2.12 ± -0.0451 $\mu g/g$ *wet soil* for the bottom 2 cm. No satisfactory explanation for the observed RDX extracted concentrations has been found. Further research is required to rectify the observed increase in extracted concentrations at the lower portion of the column.

Although the resistant concentrations obtained in the column are low, especially for RDX, it is important to note that field sites are significantly deeper than a laboratory experiment can conveniently accomodate. The advective-diffusive model would suggest that over longer column depths, a larger fraction of the total mass of MC will sorb to resistant sites. To verify this, a simulation of a 3 m column was performed. Model parameters were the same as shown in Table 4.2 with the exception of K_0^{RDX} which was set to the sensitivity value of 0.0316. Simulation parameters were the same with the exception of the feed periods. The MC solution was allowed to run for 9 days and then a flushing solution was simulated for a further 9 days. The results of this simulation are shown in Figure 4.3.

Over the 3m depth of the column, approximately 1.8% of the total RDX mass added remained resistantly bound. If this same behavior were occurring in the 10 cm column, it would be expected that less than 0.1% of the input mass would be resistantly bound. Using influent and effluent concentrations of RDX will show little if any deviation in total mass recovered due to the associated error in each measurement. Thus, the resistantly sorbed component would be unable to be distinguished from experimental uncertainty.

TNT shows a larger resistantly sorbed concentration than RDX initially, but due to degradation the resistant concentrations decrease as depth increases. However, despite this loss of mass, 4% of the total TNT added to the column is resistantly retained. Without a reverisble/resistant analysis this portion would likely be described as degraded.

The differing behavior between RDX and TNT is also shown in the depth profiles, Figure 4.3B and D. For RDX, although there is slight spreading due to dispersion, concentrations are similar throughout the column. TNT, however, shows significant differences between concentrations in the top and bottom layers. This is

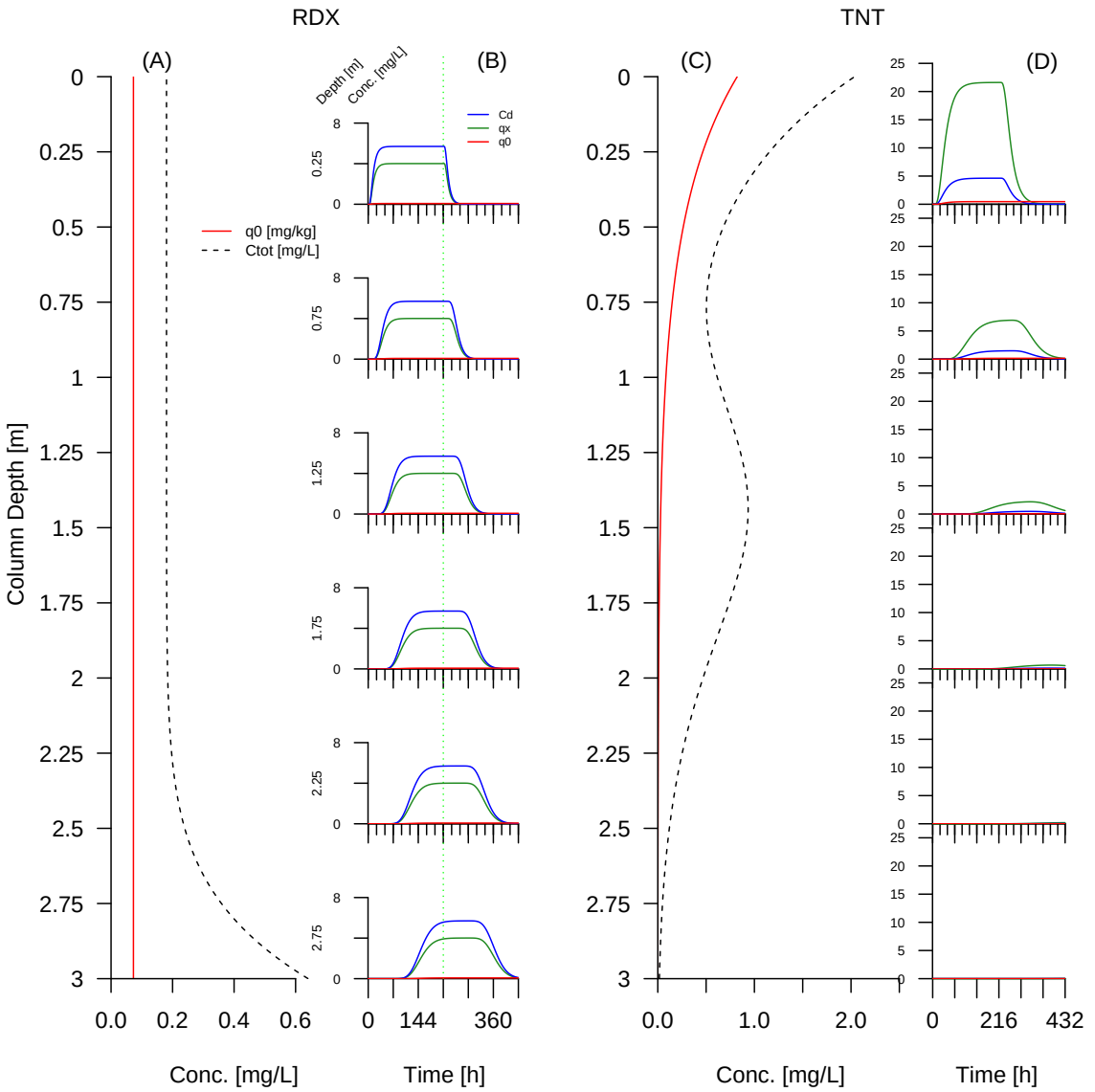


Figure 4.3: RDX and TNT sorption for an 18 d simulation using the advective-diffusive model estimated parameters and $K_x^{RDX} = 0.0316$. (A) Total concentration ($C_d + C_x + C_0$) and resistant concentration (q_0) (dashed black line and red line respectively) RDX at the end of the flushing cycle (t = 432 h) as a function of column depth. (B) Dissolved, reversible, and resistant RDX concentrations as a function of time for several column depths. (C) Total concentration ($C_d + C_x + C_0$) and resistant concentration (q_0) (dashed black line and red line respectively) TNT at the end of the flushing cycle (t = 432 h) as a function of column depth. (D) Dissolved, reversible, and resistant TNT concentrations as a function of time for several column depths.

due to degradation.

As a final simulation, the multilinear model was used to predict the effect of a resistant component in 5 soils that have previously been used for batch testing. The multilinear model as applied is:

$$K_x(j,k) = f_{OC}(j)K_{OC,x}(k) + f_{clay}(j)K_{clay,x}(k) \tag{4.11}$$

$$K_0(j,k) = f_{OC}(j)K_{OC,0}(k) + f_{clay}(j)K_{clay,0}(k) \tag{4.12}$$

where j and k refer to soil j and chemical k, respectively. Soils chosen were: Aberdeen BT, Souli, Houthalein, Rhydalog, and Zegveld. These soils were chosen as examples of a range of behavior that would be expected in the field. The simulation parameters used are shown in Table 4.5, soil properties are shown in Appendix E.2.2.

Table 4.5: Parameters used for simulation of 5 soils using multilinear model derived partition coefficients

Parameter	Value	Units	Parameter	Value	Units
MC Feed	36	[h]	Duration Simulated	120	[h]
Diameter	2.2	[cm]	Length	20	[cm]
Flowrate	0.2	[mL/min]	Pore volumes per day	0.127	$[1/d]$
Porosity	0.482*				

Figures 4.4 and 4.5 show the predicted dissolved and resistant bulk concentrations for RDX and TNT respectively, for each of the soils using the multilinear derived partition coefficients or the fully reversible model where K_P is equal to the sum of the previously determined values of K_x and K_0.

From these figures it can be observed that despite a significant amount of resistant sorption, dissolved concentrations are similar between the reversible and the reversible/resistant models regardless of depth or time. Aberdeen BT (f_{OC} = 0.07%) and Zegveld (f_{OC} = 18.23%) soils differ by a factor of 250× in the f_{OC},

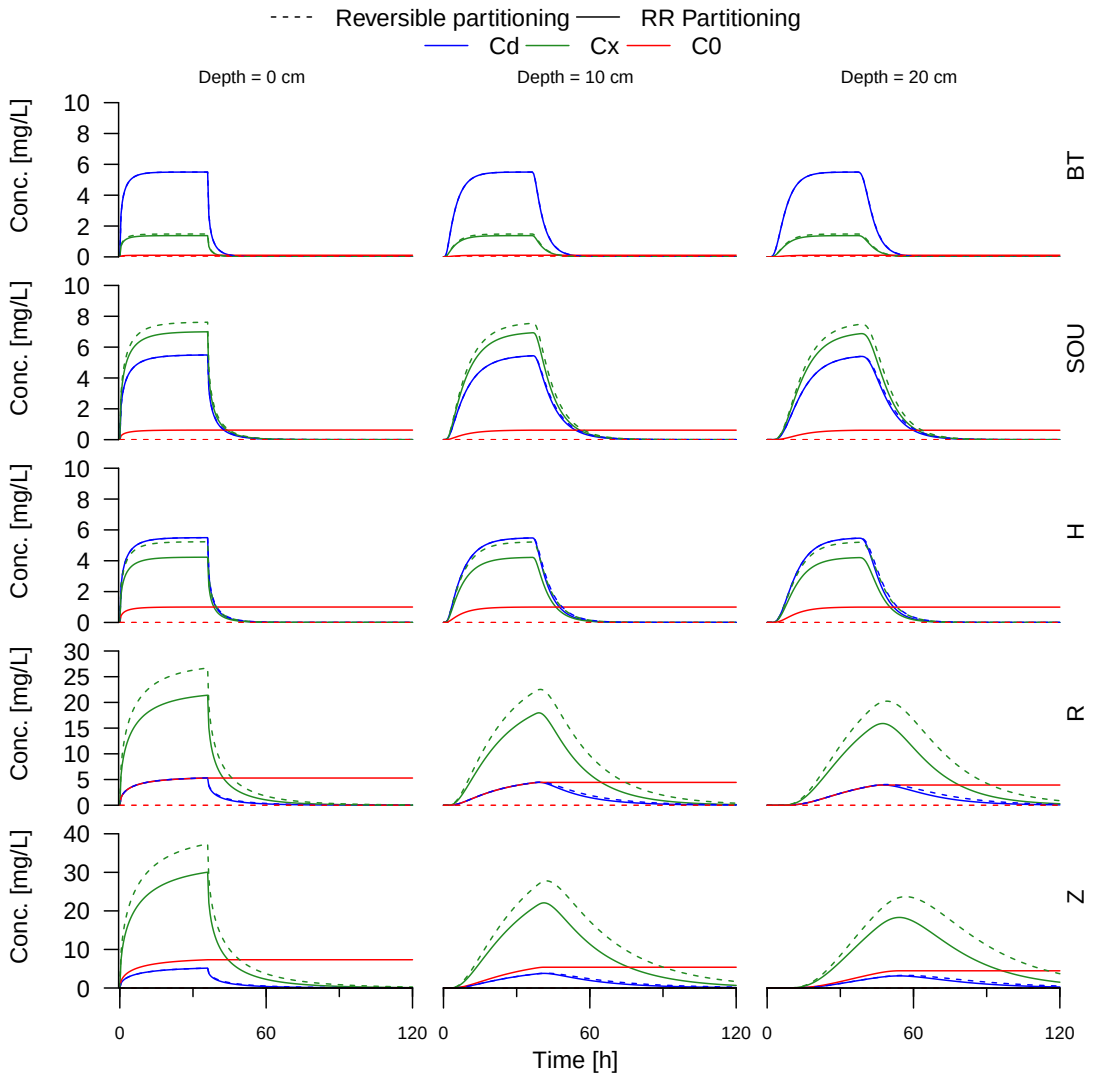


Figure 4.4: RDX bulk concentrations C_d, C_x and C_0 (blue, green, and red, respectively) for five soils: Aberdeen BT (BT), Souli (SOU), Houthalein (H), Rhydtalog (R), and Zegveld (Z). Soil properties are given in Table 4.1. Depth increases from left to right. Dashed line indicates a reversible model ($K_0 = 0$) predicted concentration. Solid lines indicate a reversible/resistant model predicted concentration.

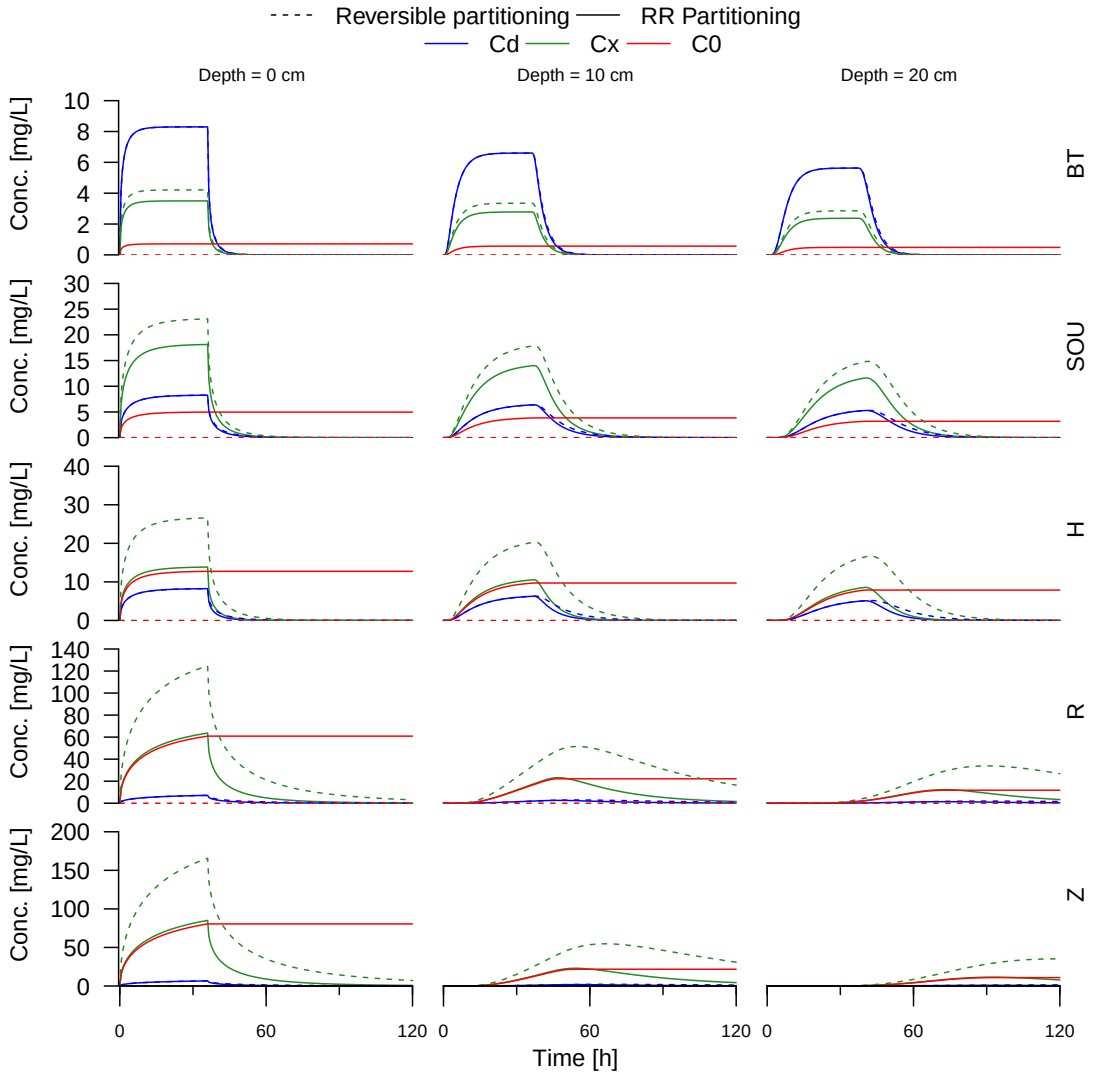


Figure 4.5: TNT bulk concentrations C_d, C_x and C_0 (blue, green, and red, respectively) for five soils: Aberdeen BT (BT), Souli (SOU), Houthalein (H), Rhydtalog (R), and Zegveld (Z). Soil properties are given in Table 4.1. Depth increases from left to right. Dashed line indicates a reversible model ($K_0 = 0$) predicted concentration. Solid lines indicate a reversible/resistant model predicted concentration.

yet show little difference in the dissolved concentration exiting the column at any time despite the addition of a much larger resistant bound concentration in Zegveld soil. This indicates that dissolved concentrations alone are not enough to show if an experiment exhibited resistant sorption.

TNT exhibits depth dependent resistant sorption, whereas RDX does not. This is due to the degradation of TNT. As chemical penetrates the column, the loss in TNT mass allows for less chemical to partition to both the reversible and resistant sites.

For all soils, a large amount of TNT is resistantly sorbed. RDX also resistantly sorbs, though less so than TNT. The non-zero resistant sorption of both of these chemicals is a point of concern because the resistantly sorbed mass may be small, rendering it undetectable without accurate extractions. This may result in unexpected resistantly sorbed masses in field scale depths.

4.3 Conclusions

The implications from this analysis of hysteresis are significant. It is evident that extractions are needed to accurately determine the mass of chemical remaining on the column soil. Further, there is a need for longer columns, which may be difficult for experimental work. This need arises from the small fractions of resistantly sorbed material in a typical laboratory scale experiment. As shown by the simulation of 5 soils, soil characteristics greatly affect the amount of resistant sorption. It is suggested that a soil exhibitng significant hysteresis be used to measure the potential for long term storage of MC in the field. Application of more rigorous methods of modeling resistant sorption should aid in determining a mechanism for the observed sorption and whether it is truly irreversible.

REFERENCES

Allen, H. E., Di Toro, D. M., Kuo, D. T. F, M. R., Michelson, K., Miglino, A., Checkai, R. T., Kuperman, R. G., Simini, M., and Hawari, J. (2015). Improving understanding of the fate and transport of munitions constituents to enhance sustainability of operational ranges. Technical report, University of Delaware. SERDP Project ER-1688.

Chappell, M. A., Price, C. L., Bourne, G. G., Pettway, B. A., and Porter, B. E. (2011). Soil vadose zone chemistry of TNT and RDX under water-saturated conditions. In *Environmental Chemistry of Explosives and Propellant Compounds in Soils and Marine Systems: Distributed Source Characterization and Remedial Technologies*, volume 1069 of *ACS Symposium Series*, pages 217–227. American Chemical Society.

Comfort, S. D., Shea, P. J., Hundal, L. S., Li, Z., Woodbury, B. L., Martin, J. L., and Powers, W. L. (1995). TNT transport and fate in contaminated soild. *Journal of Environment Quality*, 24(6):1174.

Di Toro, D. M. and Horzempa, L. M. (1982). Reversible and resistant components of pcb adsorption desorption - isotherms. *Environmental Science & Technology*, 16(9):594–602.

Dontsova, K. M., Yost, S. L., Simunek, J., Pennington, J. C., and Williford, C. W. (2006). Dissolution and transport of TNT, RDX, and Composition B in saturated soil columns. *Journal of Environmental Quality*, 35(6):2043–2054.

Gonzalez Forero, R. (2013). *Factors Controlling the Reversible and Resistant Adsorption and Desorption of Munitions Constituents on Soils*. PhD dissertation. University of Delaware.

Sharma, P., Mayes, M. A., and Tang, G. (2013). Role of soil organic carbon and colloids in sorption and transport of TNT, RDX and HMX in training range soils. *Chemosphere*, 92(8):993–1000.

Chapter 5

MODELING MUNITION CONSTITUENT ADSORPTION AND DESORPTION HYSTERESIS USING DIFFUSION LIMITED TRANSPORT

5.1 Background

In Chapters 2 and 3, it was observed that the degree of hysteresis is dependent on the duration of adsorption. This behavior was explained by using a site transformation model that correlates the increase in binding strength with an increase in adsorption duration. However, hysteretic behavior has also been explored by other researchers who have used diffusive transport as an explanation for hysteresis.

In experiments, a system is treated as though it were at equilibrium if there is no apparent change in sorbed and aqueous concentrations. This may not be true if the mass transport process is slow enough. Sabbah [Sabbah and Rebhun, 1997; Sabbah et al., 2005] and Birdwell [Birdwell et al., 2007] have attempted to elucidate if a system is in equilibrium. Without both short and long term studies it cannot be discerned if the soil has truly reached equilibrium conditions with the bulk water.

Diffusion transports material in the direction opposite to the concentration gradient. This can continue to transport material into particles even if there is no chemical in the bulk aqueous phase. Because of the long time spans it may take for intra-particle equilibration, the rate of adsorption may be significantly different than the rate of desorption. This will lead to an assumption of irreversible hysteresis, when it is in fact a transport limitation.

Diffusive processes generally use the Fick equations. Berner [Berner, 1980], for example, describes diffusion into sediments as a variant of the Fick equations where diffusion is retarded by partitioning (Eqns. 5.1 and 5.2).

$$\frac{\partial C}{\partial t} = D' \frac{\partial^2 C}{\partial x^2} \tag{5.1}$$

$$D' = \left(\frac{D_s}{1 + mK} \right) \tag{5.2}$$

where D' is the apparent diffusion coefficient $[cm^2/d]$, C is the aqueous concentration, $[mg/L]$, D_s is the true diffusion coefficient $[cm^2/d]$, m is the soil water ratio $[kg/L]$, and K is the partition coefficient $[L/kg]$.

Wu and Gschwend [Wu and Gschwend, 1986] also apply a correction to the diffusion coefficient, by including porosity, tortuosity and sorption. Tortuosity and porosity would inhibit diffusive flux and aid in retarding chemical transport. The apparent diffusion coefficient is then used in a solution to the Fick equations derived by Crank [Crank, 1956] to model hydrophobic organic compounds in sediments and soils. Although the model developed therein successfully predicts aqueous phase concentrations, the work points to the need for accurate particle size fraction information. They find that in their work, only narrowly sized particle distributions are successfully modeled.

In this work, it was suggested that particle size fractions may be responsible for the rapid uptake phase as well as slow equilibration. To model data on 5 munition constituents (MC) sorbed to 25 soils two models were investigated. One used two particle sizes, the second used a log-normal distribution of particle sizes. Although final analysis could not be completed due to time constraints, suggestions for future work are given.

5.2 Data

The data used in modeling was the 25 soil data set, described in Chapter 2 in detail. This data set was composed of 25 soils of varying properties (fraction organic carbon, $f_{OC} = 0.043\% - 18.3\%$, fraction clay, $f_{clay} = 4.02\% - 86\%$). Soil particle sizes were characterized based on the sand/silt/clay breakpoints (sand: diameter $(d) > 80\mu m$, silt: $80\mu m > d > 5\mu m$, clay: $5\mu m > d$). 5 MC were amended to the soils at two initial concentrations. Equilibration was allowed to occur over 2, 48, 240 or 720 h. After the adsorption equilibration, 4 sequential desorptions, spaced 1 h apart, were conducted by removing and sampling the supernatant and replacing it with the same volume of DI water containing $CaCl_2$ and NaN_3 each at 0.01M. A series of extractions were performed to complete the mass balance. After screening for incomplete sets and degradation greater than 20% of the initial mass, the final data set was composed of 6,640 aqueous concentration observations.

5.3 Heterogeneous particle model

It was hypothesized that small particles equilibrate rapidly, whereas large ones take significant amounts of time to reach equilibrium. Similar behavior was observed by Wu and Gschwend [Wu and Gschwend, 1986] who noted that the uptake rate decreases as the square of the particle diameter. Further, Wu and Gschwend conclude that a single particle size is only reasonable for narrow ranges of particle sizes, which are unlikely to be encountered in the field.

To analyze the data, an established water column model was modified. The Simplified Lake/Stream Analysis (SLSA) model [Di Toro and Paquin, 1984] was used. A typical lake model contains both suspended matter and a sediment component, mirroring the two particle hypothesis where suspended particles are analogous to small rapidly equilibrating material and the sediment represents larger, transport

limited particles. In light of these changes, the SLSA model was re-derived for the batch tests under study.

For a bulk aqueous phase with instantaneously equilibrating particulate matter (layer 1) and diffusively limited larger particles (layer 2), the differential equations controlling transport and degradation are:

$$\begin{aligned} V_1 \frac{dC_{T,1}}{dt} =& - v_s f_{p,1} C_{T,1} A + v_{rs} f_{p,2} C_{T,2} A - v_d A \left(f_{d,1} C_{T,1} - f_{d,2} C_{T,2} \right) \\ & - Q C_{T,1} - k_1 C_{T,1} V_1 \end{aligned} \tag{5.3}$$

$$\begin{aligned} V_2 \frac{dC_{T,2}}{dt} =& + v_s f_{p,1} C_{T,1} A - v_{rs} f_{p,2} C_{T,2} A + v_d A \left(f_{d,1} C_{T,1} - f_{d,2} C_{T,2} \right) \\ & - k_2 C_{T,2} V_2 - v_b f_{p,2} C_{T,2} A \end{aligned} \tag{5.4}$$

where V is the volume $[L]$, C_T is the total concentration $[mg/L]$, v_s is the settling velocity for particles $[1/min]$, f_d is the fraction dissolved (as defined in Eq 5.5) $[unitless]$, f_p is the fraction particulate (as defined in Eq 5.6) $[unitless]$, A is the interfacial area between 1 and 2 $[cm^2]$, v_{rs} is the resuspension velocity $[1/min]$, v_d is the diffusion velocity $[1/min]$, Q is the advective flow rate $[cm^3/min]$, k is the first order removal rate (degradation) $[1/min]$, and the subscripts 1 and 2 refer to layer 1 and 2.

The fractions particulate and dissolved for layer i are defined as [Schwarzenbach et al., 2002]:

$$f_{d,i} = \frac{1}{1 + m K_{P,i}} \tag{5.5}$$

$$f_{p,i} = \frac{m K_{P,i}}{1 + m K_{P,i}} \tag{5.6}$$

where $K_{P,i}$ is the partition coefficent for layer i and m is the soil:water ratio.

Dividing by the interfacial area yields:

$$\begin{aligned} H_1\frac{dC_{T,1}}{dt} =& - v_s f_{p,1} C_{T,1} + v_{rs} f_{p,2} C_{T,2} - v_d \left(f_{d,1} C_{T,1} - f_{d,2} C_{T,2}\right) \\ & - {}^{Q}/_{A} C_{T,1} - k_1 C_{T,1} H_1 \qquad (5.7) \\ H_2\frac{dC_{T,2}}{dt} =& + v_s f_{p,1} C_{T,1} - v_{rs} f_{p,2} C_{T,2} + v_d \left(f_{d,1} C_{T,1} - f_{d,2} C_{T,2}\right) \\ & - k_2 C_{T,2} H_2 - v_b f_{p,2} C_{T,2} \qquad (5.8) \end{aligned}$$

where H is the depth of the layer.

To simply the equation, let:

$$\begin{aligned} j_{1\to 2} &= v_s f_{p,1} + v_d f_{d,1} \\ j_{2\to 1} &= v_{rs} f_{p,2} + v_d f_{d,2} \\ s_1 &= \frac{j_{1\to 2}}{H_1} \\ s_2 &= \frac{j_{2\to 1}}{H_2} \\ s_1' &= s_1 + k_1 + \frac{1}{t_0} \\ s_2' &= s_2 + k_2 + \frac{v_b f_{p,2}}{H_2} \end{aligned}$$

where $t_0 = {}^{V}/_{Q}$.

After substitution into Eqs 5.7 and 5.8, the reduced equations are:

$$\frac{dC_{T,1}}{dt} = -s_1' C_{T,1} + s_2 \frac{H_2}{H_1} C_{T,2} \qquad (5.9)$$

$$\frac{dC_{T,2}}{dt} = s_1 \frac{H_1}{H_2} C_{T,1} - s_2' C_{T.2} \qquad (5.10)$$

The reduced equations have a known general solution of:

$$C_{T,1}(t) = C_{T,1}(0)\left(\frac{s_2' - g_1}{g_2 - g_1}e^{-g_1 t} - \frac{s_2' - g_2}{g_2 - g_1}e^{-g_2 t}\right) + C_{T,2}(0)\frac{H_2}{H_1}\frac{s_2}{g_2 - g_1}\left(e^{-g_1 t} - e^{-g_2 t}\right) \tag{5.11}$$

$$C_{T,2}(t) = C_{T,2}(0)\left(\frac{s_1' - g_1}{g_2 - g_1}e^{-g_1 t} - \frac{s_1' - g_2}{g_2 - g_1}e^{-g_2 t}\right) + C_{T,1}(0)\frac{H_1}{H_2}\frac{s_1}{g_2 - g_1}\left(e^{-g_1 t} - e^{-g_2 t}\right) \tag{5.12}$$

where

$$g_1 = {}^1\!/_2\left(s_1' + s_2'\right)\left(1 + \left(1 - \frac{4\left(s_1' s_2' - s_1 s_2\right)}{\left(s_1' + s_2'\right)^2}\right)^{1/2}\right) \tag{5.13}$$

$$g_2 = {}^1\!/_2\left(s_1' + s_2'\right)\left(1 - \left(1 - \frac{4\left(s_1' s_2' - s_1 s_2\right)}{\left(s_1' + s_2'\right)^2}\right)^{1/2}\right) \tag{5.14}$$

The system analyzed has no advection ($Q = 0$), no burial or resuspension ($v_{rs} = v_b = 0$), and no degradation since samples with significant degradation were excluded ($k = 0$). A further simplification of the model can be made:

$$s_1' = s_1 = {}^{j_1}/_{H_1} = {}^{v_d f_{d,1}}/_{H1} \tag{5.15}$$

$$s_2' = s_2 = {}^{j_2}/_{H_2} = {}^{v_d f_{d,2}}/_{H2} \tag{5.16}$$

$$\begin{aligned} g_1 =& {}^1/_2 \left(s_1' + s_2'\right) \left(1 + \left(1 - \frac{4\left(0\right)}{\left(s_1' + s_2'\right)^2}\right)^{1/2}\right) \\ =& s_1' + s_2' \end{aligned} \tag{5.17}$$

$$\begin{aligned} g_2 =& {}^1/_2 \left(s_1' + s_2'\right) \left(1 - \left(1 - \frac{4\left(0\right)}{\left(s_1' + s_2'\right)^2}\right)^{1/2}\right) \\ =& 0 \end{aligned} \tag{5.18}$$

After substitution:

$$\begin{aligned} C_{T,1}(t) =& C_{T,1}(0) \left(\frac{s_2' - \left(s_1' + s_2'\right)}{0 - \left(s_1' + s_2'\right)} e^{-\left(s_1' + s_2'\right)t} - \frac{s_2' - 0}{0 - \left(s_1' + s_2'\right)} e^{-0t}\right) \\ &+ C_{T,2}(0) \frac{H_2}{H_1} \frac{s_2}{0 - \left(s_1' + s_2'\right)} \left(e^{-\left(s_1' + s_2'\right)t} - e^{-0t}\right) \end{aligned} \tag{5.19a}$$

$$= C_{T,1}(0) \left[\frac{s_1'}{s_1' + s_2'} e^{-\left(s_1' + s_2'\right)t} + \frac{s_2'}{s_1' + s_2'}\right] - C_{T,2}(0) \frac{H_2}{H_1} \frac{s_2}{s_1' + s_2'} \left(e^{-\left(s_1' + s_2'\right)t} - 1\right) \tag{5.19b}$$

and using the initial conditions:.

$$C_{T,1}(0) = C_T(0)$$

$$C_{T,2}(0) = 0$$

$$s' = s$$

the model reduces to:

$$C_{T,1}(t) = C_{T,1}(0)\left[\frac{s_1}{s_1+s_2}e^{-(s_1+s_2)t} + \frac{s_2}{s_1+s_2}\right] \tag{5.19c}$$

Similarly for the second layer with initial conditions

$$C_{T,1}(0) = C_T(0$$
$$C_{T,2}(0) = 0$$
$$s' = s$$

The model reduces to:

$$\begin{aligned} C_{T,2}(t) =& C_{T,2}(0)\left(\frac{s_1' - (s_1'+s_2')}{0-(s_1'+s_2')}e^{-\left(s_1'+s_2'\right)t} - \frac{s_1'-0}{0-(s_1'+s_2')}e^{-0t}\right) \\ &+ C_{T,1}(0)\frac{H_1}{H_2}\frac{s_1}{0-(s_1'+s_2')}\left(e^{-\left(s_1'+s_2'\right)t} - e^{-0t}\right) \end{aligned} \tag{5.20a}$$

which is:

$$\begin{aligned} =& C_{T,2}(0)\left[\frac{s_2'}{s_1'+s_2'}e^{-\left(s_1'+s_2'\right)t} + \frac{s_1'}{s_1'+s_2'}\right] \\ &- C_{T,1}(0)\frac{H_1}{H_2}\frac{s_1}{s_1'+s_2'}\left(e^{-\left(s_1'+s_2'\right)t} - 1\right) \end{aligned} \tag{5.20b}$$

and since $C_{T,2}(0) = 0$:

$$C_{T,2}(t) = -C_{T,1}(0)\frac{H_1}{H_2}\frac{s_1}{s_1+s_2}\left[e^{-(s_1+s_2)t} - 1\right] \tag{5.20c}$$

To model the diffusive velocity the molecular diffusion coefficient, D_m, can be adjusted by using particle size information. The assumed diffusion coefficient was 1

$^{cm^2}/_d$, approximately the molecular diffusion rate. This diffusion coefficient was then reduced to a velocity by dividing by the mean particle radius, r_μ:

$$v_d = {}^{D_m}/_{r_\mu} \tag{5.21}$$

$$r_\mu = \text{lognorm}\left(f_{clay}, f_{silt}\right) \tag{5.22}$$

where the mean particle radius was determined by using the breakpoints for f_{clay} and f_{silt} to develop a log-normal distribution of particle sizes (Appendix D.1.1). A log-normal distribution of sizes has been suggested previously, as long as several measurements of size are given, [Gardner, 1956; Wagner and Ding, 1994].

The H terms of each equation were constrained in order to reduce the degrees of freedom the model could explore. H_1 and H_2 are the fraction of the total volume in each layer:

$$H_1 = \frac{V_1}{V_1 + V_2} \tag{5.23a}$$

$$H_2 = \frac{V_2}{V_1 + V_2} \tag{5.23b}$$

where the total volume is:

$$V_1 + V_2 = V_{Aq} + V_{HV} + V_{Solids} - V_{Sand} \tag{5.23c}$$

which is

$$= V_{Aq} + V_{HV} + V_{Clay} + V_{Silt} \tag{5.23d}$$

or by applying the fractions clay and silt

$$= V_{Aq} + f_{Clay}\left(V_{HV} + V_{Solids}\right) + f_{Silt}\left(V_{HV} + V_{Solids}\right) \tag{5.23e}$$

then layer 1 is

$$V_1 = V_{Aq} + f_{Clay}\left(V_{HV} + V_{Solids}\right) \tag{5.23f}$$

and layer 2 is

$$V_2 = f_{Silt}\left(V_{HV} + V_{Solids}\right) \tag{5.23g}$$

Substituting Eq 5.23f and 5.23g into 5.23a and 5.23b yields

$$H_1 = \frac{5\text{mL} + f_{Clay}\left(V_{HV} + {}^{5\text{g}}/_{\rho_{solids}}\right)}{5\text{mL} + V_{HV} + {}^{5\text{g}}/_{\rho_{solids}}\left(1 - f_{Sand}\right)} \tag{5.23h}$$

$$H_2 = \frac{f_{Silt}\left(V_{HV} + {}^{5\text{g}}/_{\rho_{solids}}\right)}{5\text{mL} + V_{HV} + {}^{5\text{g}}/_{\rho_{solids}}\left(1 - f_{Sand}\right)} \tag{5.23i}$$

where 5 mL is equal to the volume in excess of the hydration volume and is equivalent to V_{aq}, 5 g is the average mass of solid in each sample, ρ is the dry density of the soil, and V is the volume of the hydration (HV), Clay, or Silt phases as denoted by the subscript. f refers to the fraction of total soil in the silt, sand, or clay regions (by particle size) as denoted by the subscript.

Then, the equations for the two layers are:

$$C_{T,1}(t) = C_{T,1}(0)\left[\frac{f_{d,1}}{f_{d,1} + f_{d,2}{}^{H_1}/_{H_2}} e^{-\left(f_{d,1}/H_1 + f_{d,2}/H_2\right)\left(D_m/r_\mu\right)t} + \frac{f_{d,2}}{f_{d,1}{}^{H_2}/_{H_1} + f_{d,2}}\right] \tag{5.24}$$

$$C_{T,2}(t) = -C_{T,1}(0)\frac{f_{d,1}}{f_{d,1}{}^{H_2}/_{H_1} + f_{d,2}}\left[e^{-\left(f_{d,1}/H1 + f_{d,2}/H2\right)\left(D_m/r_\mu\right)t} - 1\right] \tag{5.25}$$

where H_1 and H_2 are defined in Eqs 5.23h and 5.23i. The two-particle model, Eqs 5.24 and 5.25, gives the aqueous phase concentration for a non-desorbing process.

To model a desorption, let t' be the time at which desorption occurs. Let C' be the concentration for the first desorption and $C_{d,i}(t')$ be the aqueous concentration in layer i at time $= t'$. The solution for a single desorption is:

$$C'_{T,1}(t) = C_{T,1}(t) - \frac{C_{d,1}(t')}{C_{T,1}(0)} C_{T,1}(t - t') \tag{5.26}$$

$$C'_{T,2}(t) = C_{T,2}(t) - \frac{C_{d,2}(t')}{C_{T,1}(0)} C_{T,2}(t - t') \tag{5.27}$$

for $t \geq t'$

By this reasoning, the concentrations for the fourth desorption are:

$$C''''_{T,1}(t) = C'''_{T,1}(t) - \frac{C_{d,1}(t'''')}{C_{T,1}(0)} C_{T,1}(t - t'''') \tag{5.28}$$

$$C''''_{T,2}(t) = C'''_{T,2}(t) - \frac{C_{d,2}(t'''')}{C_{T,1}(0)} C_{T,2}(t - t'''') \tag{5.29}$$

for $t \geq t''''$.

Using this technique, the aqueous concentrations during adsorption and the four sequential desorptions can be modeled.

Model Fitting and Analysis

The 2 particle model was fit using R statistical software [R Core Team, 2014] using the *optim* nonlinear fitting package and the Brent method. The sum of square residuals between observed (obs) and modeled (mod) aqueous concentrations was used as the forcing function, Eq 5.30.

$$ssq = \sum_{k=1}^{n} \left(C_{d,obs}(k) - C_{d,mod}(k)\right)^2 \tag{5.30}$$

where n is the total number of observations and $C_d(k)$ is the k observation of an aqueous concentration. Linear residuals were used because log residuals favored low concentrations, such as those found in the third and fourth desorption, instead of the adsorption point.

As a measure of how well the model fit, residuals were plotted for each MC and sorbent, Figure 5.1. Although the model appears to predict the behavior of high f_{OC} sorbents better than low f_{OC}, this is misleading. High f_{OC} sorbents result in small aqueous concentrations. The model applied overly large f_p such that the majority of chemical was sorbed, leading to very low aqueous concentrations and therefore, low residuals.

From the results, the assumption of two K_P, one for each particle size is reasonable for small ranges of particle sizes. As the range of particle diameters range over several orders of magnitude, two particle sizes may not be sufficient for modeling. To more accurately model the behavior of sorption, the two-particle model was extended to an n-particle mode.

n-Particle Model

Using a log-normal distribution of particle sizes, the two-layer model can be extended to an n-particle model using solutions in terms of exponential matrices. If the model is developed in the form

$$\vec{x}(t) = e^{At}\vec{x}(0) \tag{5.31}$$

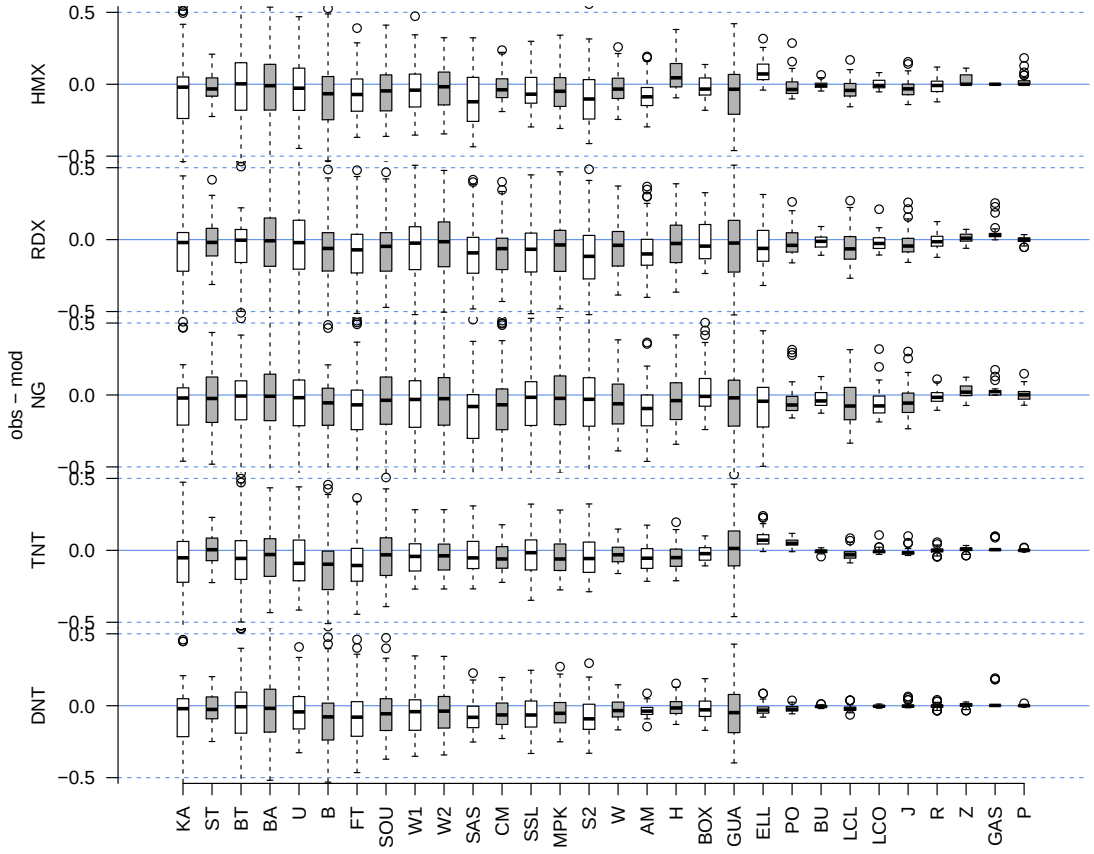


Figure 5.1: Linear residuals from the two-particle model for 5 MC. Soils are ordered from low to high f_{OC} from left to right.

where x is a vector of $n+1$ concentrations and $\mathbf{A}$ is a $n+1 \times n+1$ matrix, then a solution can be found.

Let matrix $\mathbf{A}$ be an $n+1 \times n+1$ matrix where n is the number of representative particle sizes. Then $\mathbf{A}$ is:

$$A = \begin{pmatrix} a_{1,1} & a_{1,2} & \cdots & a_{1,n+1} \\ a_{2,1} & a_{2,2} & \cdots & a_{2,n+1} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n+1,1} & a_{n+1,2} & \cdots & a_{n+1,n+1} \end{pmatrix} \tag{5.32}$$

where each element of $\mathbf{A}$ is the transport to or from each particle and the bulk phase. For example, element $a_{1,3}$ is the transport from the bulk phase (1) to particle size 2.

Then, the elements of $\mathbf{A}$ are:

$$a_{i,1} = \sum_{j=1}^{n} \frac{v_{d,j} A_j f_{d,j} V_j}{V_i} \tag{5.33}$$

$$a_{i \neq 1,j} = \frac{v_{d,i} A_i f_{d,i} V_i}{V_j} \tag{5.34}$$

where variables are defined as above. Subscripts i and j index the bulk ($i = 1$ or $j = 1$) and particle phases ($i > 1$ or $j > 1$).

The vector, $\vec{x}(t)$ is the concentration in each particle and bulk phase at time t:

$$\vec{x}(t) = \begin{pmatrix} x_1 = C_{bulk} \\ x_2 = C_{p(1)} \\ \vdots \\ x_{n+1} = C_{p(n)} \end{pmatrix} \tag{5.35}$$

where C_{bulk} is the concentration associated with the bulk phase and $C_{p(n)}$ is the total

concentration associated with the n^{th} particle size.

To solve the equation, $\vec{x}(t) = e^{At}\vec{x}(0)$, for any time, first we find the eigenvalues (λ) and eigenvectors of **A**. Then form a diagonal matrix of the eigenvalues of **A**:

$$D = \begin{bmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \lambda_n \end{bmatrix} \tag{5.36}$$

The exponential of D is:

$$e^{Dt} = \begin{bmatrix} e^{\lambda_1} & 0 & \cdots & 0 \\ 0 & e^{\lambda_2} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & e^{\lambda_n} \end{bmatrix} \tag{5.37}$$

To solve the exponential, we need

$$e^{At} = Se^{Dt}S^{-1} \tag{5.38}$$

where S is a vector of the eigenvectors of **A**. The solution to Eq 5.38 at t=0 is $\vec{x}(0)$ in Eq 5.31.

Finally, by solving Eq 5.38 for any time we can multiply by $\vec{x}(0)$ and determine a solution to Eq 5.31. After which, by using the same technique as in the two-layer model (Eqs 5.26 - 5.29), we can determine a concentration at any time with any number of desorptions.

After an initial simulation to determine if the model was performing properly,

it was determined that the assumption of f_{OC} evenly distributed across size fractions yielded inaccurate results, especially when correlations are to be drawn between model parameters and sorbent/sorbate properties. A method of sieving soils into 10 or more size fractions and then determining f_{OC}, sand, silt, and clay fractions for each was suggested. As the time required to perform such an analysis was prohibitive, the remainder of the analysis is left to a subsequent investigator.

5.4 Conclusions

As other investigators have shown, diffusive transport can be the cause of observations of hysteresis. We have shown that a multi-particle size approach can be used to explain both rapid and slow sorption. The two-layer model requires few parameters but yields results that, although useful, are not sufficient to discern if the model is accurate in the portrayal of hysteresis. The extension of the two-particle model to an n-particle model suggests stronger correlations to sorbent properties could be made, however, data requirements for the model are more extensive than currently available. A future investigation of f_{OC} content in several size fraction as well as the application to n-particle modeling is left to future investigators.

REFERENCES

Berner, R. A. (1980). *Early Diagenesis*. Princeton University Press, Princeton, NJ.

Birdwell, J., Cook, R. L., and Thibodeaux, L. J. (2007). Desorption kinetics of hydrophobic organic chemicals from sediment to water: A review of data and models. *Environmental Toxicology and Chemistry*, 26(3):424–434.

Crank, J. (1956). *The Mathematics of Diffusion*. Claredon Press, Oxford, 2nd edition.

Di Toro, D. M. and Paquin, P. R. (1984). Time variable model of the fate of DDE and lindane in a quarry. *Environmental Toxicology and Chemistry*, 3(2):335–353.

Gardner, W. R. (1956). Representation of soil aggregate-size distribution by a logarithmic-normal distribution. *Soil Science Society of America Journal*, 20(2):151.

R Core Team (2014). *R: A Language and Environment for Statistical Computing*. R Foundation for Statistical Computing, Vienna, Austria.

Sabbah, I., Ball, W. P., Young, D. F., and Bouwer, E. J. (2005). Misinterpretations in the modeling of contaminant desorption from environmental solids when equilibrium conditions are not fully understood. *Environmental Engineering Science*, 22(3):350–366.

Sabbah, I. and Rebhun, M. (1997). Adsorption-desorption of trichlorophenol in water-soil systems. *Water Environment Research*, 69(5):1032–1038.

Schwarzenbach, R. P., Gschwend, P. M., and Imboden, D. M. (2002). *Environmental Organic Chemistry*. John Wiley & Sons, Inc, Hoboken, NJ, USA.

Wagner, L. and Ding, D. (1994). Representing aggregate size distributions as modified lognormal distributions. *Transactions of the ASAE*, 37(3):815–821.

Wu, S. C. and Gschwend, P. M. (1986). Sorption kinetics of hydrophobic organic-compounds to natural sediments and soils. *Environmental Science & Technology*, 20(7):717–725.

Chapter 6

CONCLUSIONS

In Chapter 2 I showed that an analysis of sorption data using a reversible model was not sufficient to describe desorption behavior for longer adsorption contact times and/or high (> 0.03) f_{OC} sorbents. To accurately model these situations, a hysteretic model was required. The reversible/resistant model was chosen to model hysteresis. Reversible partition coefficients, had no relationship to adsorption contact time, but were correlated to f_{OC} and f_{clay}. The resistant partition coefficient, however, showed a strong correlation to adsorption contact time. Moreover, the partition coefficient was correlated strongly to f_{OC}. Based on the fraction of the total partition coefficient associated with reversible sorption, it was observed that as f_{OC} increases, the degree of hysteresis increased. In addition, as the adsorption contact time increased, more sorbents showed hysteretic behavior. This time dependence, however, was not explained using this modeling framework.

Chapter 3 expanded on the findings of the reversible resistant model. Hysteresis was described using the site transformation model for both linear and Langmuir isotherms. More importantly, however, time dependent hysteresis was incorporated into a site transformation term. This term, f_{ST}, behaved in a regular and predictable manner allowing correlations to be drawn between it, sorbent properties and the adsorption contact time. A comparison to the reversible resistant model results from Chapter 2 suggested an overall improvement when using the site transformation

model. Finally, a modification to the model using regressions to sorbate and sorbent properties as well as adsorption contact time yielded a predictive model for linear sorption. This model compared well to the observed data, with residuals generally within a factor of 2. Future investigation is suggested to strengthen the correlations made.

The fourth chapter discussed the importance of incorporating a resistant modeling framework into column studies. I showed that in bench scale tests, only minimal, if any, hysteresis will be seen and would likely be attributed to degradation. When applied to field scale sites, however, a significant amount of chemical can be resistantly bound. I provided suggestions for future research to better understand hysteresis during column studies and provided strategies for future bench scale testing of hysteretic chemicals.

In the fifth chapter, I explored one of the more common suggestions for hysteretic behavior, diffusive transport. I applied both a two and an n-particle model to a large data set encompassing multiple soil types. From the analysis it was observed that diffusive processes could potentially explain the observed behavior, but applicability was limited due to the requirement of particle characteristic data. Future work was suggested.

Overall, I successfully investigated the key topics, as outlined in the first chapter. Although there is not a clear answer for hysteretic behavior, this work shows strong correlations to the organic carbon fraction in soil matrices. Results from the site transformation model suggest that organic carbon partitioning can vary in binding strength, which suggests OC deformation hypothesis as a mechanism. Further, the site transformation model shows promise as a remediation tool. The experimental burden is low, allowing for applicability to new soils and sorbents.

As suggestions for future work, further analysis of the time variant behavior

of the site transformation factor must be explored. Doing so requires studies of both short and long adsorption duration periods (e.g. 72 h, 120 h, 1440 h, etc.). This will have the benefit of increasing our understanding of the transformation factor and if/when it will saturate. In addition, analyses of differing compounds must be made using the batch experimental and STM framework. The sorbates under study herein are similar in properties and behavior. Sorbates with stronger sorption should be used to determine if the behavior noted for the MC is applicable to other compounds. Further, using sorbates with different properties will enable an analysis of the sorbate independence of the site transformation factor.

Also, chemicals that were not studied in this work require a prediction of K_{OC} and K_{clay} to allow *apriori* analyses of sites. Since the multilinear model suggests that only binding to organic carbon is a factor for $f_{OC} > \approx 2\%$, Abraham type LFER models can be used to predict behavior. Determination of similar regression models for the clay size particle contribution can enable more accurate predictions for a larger range of sorbates.

The column work also points to further work. Much longer sorption durations are required to develop an appreciable resistant fraction. Longer duration tests are required to determine the extent of hysteresis in column systems.

Finally, as suggested in the fifth chapter, a robust set of sorbent properties will allow analysis of the adsorption and desorption behavior for these chemicals. To correctly model the behavior of MC on soil, a wide range of particle sizes is needed and each size class requires organic carbon content information. This information, along with a heterogenous particle model, such as the n-particle model developed in Chapter 5, can elucidate the role of diffusive transport as it pertains to hysteretic sorption.

Appendix A

NORMALIZED REVERSIBLE AND RESISTANT SORPTION SUPPLEMENTAL INFORMATION

A.1 Data treatment

A.1.1 Normalized aqueous and sorbed concentrations

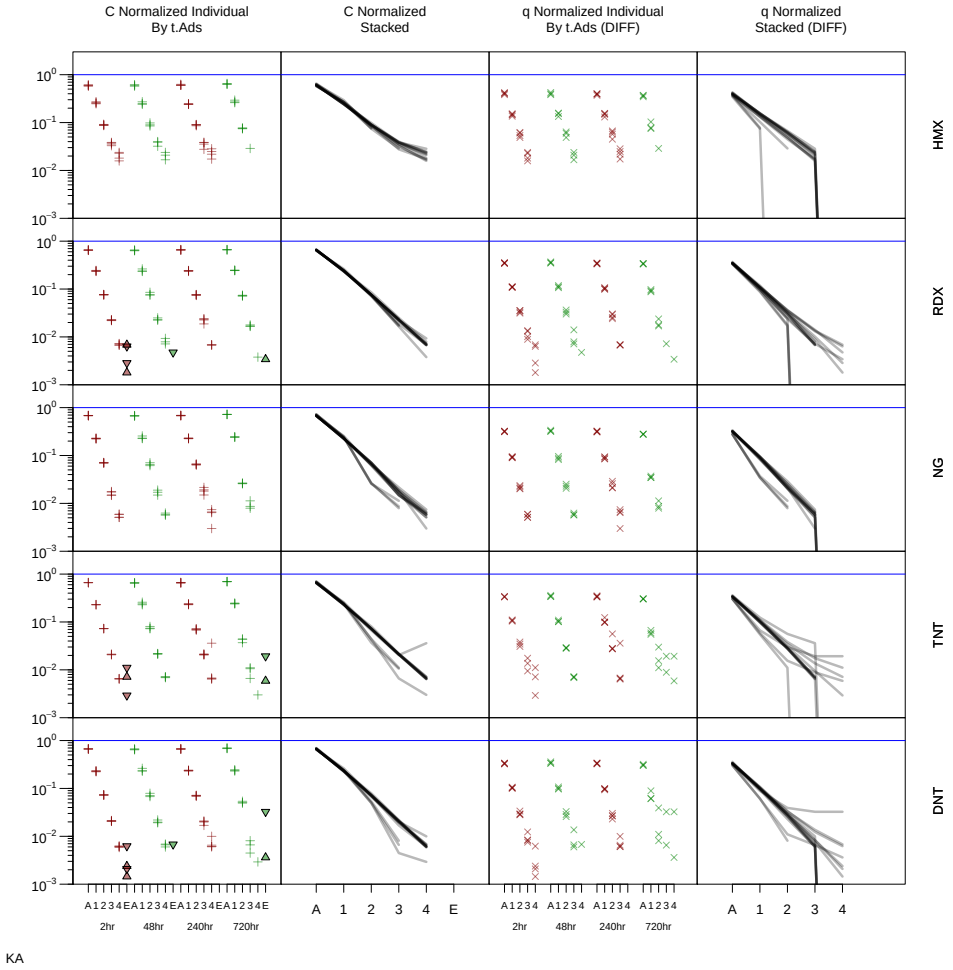
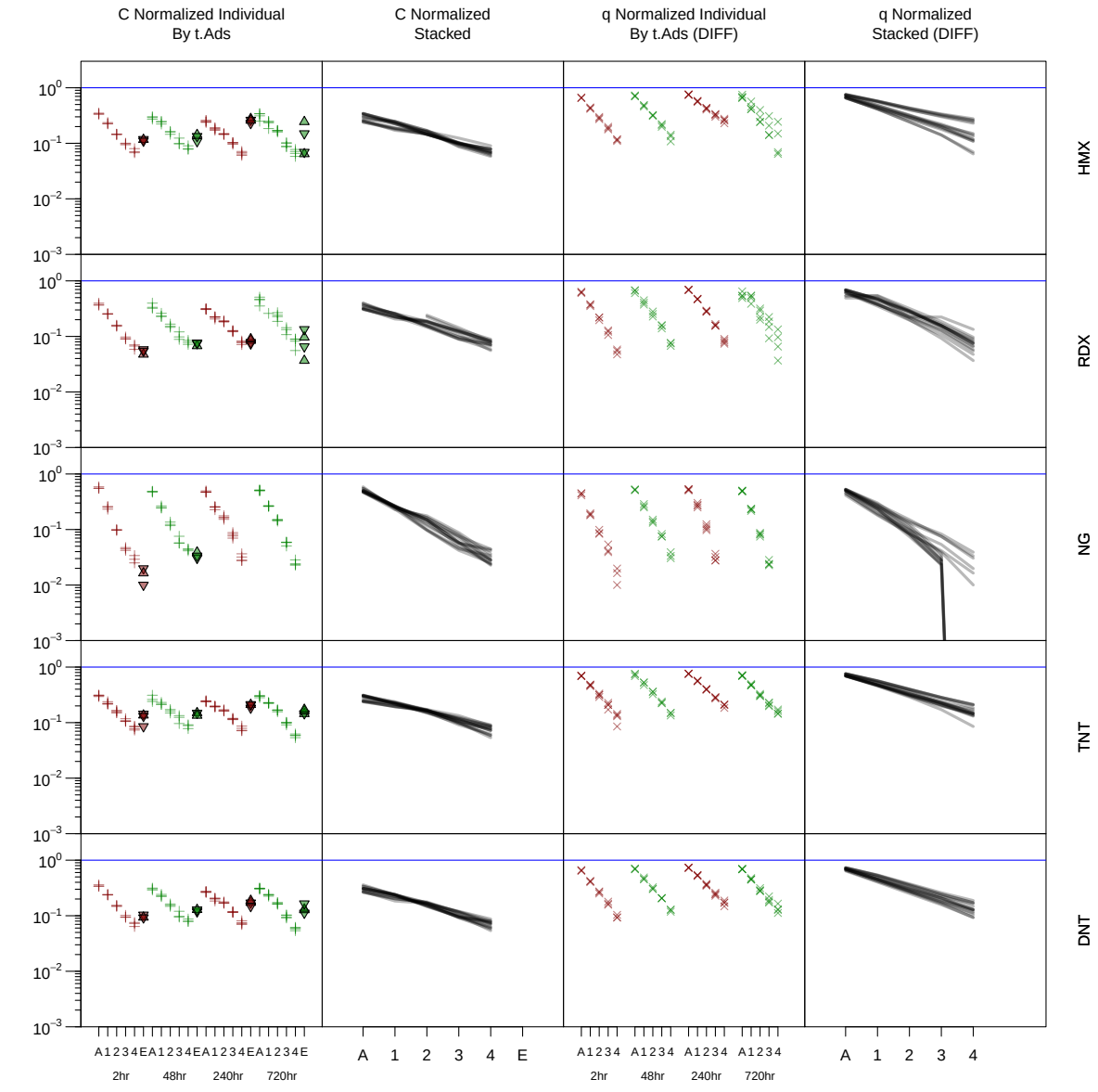
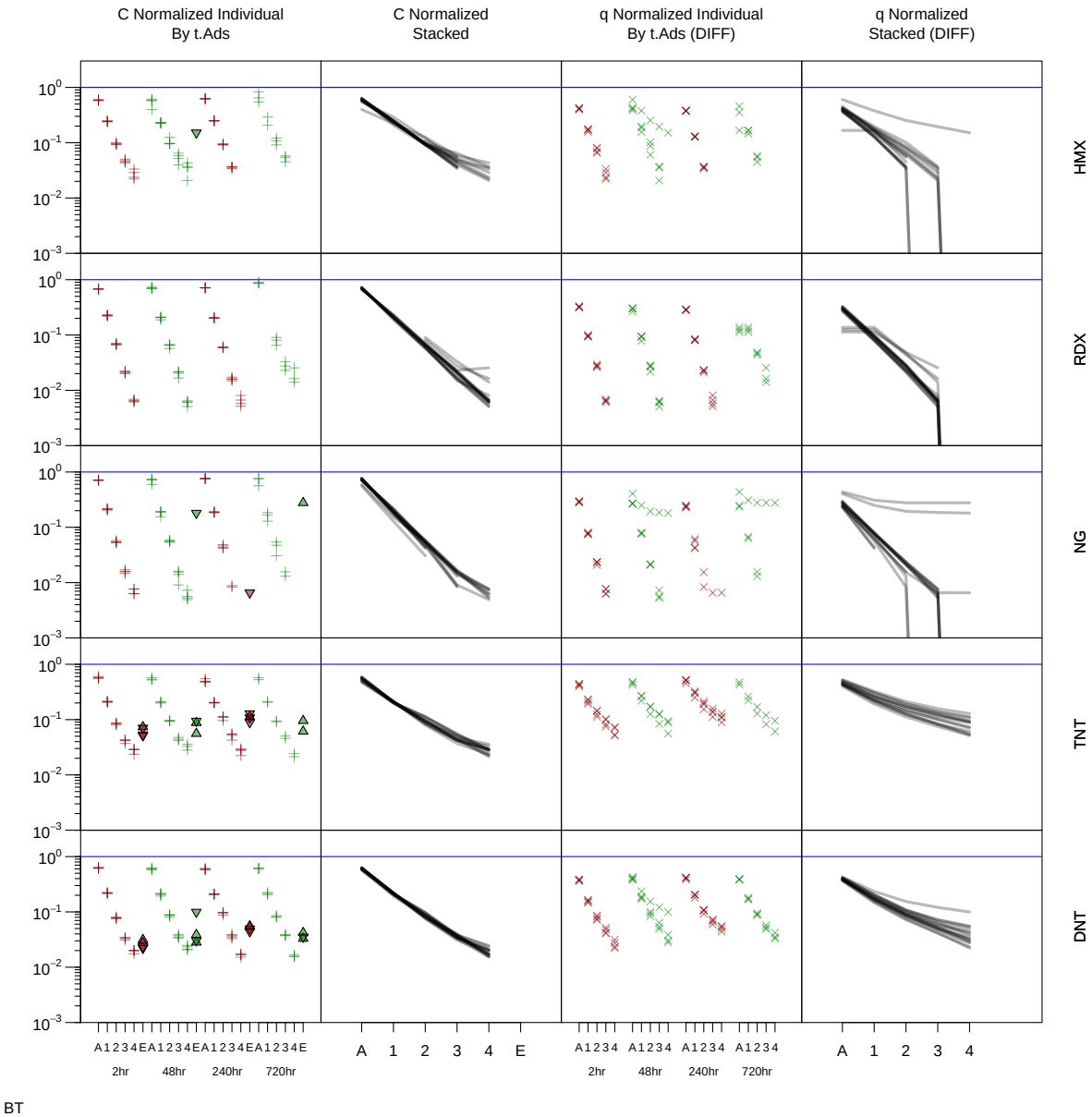
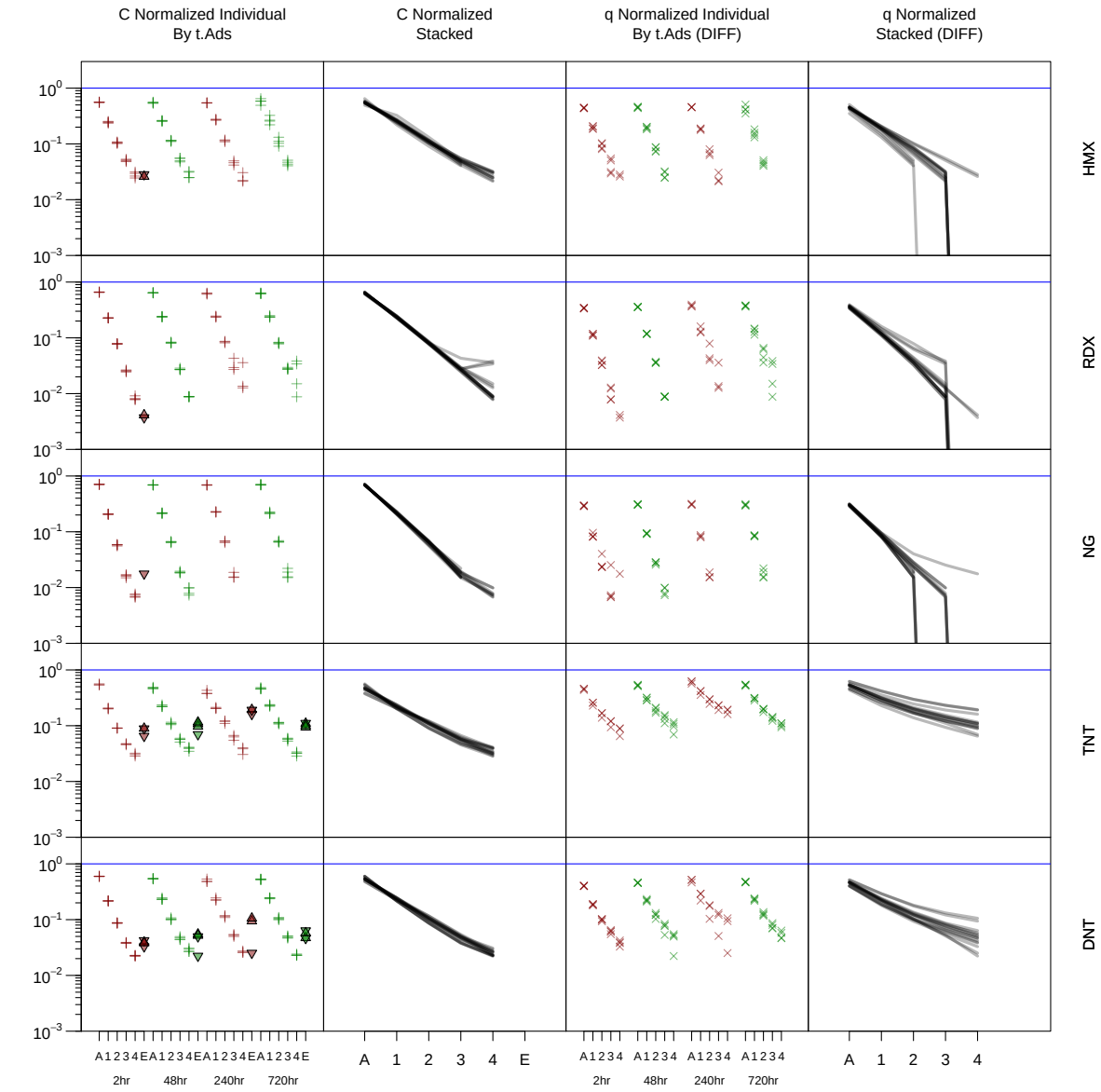


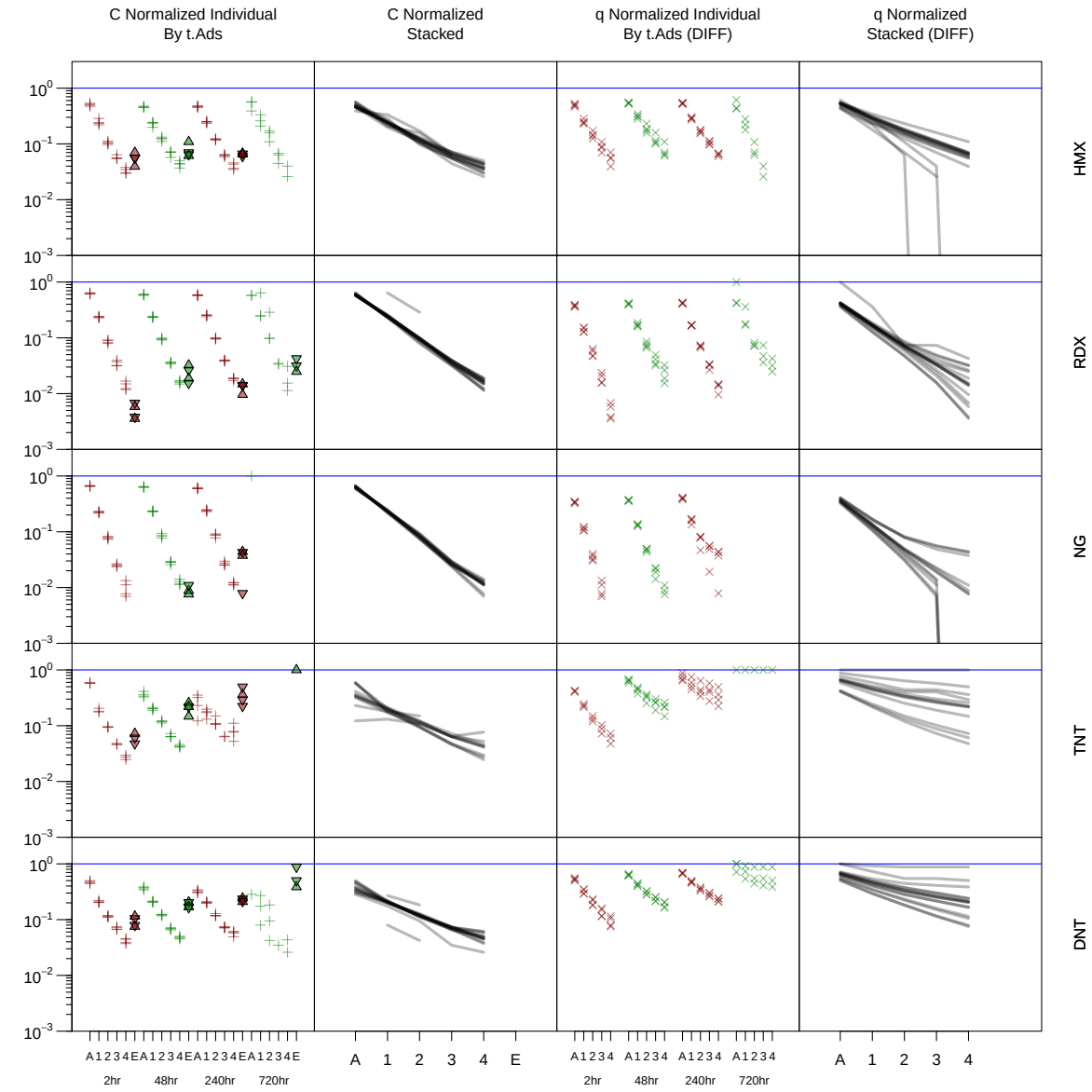
Figure A.1: Normalized aqueous and sorbed concentrations


C Normalized Individual
By t.Ads
C Normalized
Stacked
q Normalized Individual
By t.Ads (DIFF)
q Normalized
Stacked (DIFF)
HMX
RDX
NG
TNT
DNT
A1234EA1234EA1234EA1234EA1234E
2hr
48hr
240hr
720hr
A 1 2 3 4 E
A1234 A1234 A1234 A1234
A 1 2 3 4
ST

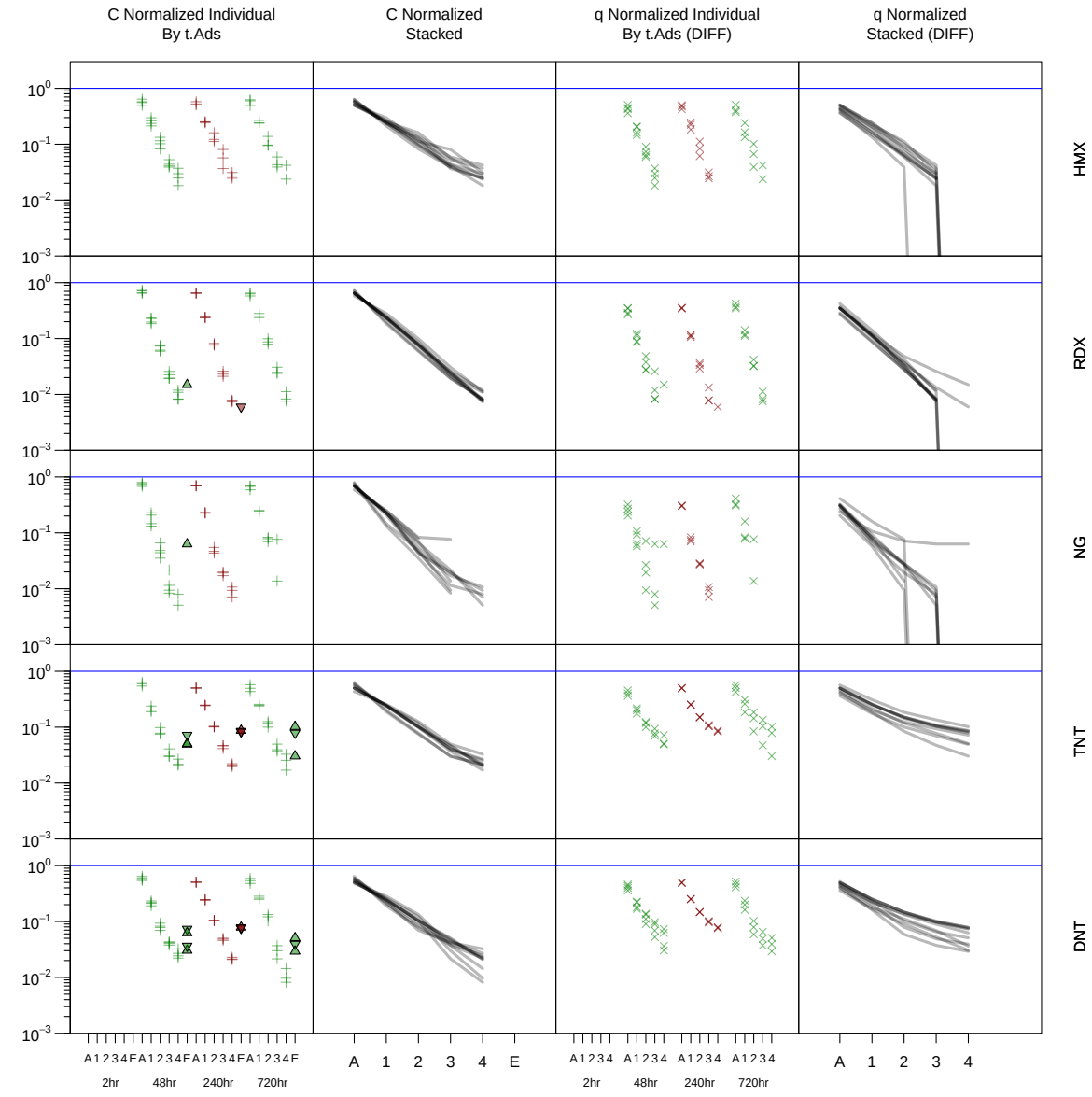

C Normalized Individual
By t.Ads
C Normalized
Stacked
q Normalized Individual
By t.Ads (DIFF)
q Normalized
Stacked (DIFF)
HMX
RDX
NG
TNT
DNT
10^{0}
10^{-1}
10^{-2}
10^{-3}
A1234EA1234EA1234EA1234EA1234E
2hr
48hr
240hr
720hr
A 1 2 3 4 E
A1234 A1234 A1234 A1234
A 1 2 3 4
BT


C Normalized Individual
By t.Ads
C Normalized
Stacked
q Normalized Individual
By t.Ads (DIFF)
q Normalized
Stacked (DIFF)
HMX
RDX
NG
TNT
DNT
A1234EA1234EA1234EA1234EA1234E
2hr
48hr
240hr
720hr
A 1 2 3 4 E
A1234 A1234 A1234 A1234
A 1 2 3 4

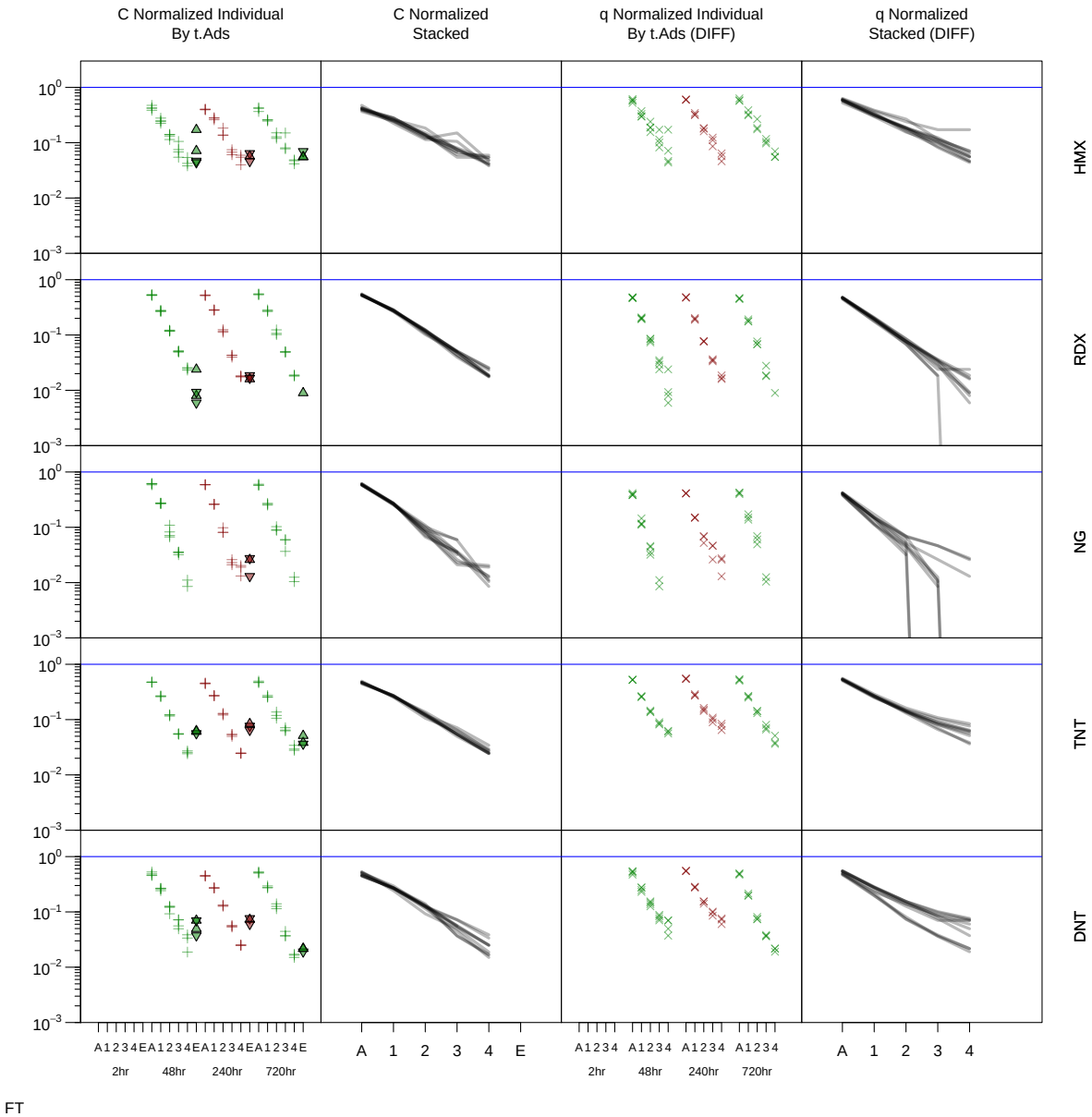
BA

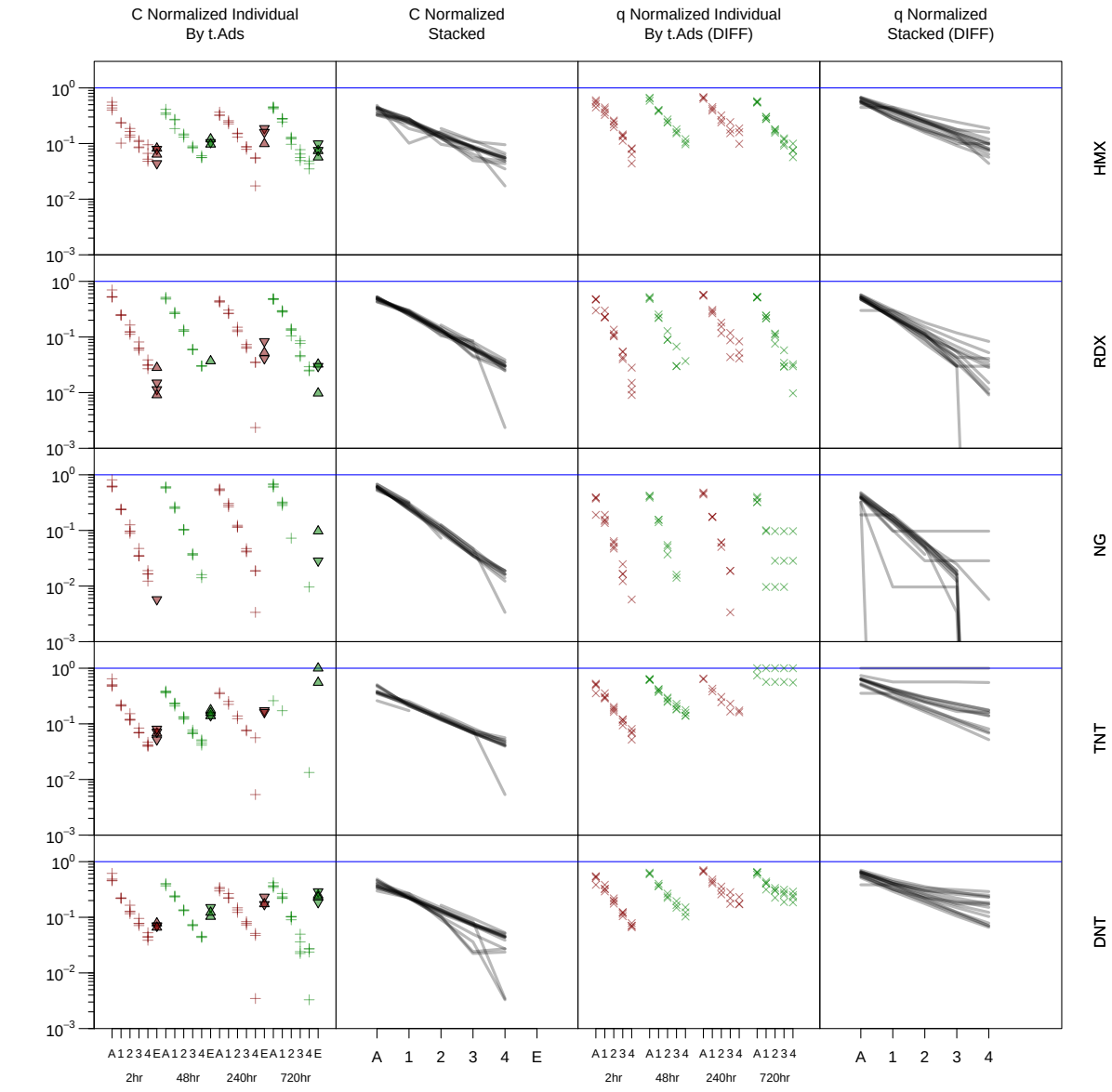

C Normalized Individual
By t.Ads
C Normalized
Stacked
q Normalized Individual
By t.Ads (DIFF)
q Normalized
Stacked (DIFF)
HMX
RDX
NG
TNT
DNT
A1234EA1234EA1234EA1234EA1234E
2hr
48hr
240hr
720hr
A 1 2 3 4 E
A1234 A1234 A1234 A1234
A 1 2 3 4

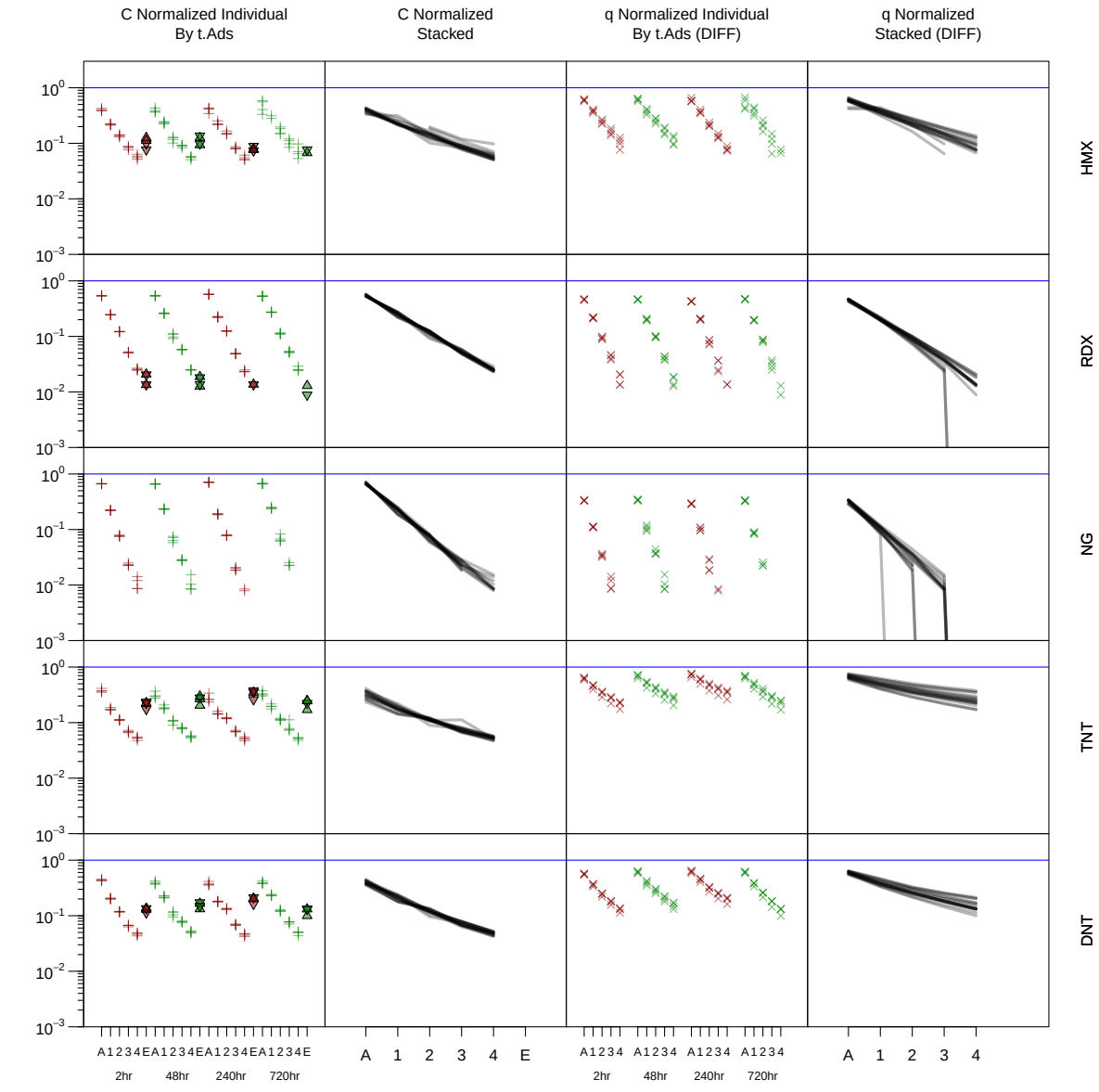
U


C Normalized Individual
By t.Ads
C Normalized
Stacked
q Normalized Individual
By t.Ads (DIFF)
q Normalized
Stacked (DIFF)
HMX
RDX
NG
TNT
DNT
A1234EA1234EA1234EA1234EA1234E
2hr
48hr
240hr
720hr
A 1 2 3 4 E
A1234 A1234 A1234 A1234
A 1 2 3 4

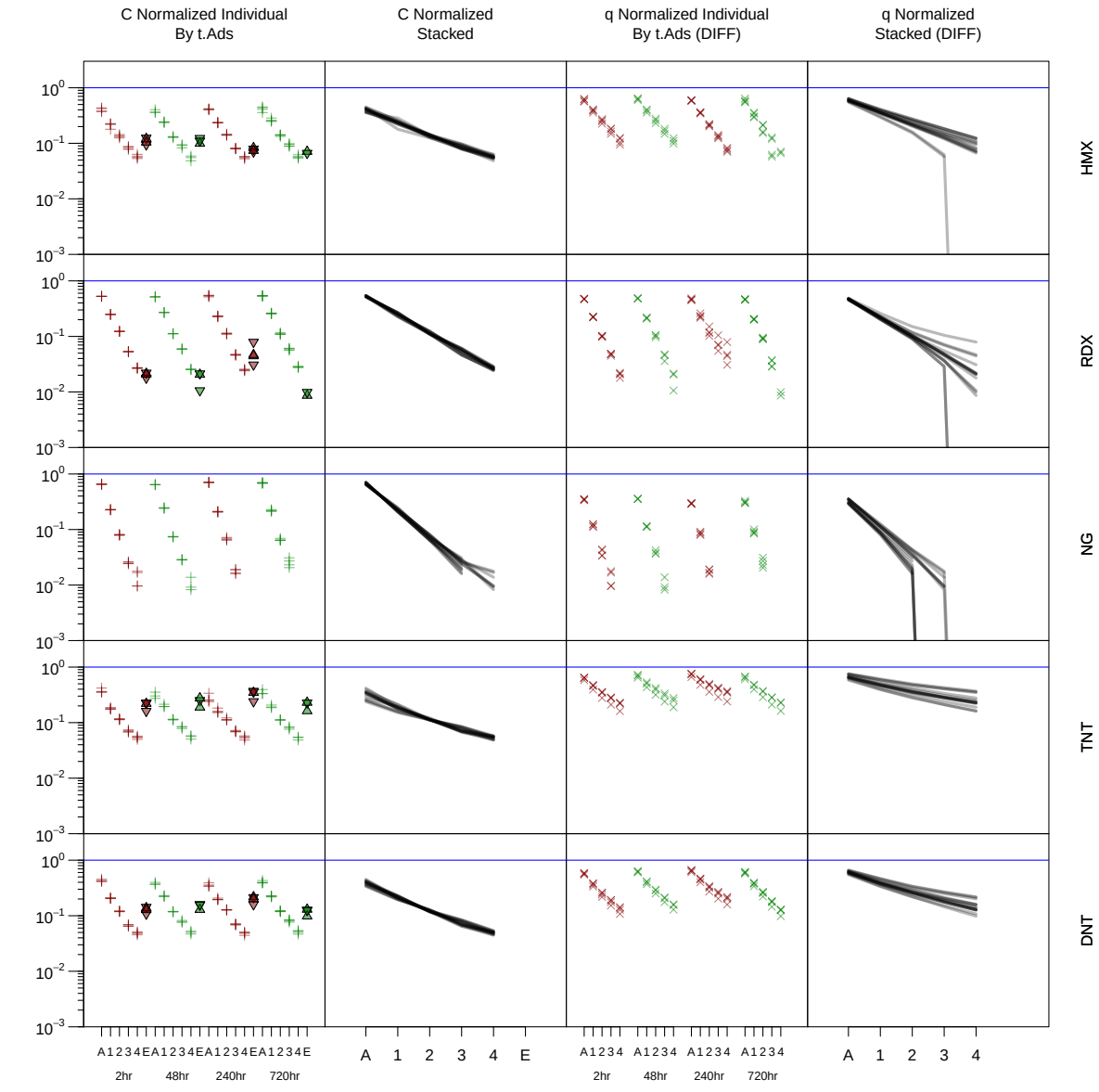
B


C Normalized Individual
By t.Ads
C Normalized
Stacked
q Normalized Individual
By t.Ads (DIFF)
q Normalized
Stacked (DIFF)
HMX
RDX
NG
TNT
DNT
A1234EA1234EA1234EA1234EA1234E
2hr
48hr
240hr
720hr
A 1 2 3 4 E
A1234 A1234 A1234 A1234
A 1 2 3 4
FT

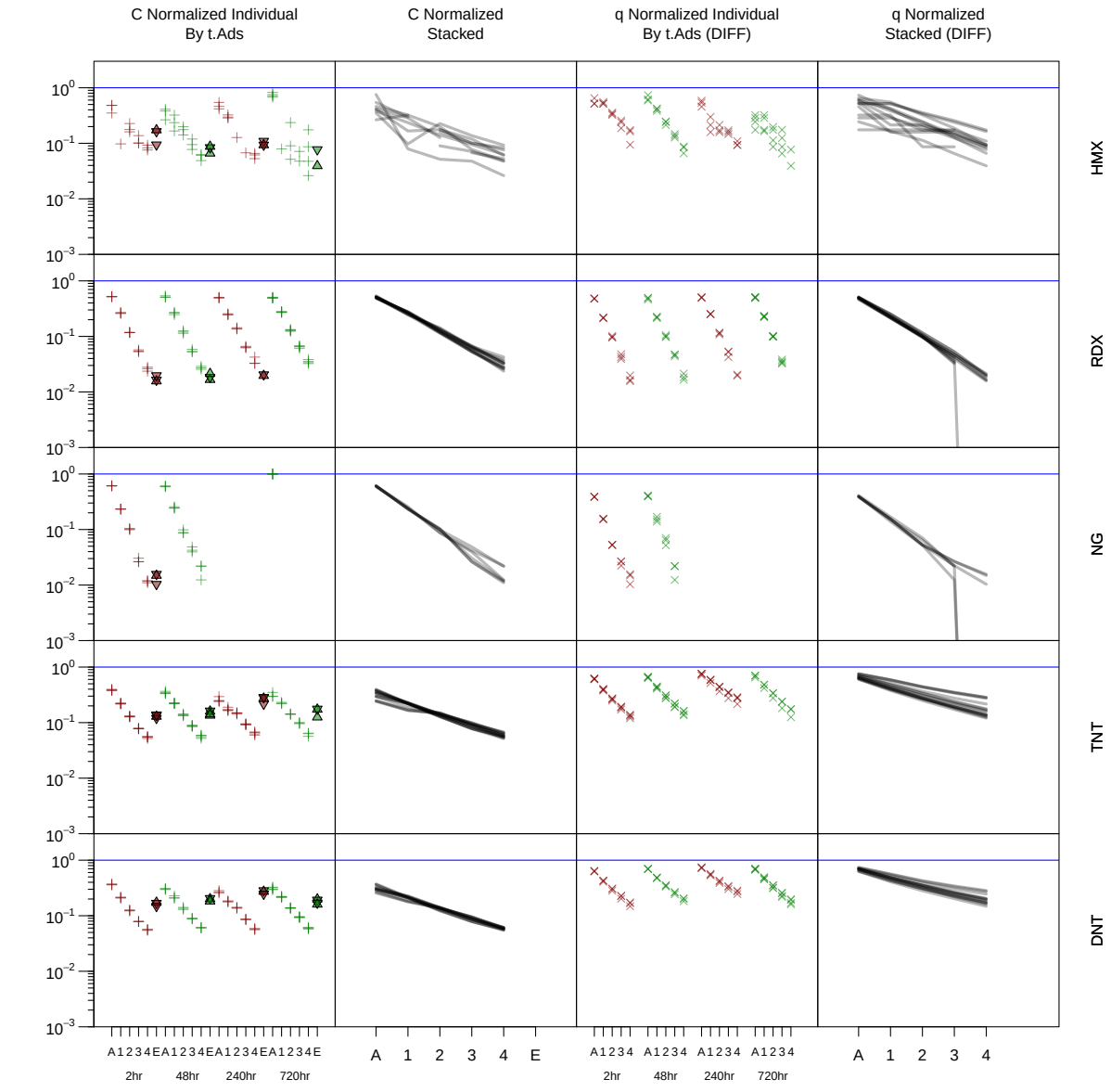

C Normalized Individual
By t.Ads
C Normalized
Stacked
q Normalized Individual
By t.Ads (DIFF)
q Normalized
Stacked (DIFF)
HMX
RDX
NG
TNT
DNT
10^{0}
10^{-1}
10^{-2}
10^{-3}
A1234EA1234EA1234EA1234EA1234E
2hr
48hr
240hr
720hr
A 1 2 3 4 E
A1234 A1234 A1234 A1234
A 1 2 3 4
SOU


C Normalized Individual
By t.Ads
C Normalized
Stacked
q Normalized Individual
By t.Ads (DIFF)
q Normalized
Stacked (DIFF)
HMX
RDX
NG
TNT
DNT
A1234EA1234EA1234EA1234EA1234E
2hr
48hr
240hr
720hr
A 1 2 3 4 E
A1234 A1234 A1234 A1234
A 1 2 3 4

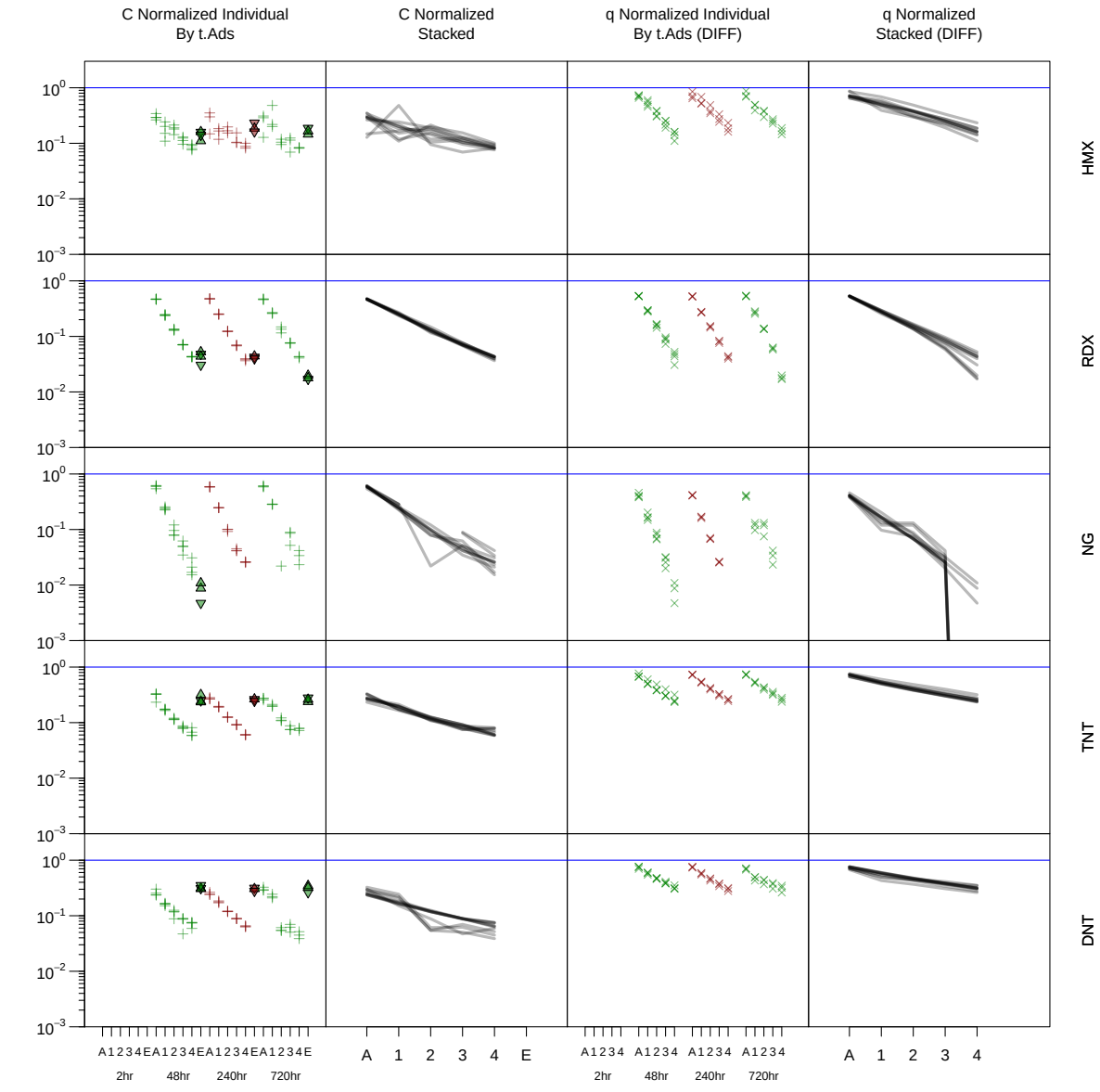
W1

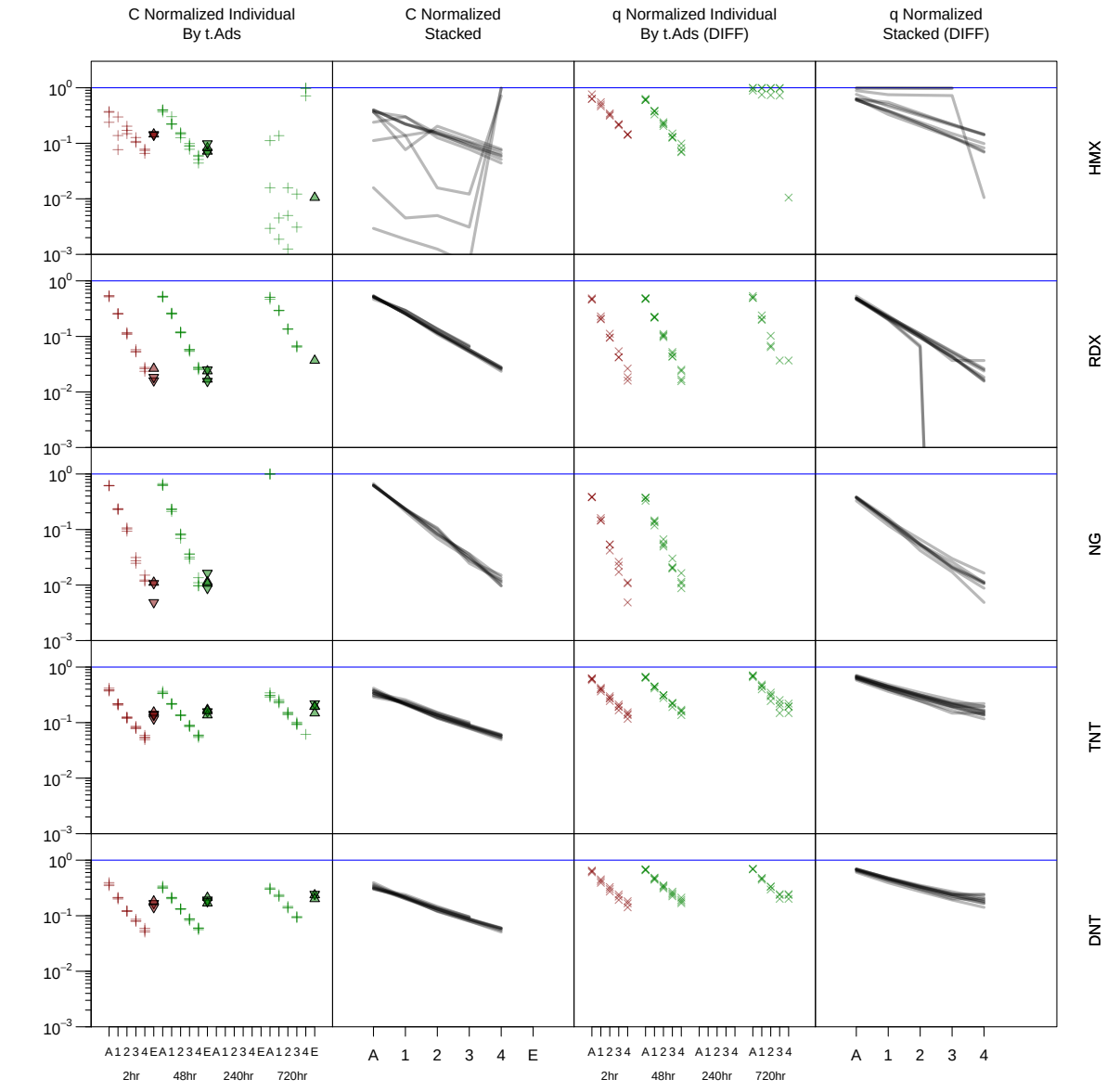

C Normalized Individual
By t.Ads
C Normalized
Stacked
q Normalized Individual
By t.Ads (DIFF)
q Normalized
Stacked (DIFF)
HMX
RDX
NG
TNT
DNT
A1234EA1234EA1234EA1234EA1234E
2hr
48hr
240hr
720hr
A 1 2 3 4 E
A1234 A1234 A1234 A1234
A 1 2 3 4

W2

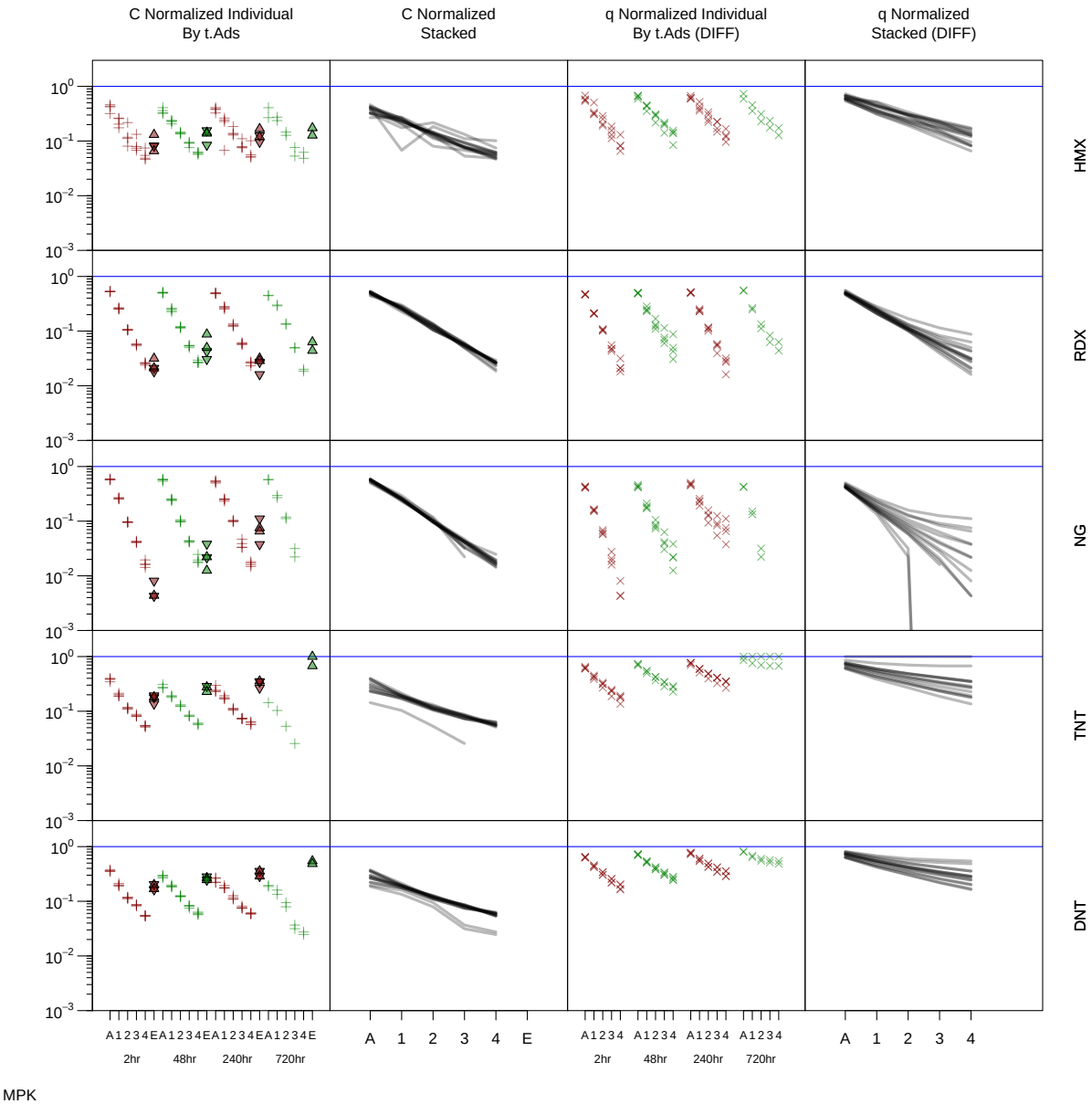

C Normalized Individual
By t.Ads
C Normalized
Stacked
q Normalized Individual
By t.Ads (DIFF)
q Normalized
Stacked (DIFF)
HMX
RDX
NG
TNT
DNT
A1234EA1234EA1234EA1234EA1234E
2hr
48hr
240hr
720hr
A 1 2 3 4 E
A1234 A1234 A1234 A1234
A 1 2 3 4

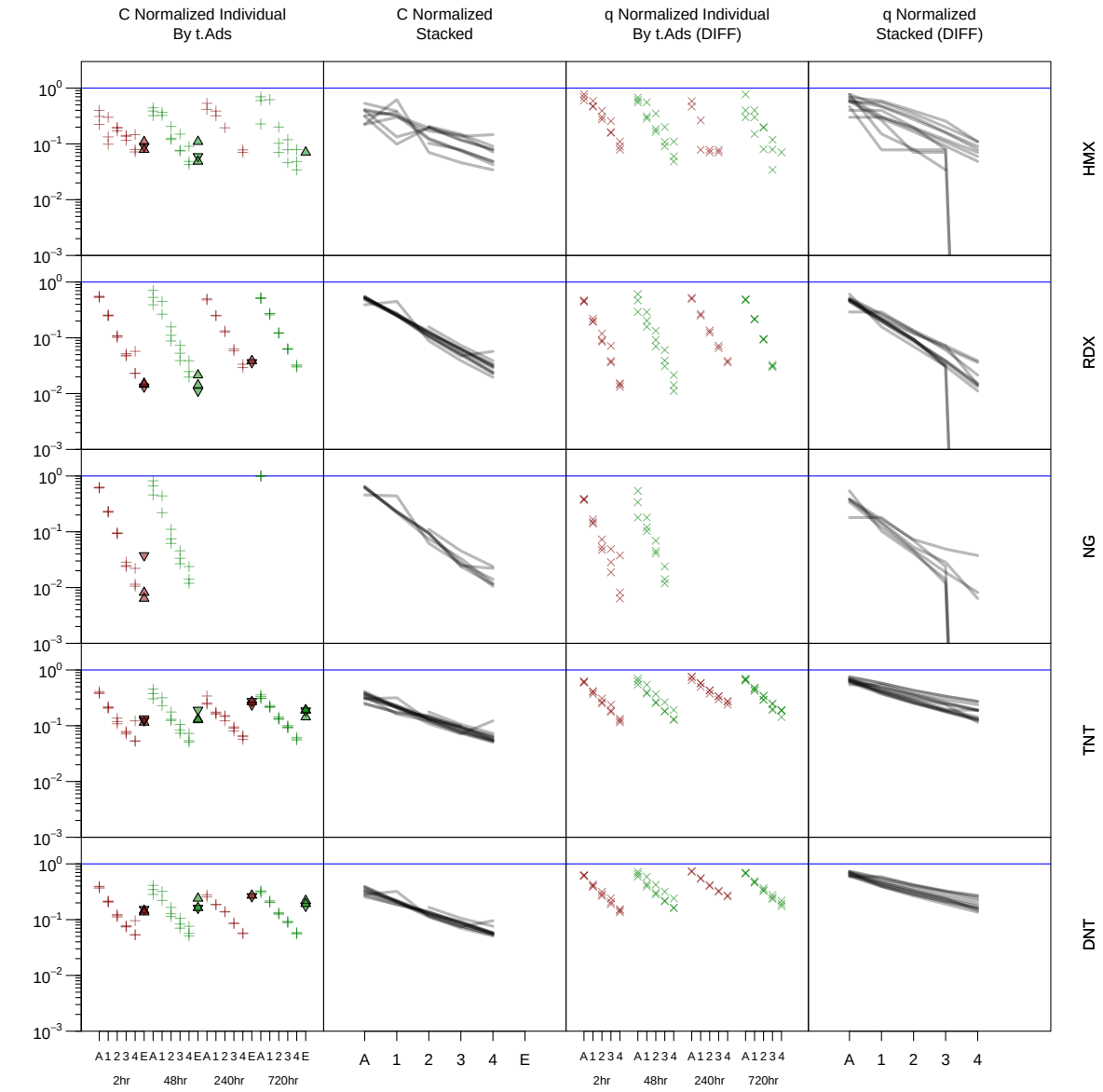
SAS


C Normalized Individual
By t.Ads
C Normalized
Stacked
q Normalized Individual
By t.Ads (DIFF)
q Normalized
Stacked (DIFF)
HMX
RDX
NG
TNT
DNT
10^{0}
10^{-1}
10^{-2}
10^{-3}
A1234EA1234EA1234EA1234EA1234E
2hr
48hr
240hr
720hr
A 1 2 3 4 E
A1234 A1234 A1234 A1234
A 1 2 3 4
CM

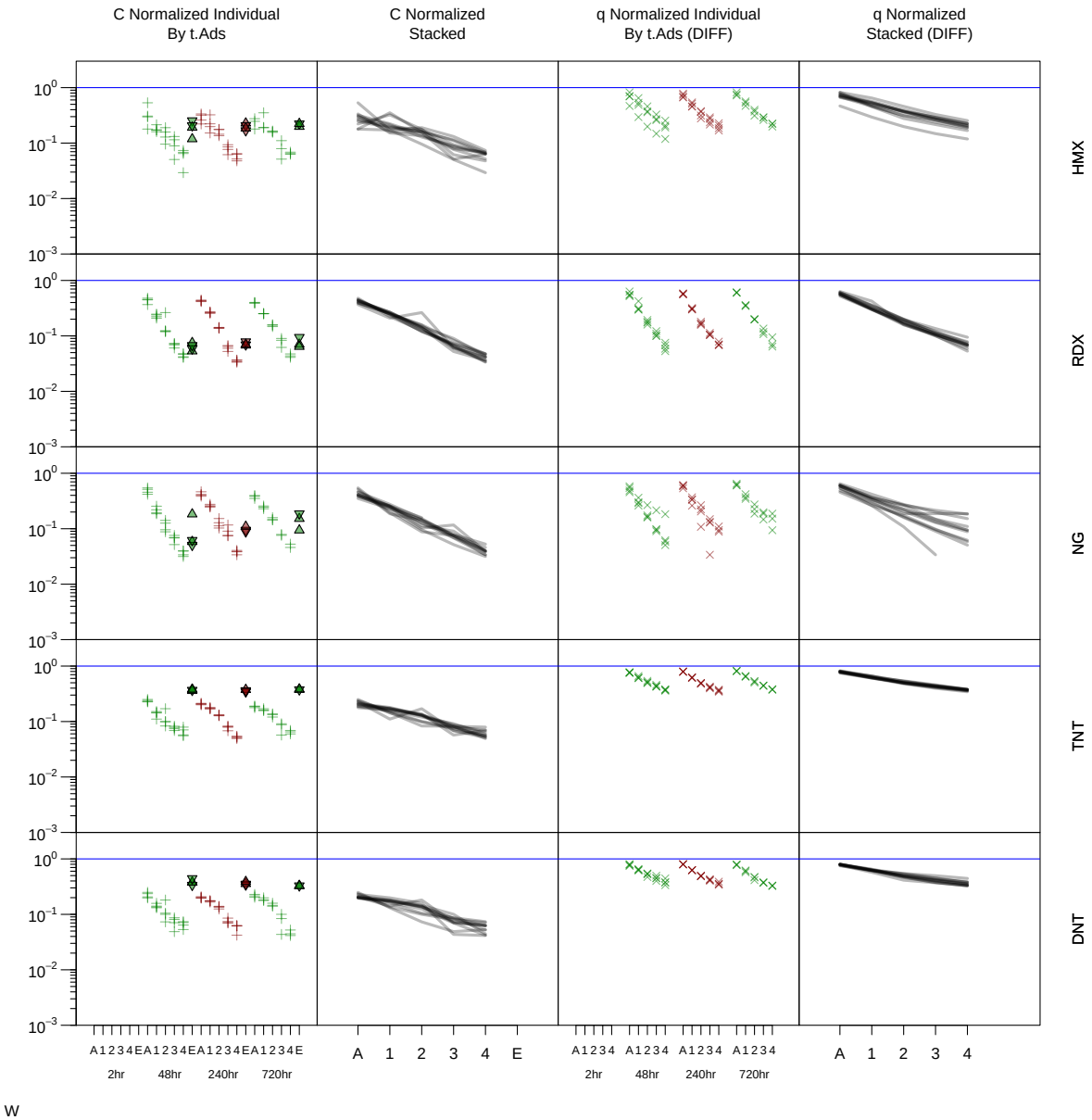

C Normalized Individual
By t.Ads
C Normalized
Stacked
q Normalized Individual
By t.Ads (DIFF)
q Normalized
Stacked (DIFF)
HMX
RDX
NG
TNT
DNT
A1234EA1234EA1234EA1234EA1234E
2hr
48hr
240hr
720hr
A 1 2 3 4 E
A1234 A1234 A1234 A1234
A 1 2 3 4

SSL

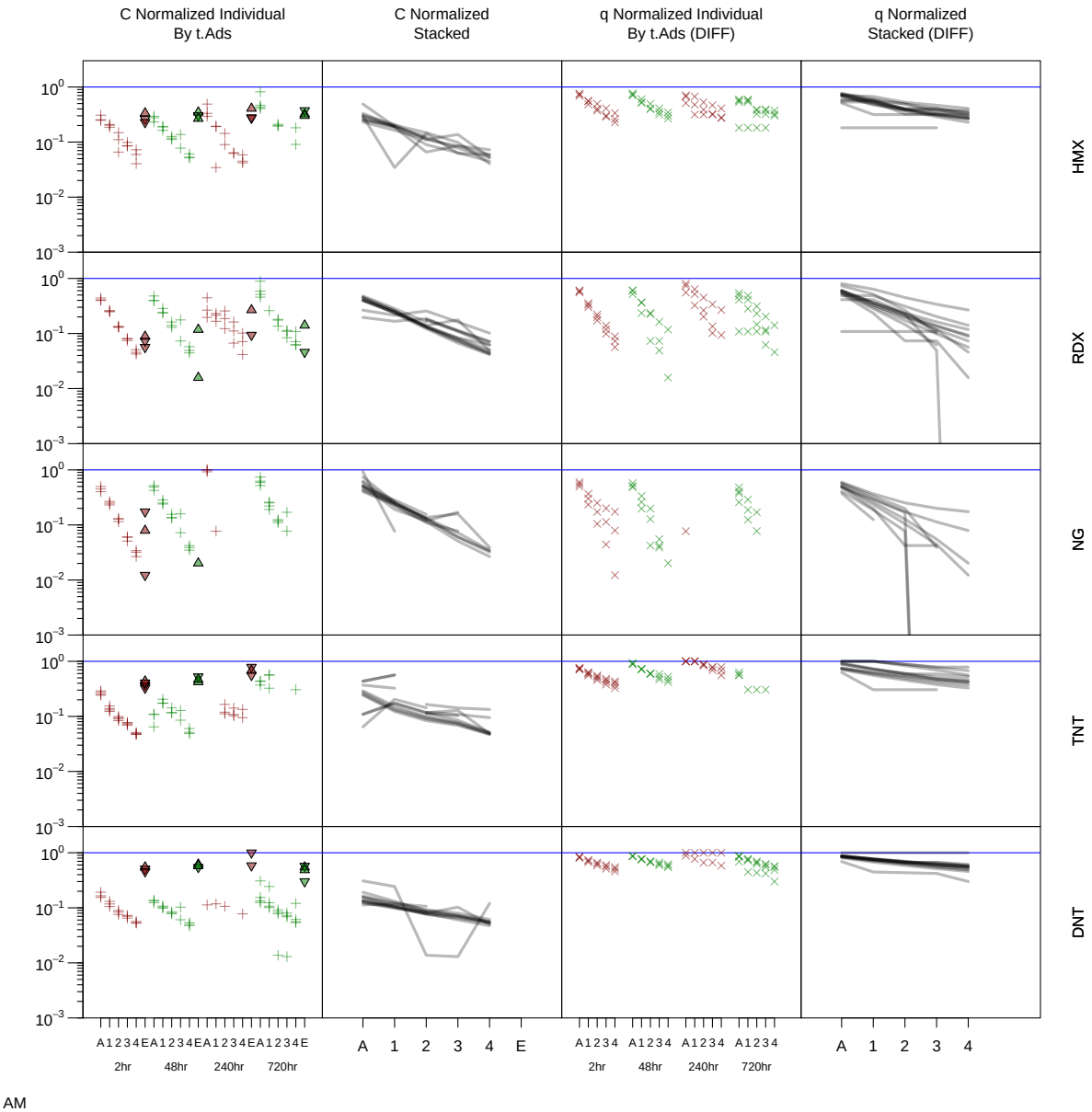

C Normalized Individual
By t.Ads
C Normalized
Stacked
q Normalized Individual
By t.Ads (DIFF)
q Normalized
Stacked (DIFF)
HMX
RDX
NG
TNT
DNT
10^{0}
10^{-1}
10^{-2}
10^{-3}
A1234EA1234EA1234EA1234EA1234E
2hr
48hr
240hr
720hr
A 1 2 3 4 E
A1234 A1234 A1234 A1234
A 1 2 3 4
MPK

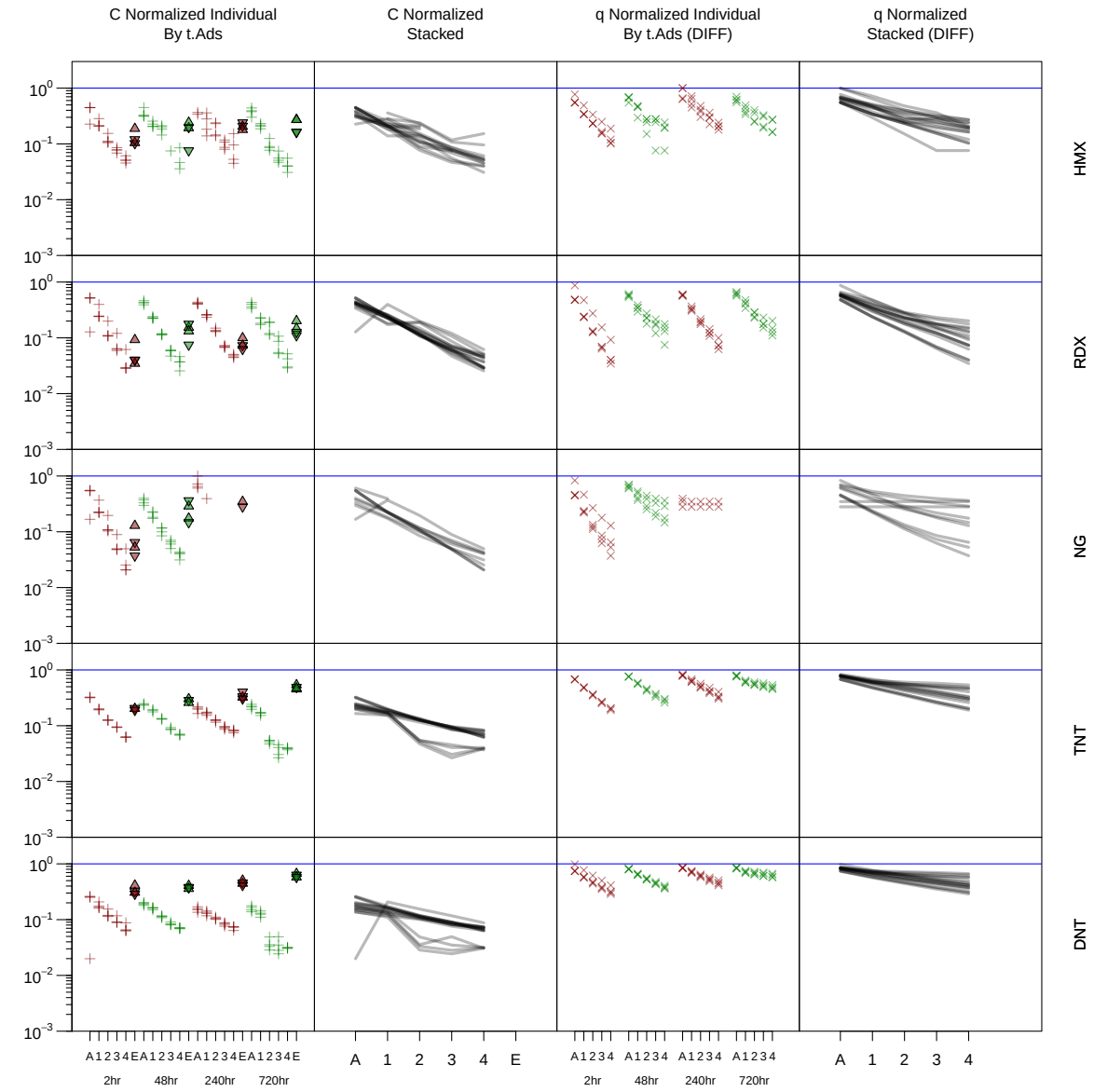

C Normalized Individual
By t.Ads
C Normalized
Stacked
q Normalized Individual
By t.Ads (DIFF)
q Normalized
Stacked (DIFF)
HMX
RDX
NG
TNT
DNT
A1234EA1234EA1234EA1234EA1234E
2hr
48hr
240hr
720hr
A 1 2 3 4 E
A1234 A1234 A1234 A1234
A 1 2 3 4

S2

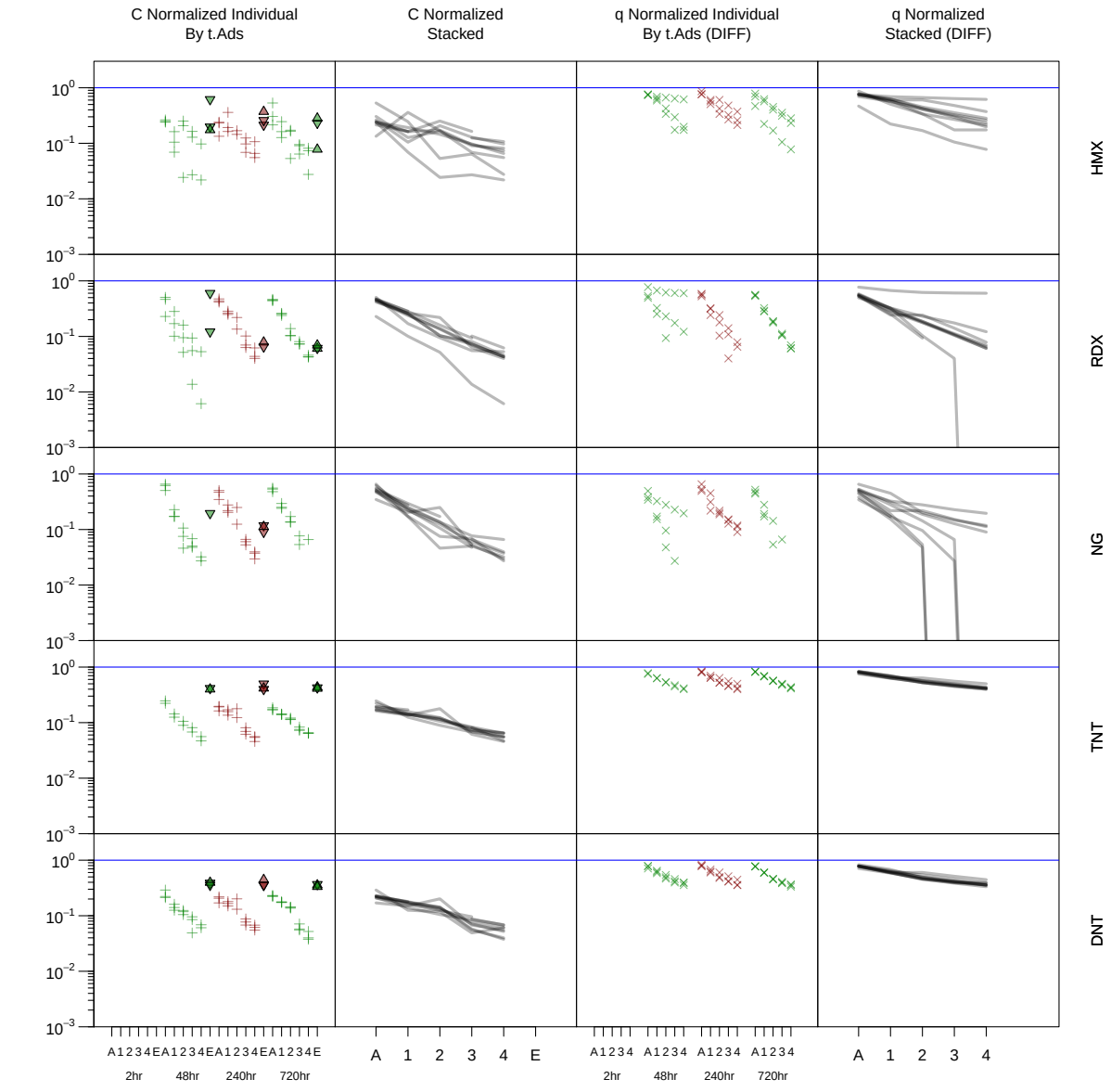

C Normalized Individual
By t.Ads
C Normalized
Stacked
q Normalized Individual
By t.Ads (DIFF)
q Normalized
Stacked (DIFF)
HMX
RDX
NG
TNT
DNT
A1234EA1234EA1234EA1234EA1234E
2hr
48hr
240hr
720hr
A 1 2 3 4 E
A1234 A1234 A1234 A1234
A 1 2 3 4

W

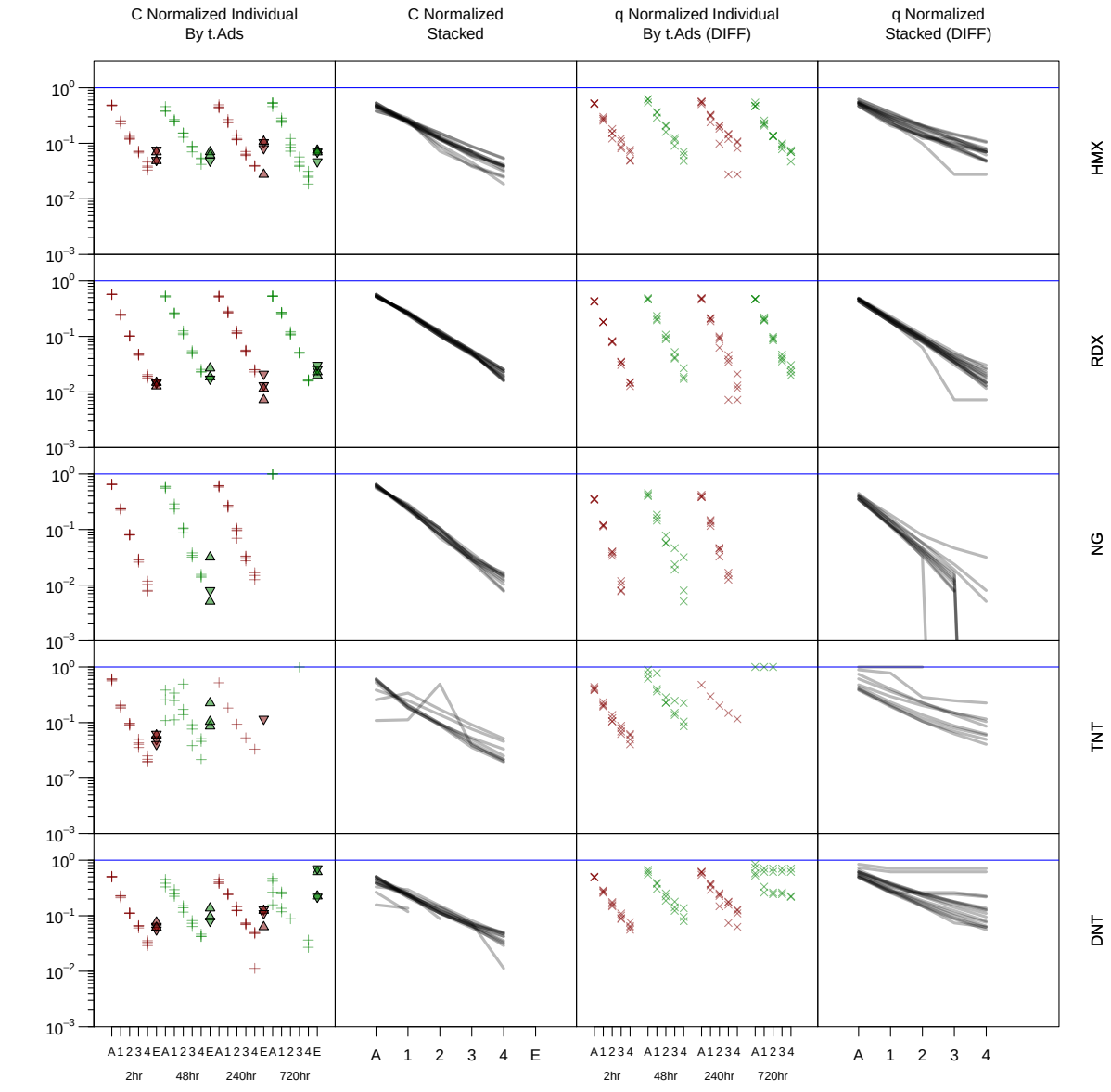

C Normalized Individual
By t.Ads
C Normalized
Stacked
q Normalized Individual
By t.Ads (DIFF)
q Normalized
Stacked (DIFF)
HMX
RDX
NG
TNT
DNT
A1234EA1234EA1234EA1234EA1234E
2hr
48hr
240hr
720hr
A 1 2 3 4 E
A1234 A1234 A1234 A1234
A 1 2 3 4
AM


C Normalized Individual
By t.Ads
C Normalized
Stacked
q Normalized Individual
By t.Ads (DIFF)
q Normalized
Stacked (DIFF)
HMX
RDX
NG
TNT
DNT
10^{0}
10^{-1}
10^{-2}
10^{-3}
A1234EA1234EA1234EA1234EA1234E
2hr
48hr
240hr
720hr
A 1 2 3 4 E
A1234 A1234 A1234 A1234
A 1 2 3 4

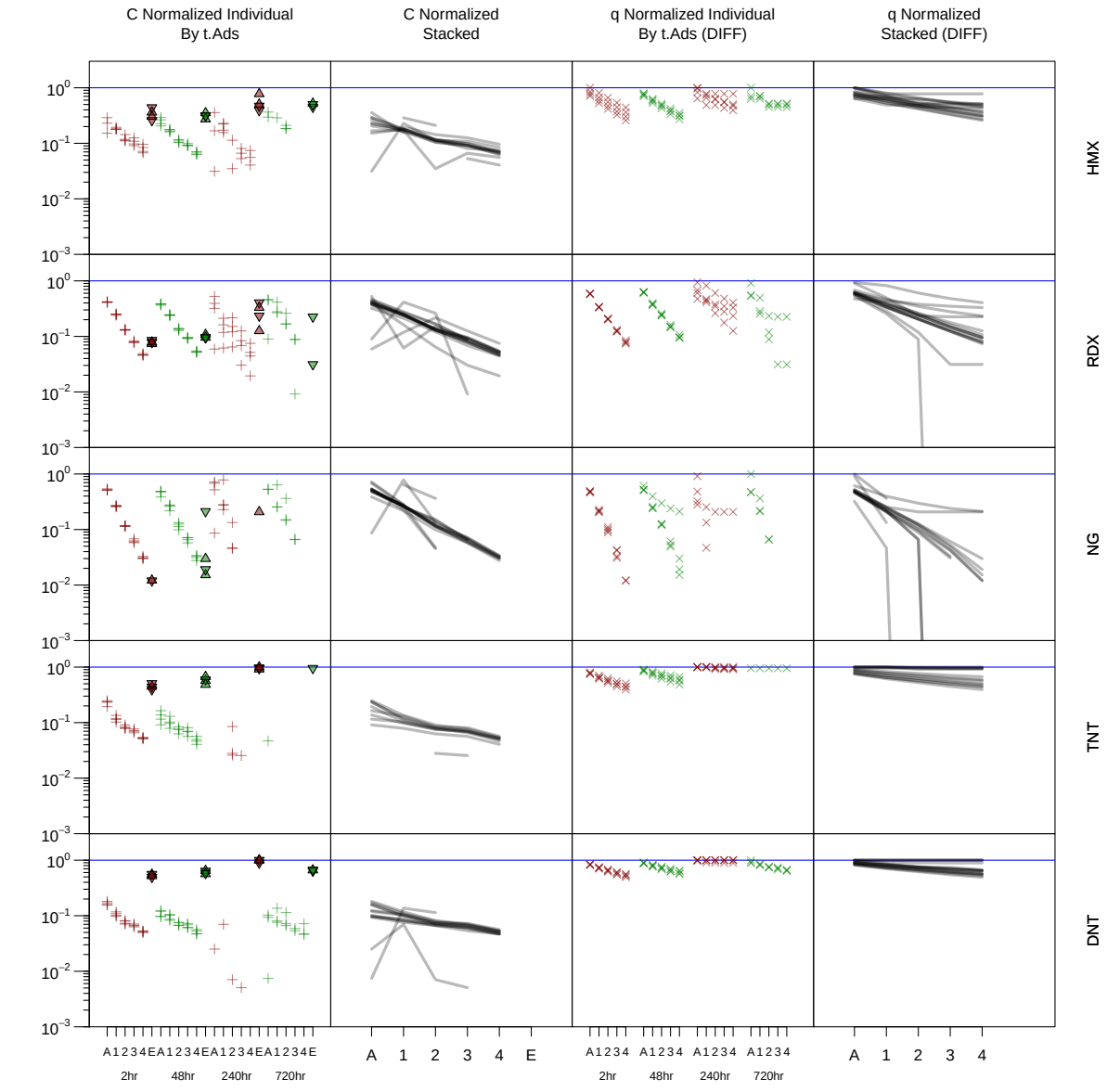
H

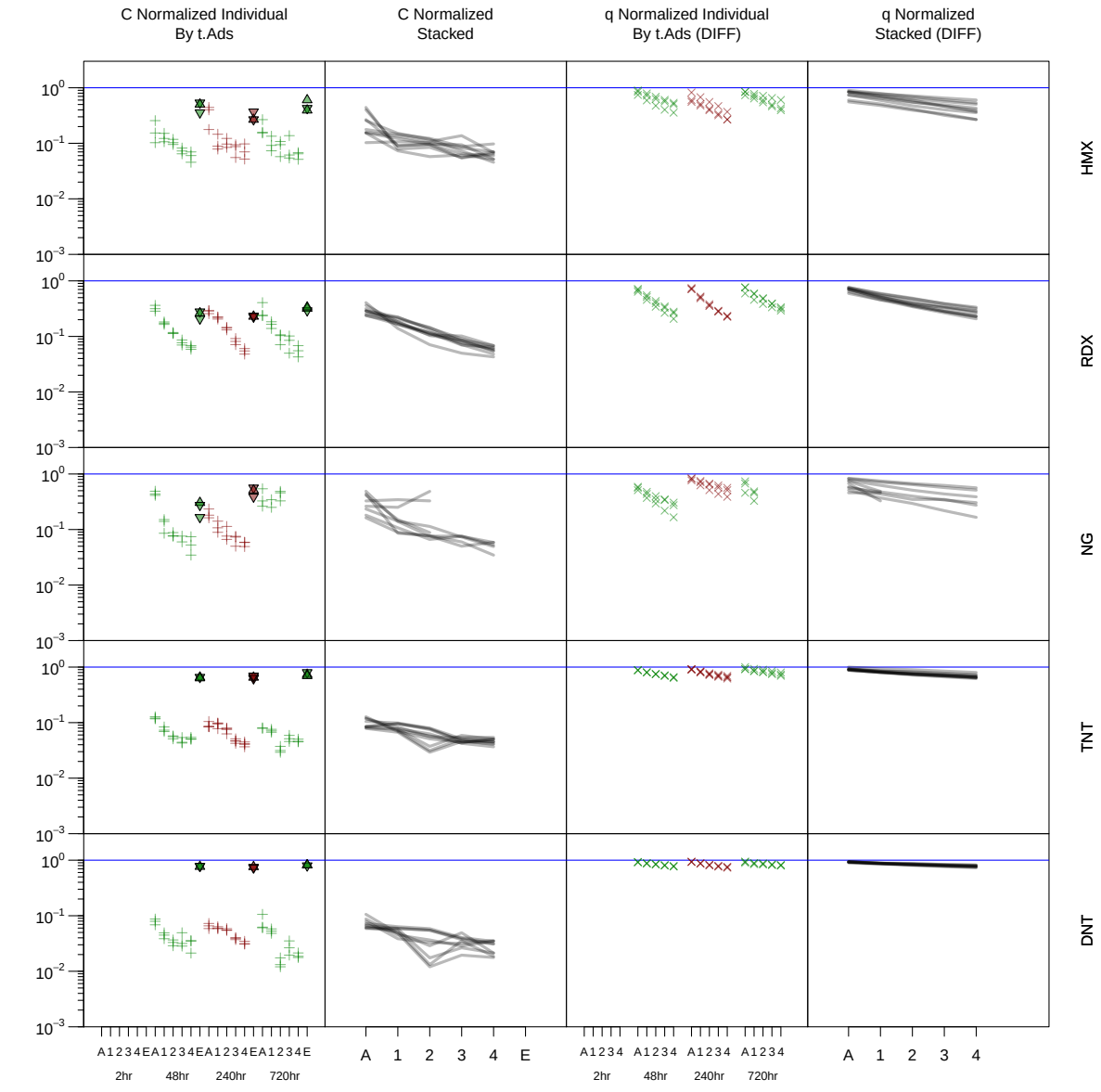

C Normalized Individual
By t.Ads
C Normalized
Stacked
q Normalized Individual
By t.Ads (DIFF)
q Normalized
Stacked (DIFF)
HMX
RDX
NG
TNT
DNT
10^{0}
10^{-1}
10^{-2}
10^{-3}
A1234EA1234EA1234EA1234EA1234E
2hr
48hr
240hr
720hr
A 1 2 3 4 E
A1234 A1234 A1234 A1234
A 1 2 3 4

BOX

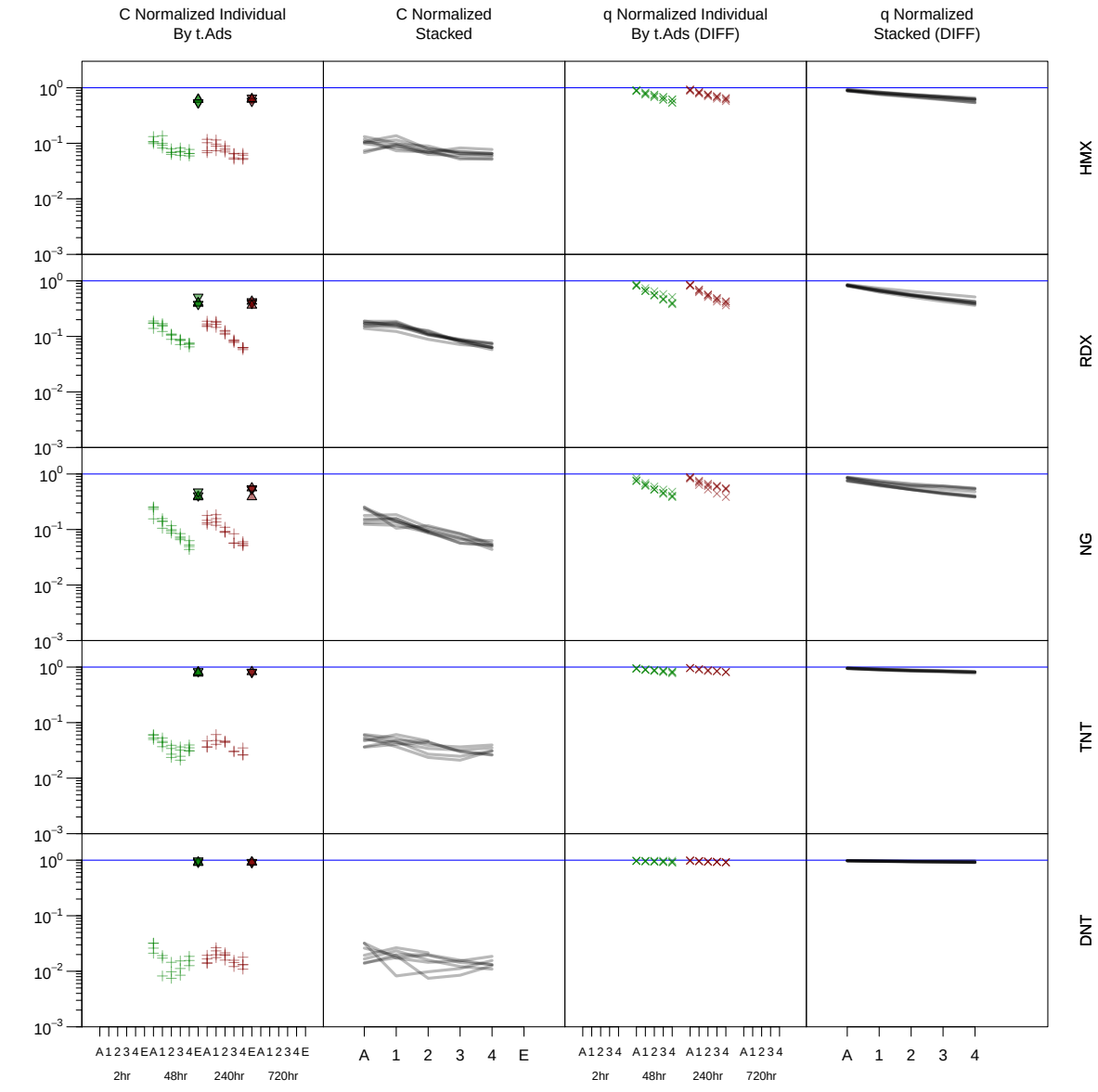

C Normalized Individual
By t.Ads
C Normalized
Stacked
q Normalized Individual
By t.Ads (DIFF)
q Normalized
Stacked (DIFF)
HMX
RDX
NG
TNT
DNT
A1234EA1234EA1234EA1234EA1234E
2hr
48hr
240hr
720hr
A 1 2 3 4 E
A1234 A1234 A1234 A1234
A 1 2 3 4

GUA

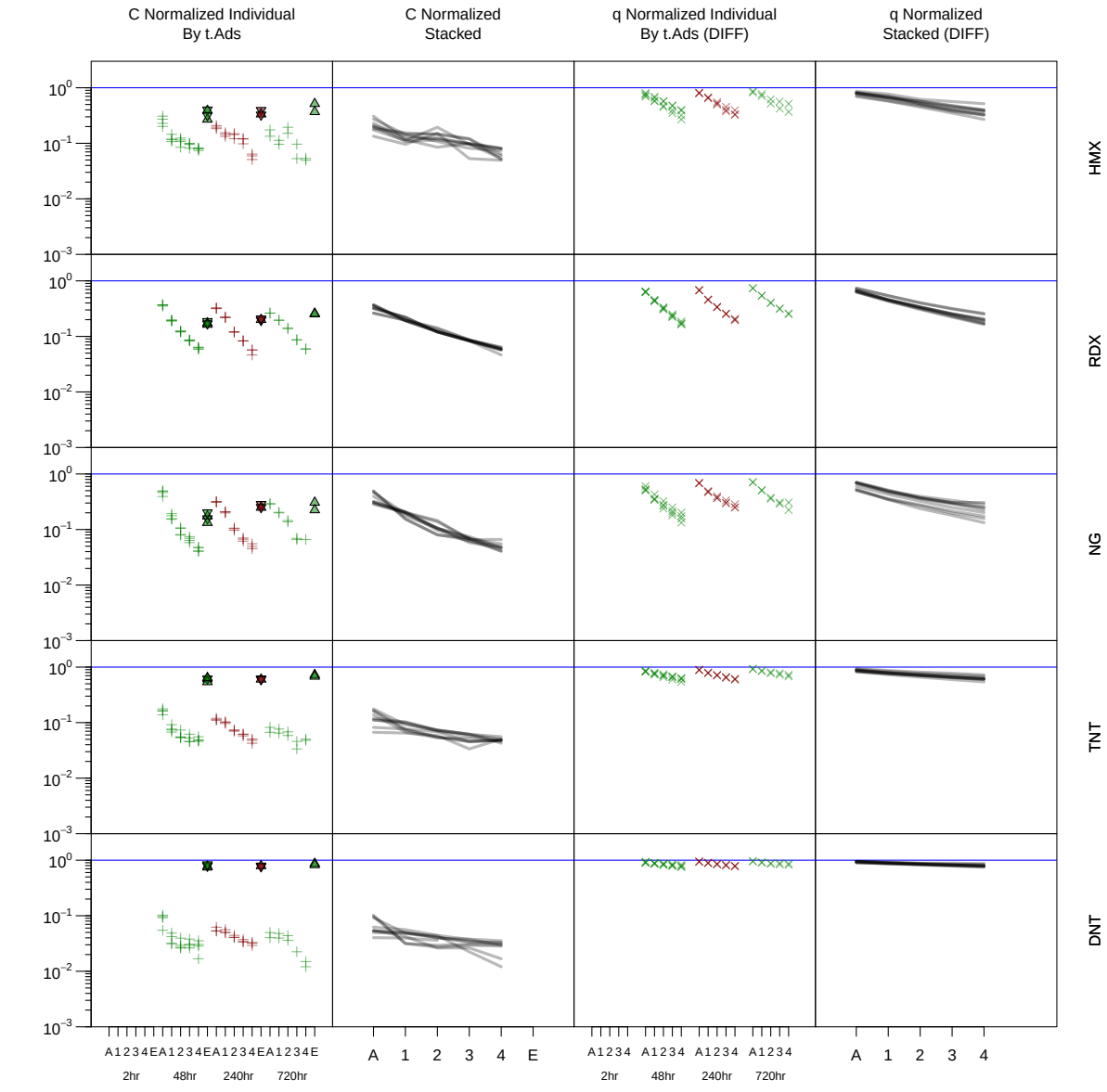

C Normalized Individual
By t.Ads
C Normalized
Stacked
q Normalized Individual
By t.Ads (DIFF)
q Normalized
Stacked (DIFF)
HMX
RDX
NG
TNT
DNT
10^{0}
10^{-1}
10^{-2}
10^{-3}
A1234EA1234EA1234EA1234EA1234E
2hr
48hr
240hr
720hr
A 1 2 3 4 E
A1234 A1234 A1234 A1234
A 1 2 3 4
ELL


C Normalized Individual
By t.Ads
C Normalized
Stacked
q Normalized Individual
By t.Ads (DIFF)
q Normalized
Stacked (DIFF)
HMX
RDX
NG
TNT
DNT
A1234EA1234EA1234EA1234EA1234E
2hr
48hr
240hr
720hr
A 1 2 3 4 E
A1234 A1234 A1234 A1234
A 1 2 3 4

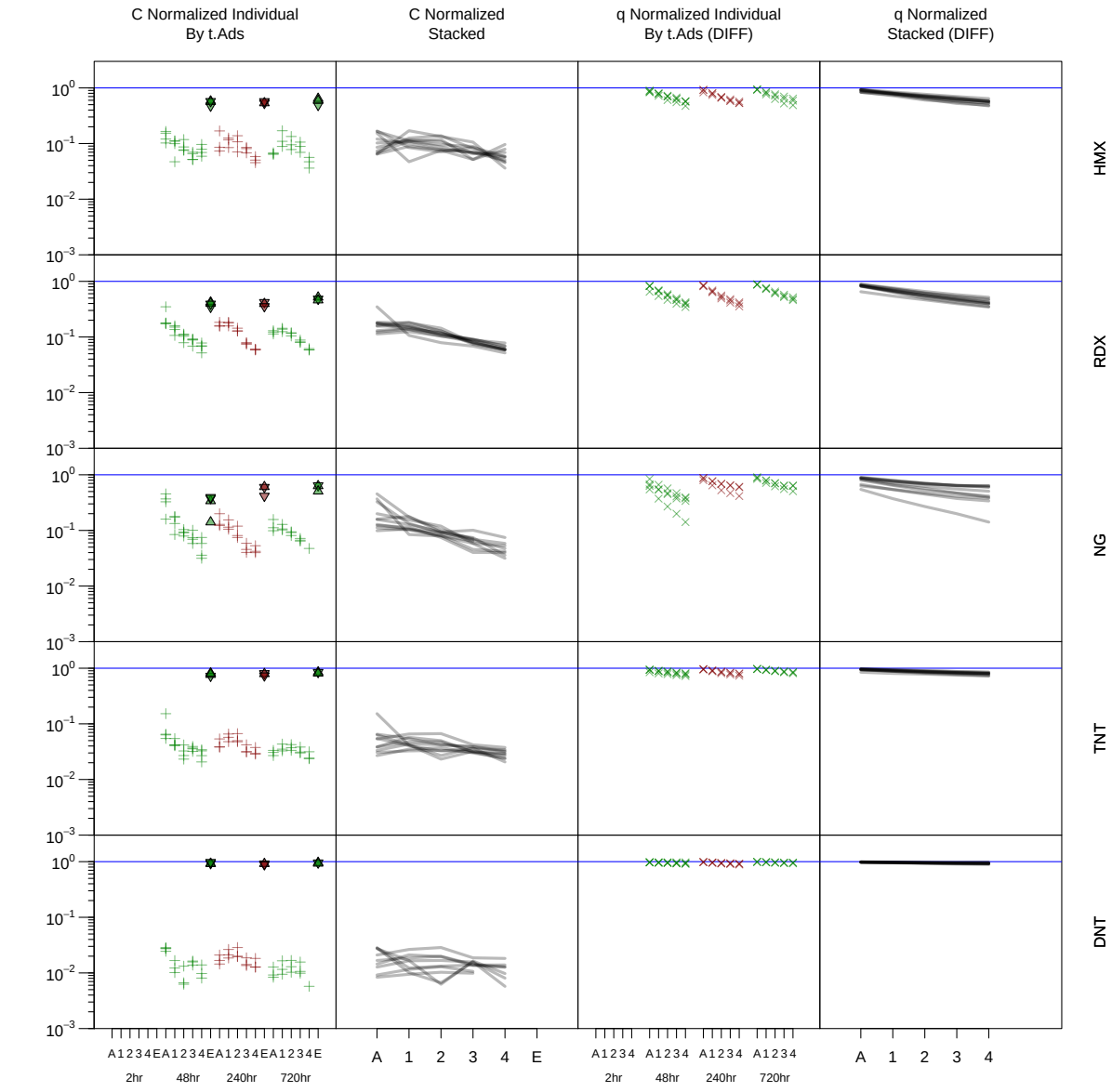
PO


C Normalized Individual
By t.Ads
C Normalized
Stacked
q Normalized Individual
By t.Ads (DIFF)
q Normalized
Stacked (DIFF)
HMX
RDX
NG
TNT
DNT
A1234EA1234EA1234EA1234EA1234E
2hr
48hr
240hr
720hr
A 1 2 3 4 E
A1234 A1234 A1234 A1234
A 1 2 3 4

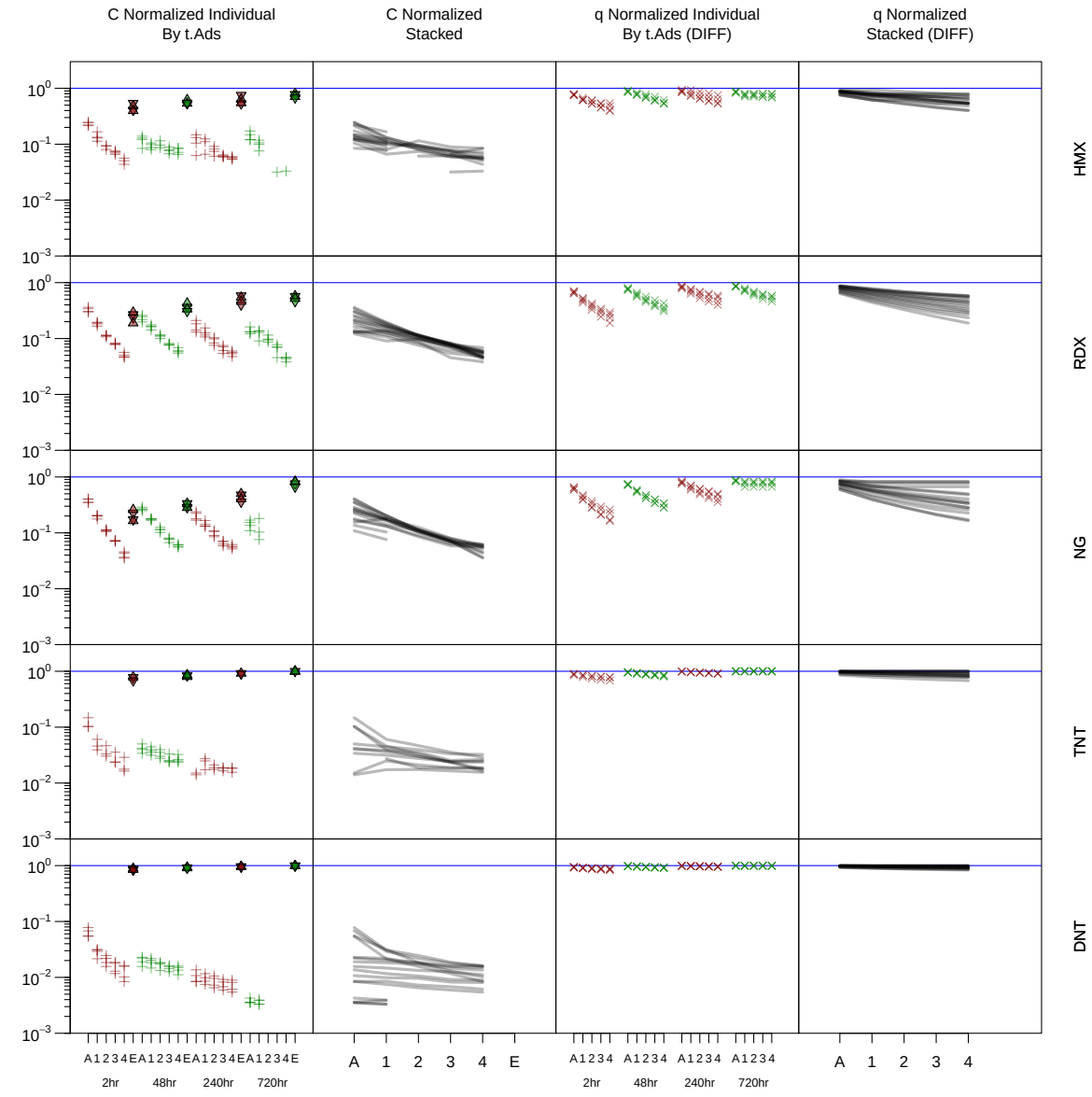
BU


C Normalized Individual
By t.Ads
C Normalized
Stacked
q Normalized Individual
By t.Ads (DIFF)
q Normalized
Stacked (DIFF)
HMX
RDX
NG
TNT
DNT
10^{0}
10^{-1}
10^{-2}
10^{-3}
A1234EA1234EA1234EA1234EA1234E
2hr
48hr
240hr
720hr
A 1 2 3 4 E
A1234 A1234 A1234 A1234
A 1 2 3 4

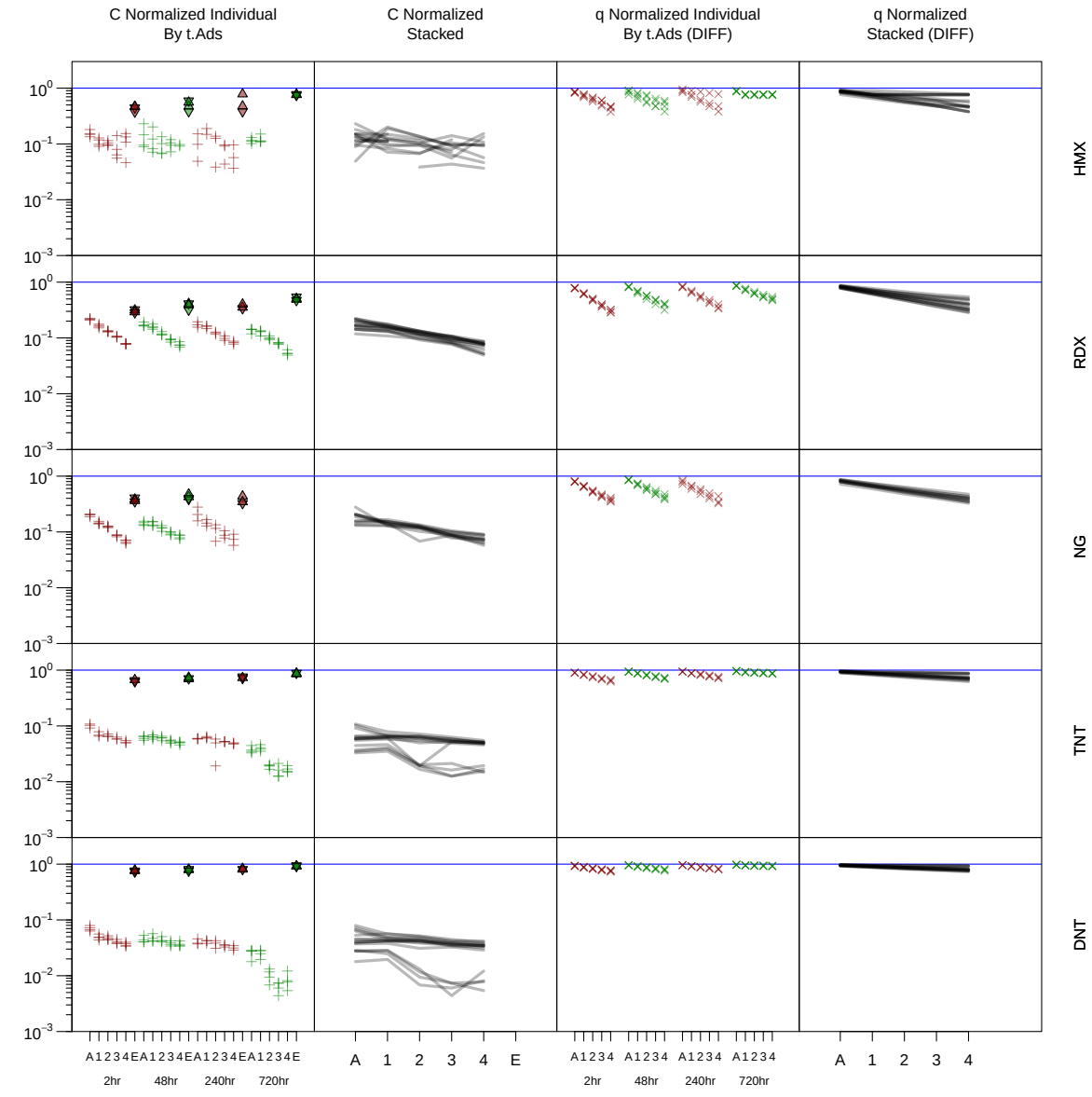
LCL


C Normalized Individual
By t.Ads
C Normalized
Stacked
q Normalized Individual
By t.Ads (DIFF)
q Normalized
Stacked (DIFF)
HMX
RDX
NG
TNT
DNT
A1234EA1234EA1234EA1234EA1234E
2hr
48hr
240hr
720hr
A 1 2 3 4 E
A1234 A1234 A1234 A1234
A 1 2 3 4

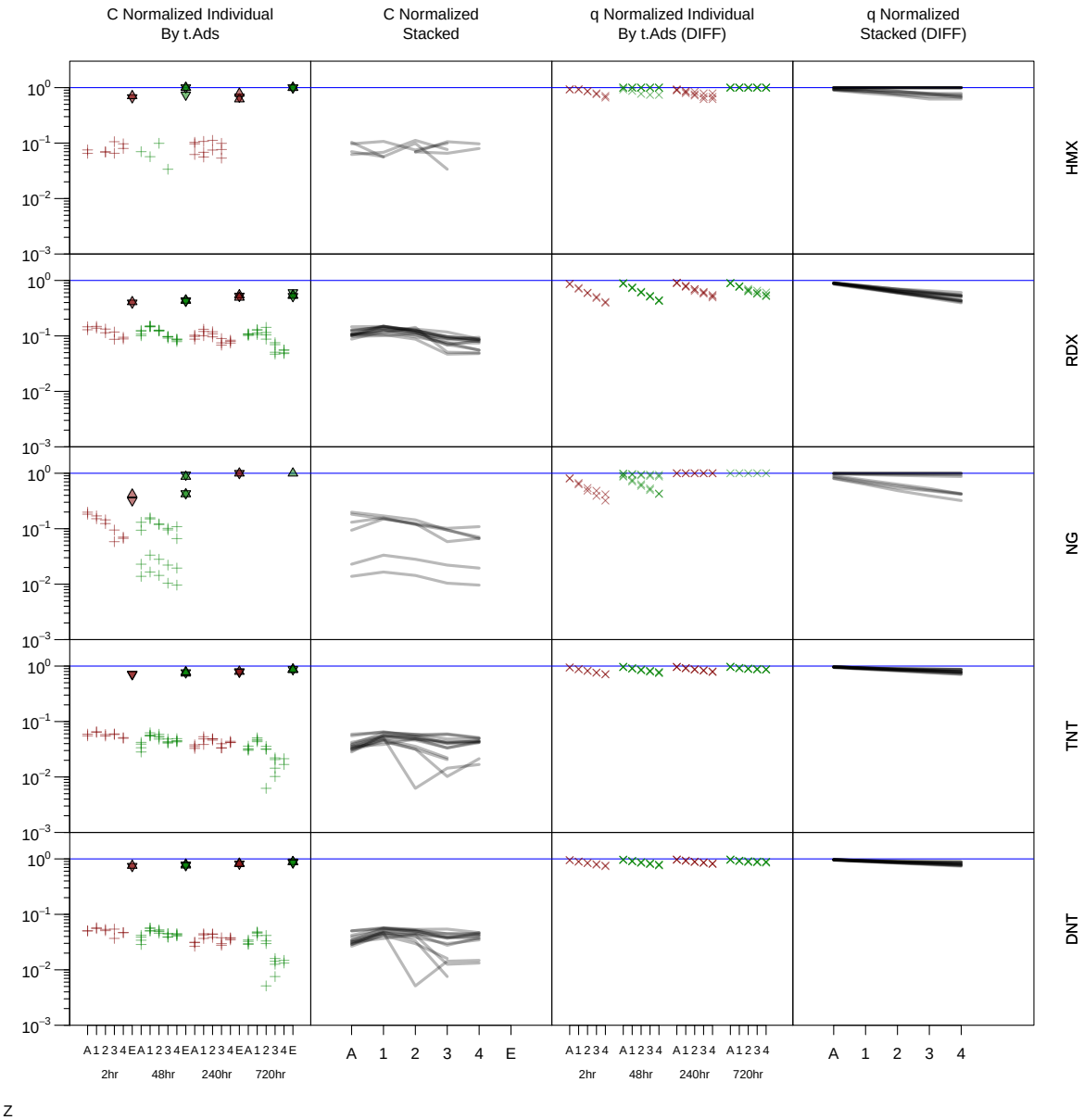
LCO

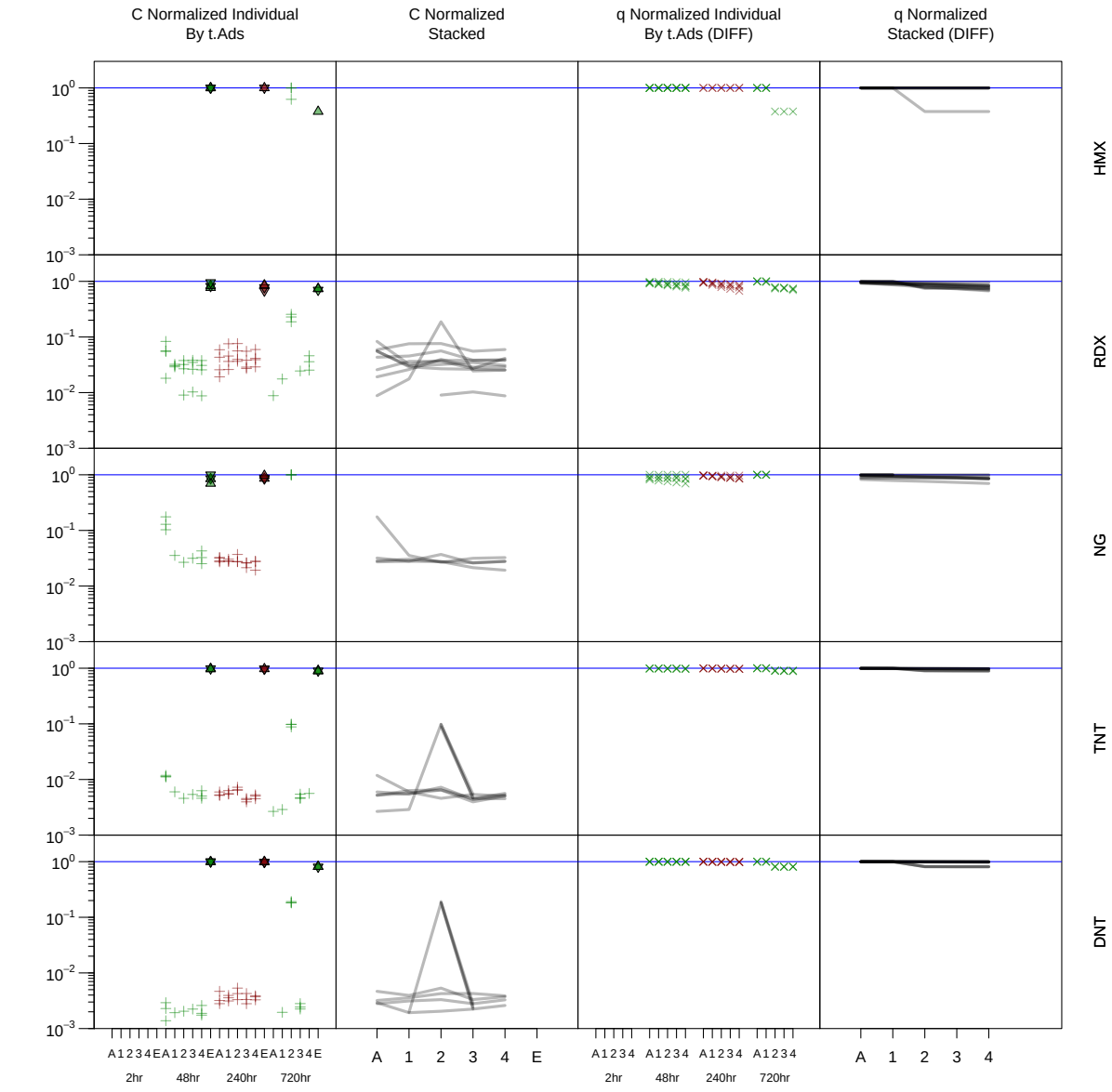

C Normalized Individual
By t.Ads
C Normalized
Stacked
q Normalized Individual
By t.Ads (DIFF)
q Normalized
Stacked (DIFF)
HMX
RDX
NG
TNT
DNT
A1234EA1234EA1234EA1234EA1234E
2hr
48hr
240hr
720hr
A 1 2 3 4 E
A1234 A1234 A1234 A1234
A 1 2 3 4

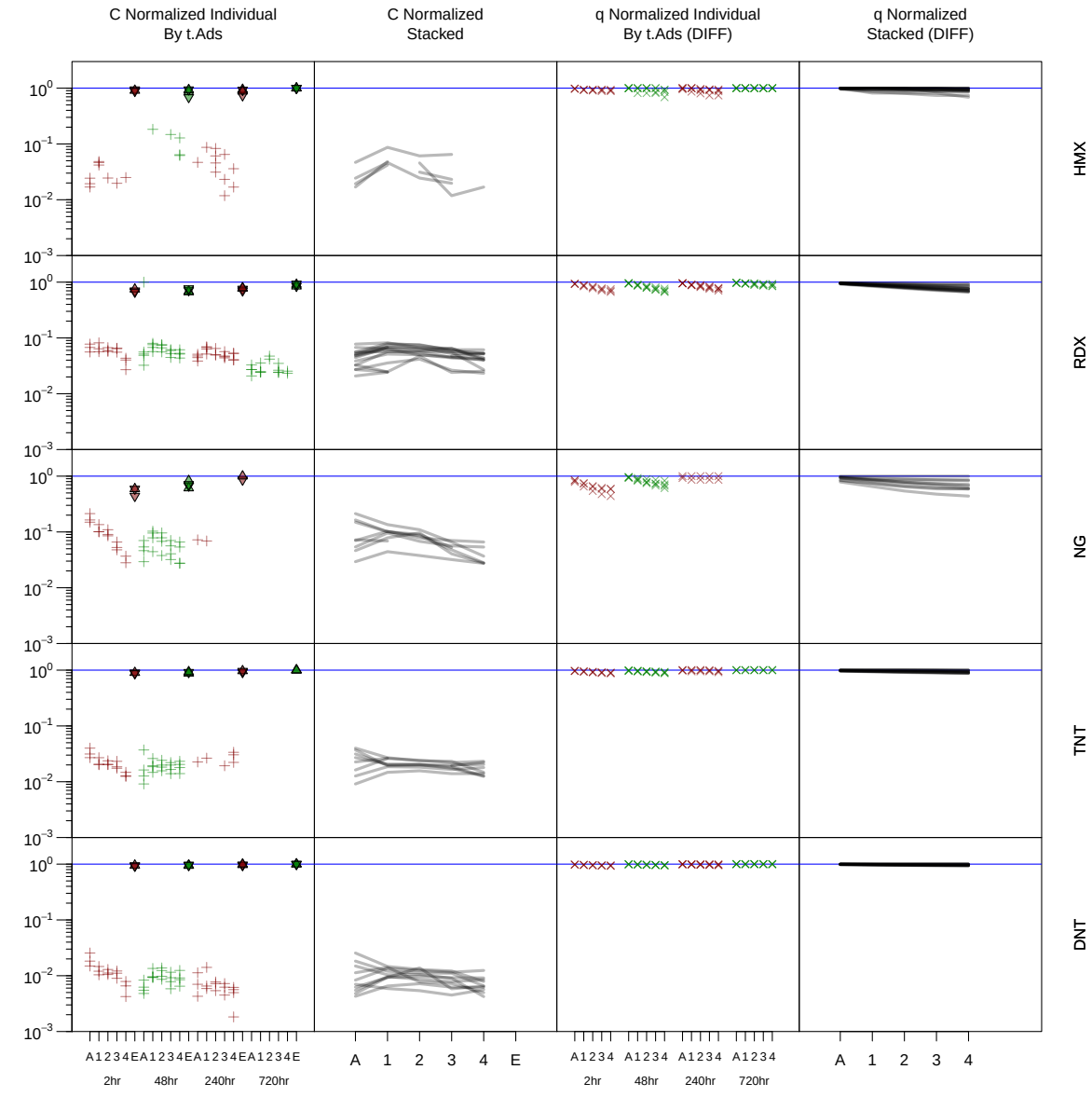
J


C Normalized Individual
By t.Ads
C Normalized
Stacked
q Normalized Individual
By t.Ads (DIFF)
q Normalized
Stacked (DIFF)
HMX
RDX
NG
TNT
DNT
A1234EA1234EA1234EA1234EA1234E
2hr
48hr
240hr
720hr
A 1 2 3 4 E
A1234 A1234 A1234 A1234
A 1 2 3 4

R


C Normalized Individual
By t.Ads
C Normalized
Stacked
q Normalized Individual
By t.Ads (DIFF)
q Normalized
Stacked (DIFF)
HMX
RDX
NG
TNT
DNT
A1234EA1234EA1234EA1234EA1234E
2hr
48hr
240hr
720hr
A 1 2 3 4 E
A1234 A1234 A1234 A1234
A 1 2 3 4
Z


C Normalized Individual
By t.Ads
C Normalized
Stacked
q Normalized Individual
By t.Ads (DIFF)
q Normalized
Stacked (DIFF)
HMX
RDX
NG
TNT
DNT
A1234EA1234EA1234EA1234EA1234E
2hr
48hr
240hr
720hr
A 1 2 3 4 E
A1234 A1234 A1234 A1234
A 1 2 3 4
GAS


C Normalized Individual
By t.Ads
C Normalized
Stacked
q Normalized Individual
By t.Ads (DIFF)
q Normalized
Stacked (DIFF)
HMX
RDX
NG
TNT
DNT
A1234EA1234EA1234EA1234EA1234E
2hr
48hr
240hr
720hr
A 1 2 3 4 E
A1234 A1234 A1234 A1234
A 1 2 3 4

P

A.2 Reversible model

A.2.1 Derivation of linear model

$$C_t^N(0) = 1 \tag{A.1}$$

$$C_d^N(0) = \frac{1}{1+K_p} C_t^N(0) = f_d \tag{A.2}$$

$$C_p^N(0) = \frac{K_p}{1+K_p} C_t^N(0) = f_p = (1-f_d) \tag{A.3}$$

$$C_t^N(1) = f_p \tag{A.4}$$

$$C_d^N(1) = f_d f_p = f_d(1-f_d) \tag{A.5}$$

$$C_t^N(2) = f_p C_t^N(1) = f_p f_p = (1-f_d)^2 \tag{A.6}$$

$$C_d^N(2) = f_d(1-f_d)^2 \tag{A.7}$$

$$C_d^N(3) = f_d(1-f_d)^3 \tag{A.8}$$

$$\vdots \tag{A.9}$$

$$C_d^N(k) = f_d(1-f_d)^k \tag{A.10}$$

A.2.2 R code for linear fit

```
# Read HPLC Data
hplc.raw     <-  read.table('../data/hplc_data.csv',header=TRUE,
    stringsAsFactor=FALSE,sep=',',as.is=TRUE)

# Read Soil Data
prop.raw     <-  read.table('../data/soil_properties.csv',header=TRUE,
    stringsAsFactors=FALSE,sep=',',as.is=TRUE)

# Convert % to fractional
foc          <-  prop.raw$TOC/100
fclay        <-  prop.raw$Clay/100

# Order soil names by foc content
soil_order   <-  prop.raw[prop.raw[,1] %in% unique(hplc.raw[,2]),]
soil_foc     <-  soil_order[order(soil_order$TOC),]
soil_order   <-  soil_order[order(soil_order$TOC),]$SoilCode
nSoil        <-  length(soil_order)

mc_list      <-  c('HMX','RDX','NG','TNT','DNT')
nMC          <-  length(mc_list)

# Determine total mass
hplc.raw$MTOT   <-  hplc.raw$A.C*hplc.raw$V.A+
                    hplc.raw$D1.C*hplc.raw$V.D1+
                    hplc.raw$D2.C*hplc.raw$V.D2+
                    hplc.raw$D3.C*hplc.raw$V.D3+
                    hplc.raw$D4.C*hplc.raw$V.D4+
                    hplc.raw$E1.C*hplc.raw$V.E1+
                    hplc.raw$E2.C*hplc.raw$V.E2+
                    hplc.raw$E3.C*hplc.raw$V.E3

# Determine extracted mass
hplc.raw$M.EXT  <-  hplc.raw$E1.C*hplc.raw$V.E1+
                    hplc.raw$E2.C*hplc.raw$V.E2+
                    hplc.raw$E3.C*hplc.raw$V.E3

# Read mass balance check file (mbal = 0 ==> bad mass balance)
mbal.yesno  <-  read.table(file='../data/MB_yesno_v3.csv',sep=',',as.is=
    TRUE,stringsAsFactors=FALSE)

# Set up output file
mbal.yesno  <-  read.table(file='D:/Users/Dropbox/Research/SERDP_1/
    Project_3-Rapid_Sorption/data/MB_yesno_v3.csv',sep=',',as.is=TRUE,
    stringsAsFactors=FALSE)

zout     <-  matrix(NA,ncol=10,nrow=nSoil*nMC)

# Loop over MC
for (ii in 1:nSoil) {
```

```
45      sub.soil    <-  hplc.raw[hplc.raw$SOILCODE==soil_order[ii],]
46      # Loop over soils
47      for (jj in 1:nMC) {
48          sub.mc  <-  sub.soil[sub.soil$MC==mc_list[jj],]
49
50          zout[nSoil*(jj-1)+ii,1] <-  soil_order[ii]
51          zout[nSoil*(jj-1)+ii,2] <-  mc_list[jj]
52
53
54          # Loop over adsorption times
55          for (kk in 1:4) {
56              sub.ads <-  sub.mc[sub.mc$VIAL>c(0,5,10,15)[kk] & sub.mc$
                    VIAL<=c(5,10,15,20)[kk],]
57
58              # Normalize data
59              obs.soil    <-  matrix(c(sub.ads$A.C*sub.ads$V.A/sub.ads$
                    MTOT,
60                                       sub.ads$D1.C*sub.ads$V.A/sub.ads$
                                             MTOT,
61                                       sub.ads$D2.C*sub.ads$V.A/sub.ads$
                                             MTOT,
62                                       sub.ads$D3.C*sub.ads$V.A/sub.ads$
                                             MTOT,
63                                       sub.ads$D4.C*sub.ads$V.A/sub.ads$
                                             MTOT),ncol=5)
64
65              is.na(obs.soil)  <-  is.nan(obs.soil)
66
67              # Set groups with poor MB to NA (mbal = 0 ==> bad mass
                    balance)
68              mbok    <-  mbal.yesno[mbal.yesno[,1]==soil_order[ii] & mbal
                    .yesno[,2]>c(0,5,10,15)[kk] & mbal.yesno[,2]<=c
                    (5,10,15,20)[kk] & mbal.yesno[,3]==mc_list[jj],]
69
70              mbna    <-  matrix(rep(mbok[,4],5),nrow=5)
71              is.na(obs.soil) <-  mbna==0
72              is.na(obs.soil[,1]) <-  obs.soil[,1]==0
73              # Drop sets with missing data
74              obs.na      <-  obs.soil[complete.cases(obs.soil),]
75              if (is.null(nrow(obs.na))) {
76                  # If there is only 1 adsorption point, that's the fd
77                  fd.fit      <-  obs.na[1]
78                  kp.fit      <-  1/fd.fit-1
79              } else if (sum(is.na(obs.na))!=nrow(obs.na)) {
80                  # Fit Kp for adsorption point and calculate error
81                  cd.obs  <-  obs.na[,1]
82                  nls.fit <-  nls(cd.obs~1/(1+kp),start=list(kp=1))
83
84                  kp.fit      <-  summary(nls.fit)$par[1]
85                  kp.err      <-  summary(nls.fit)$par[2]
86              } else {
```

```
87                  # No data, so set fit to NA
88                  kp.fit      <- NA
89                  kp.err      <- NA
90                  serr        <- NA
91                  nerr        <- NA
92              }
93              # Place fit into output file
94              zout[nSoil*(jj-1)+ii,1+(kk*2)]      <-   kp.fit
95              zout[nSoil*(jj-1)+ii,2+(kk*2)]      <-   kp.err
96          }
97      }
98  }
99  # Generate csv from fit
100 write.table(x=zout,file=paste(dat_path,'IRP_wErr_v4.csv',sep=''),sep=','
        )
```

A.2.3 Reversible model parameters

Table A.1: Parameters for reversible model derived adsorption partition coefficient * Indicates noncoverged model. NA indicates "Not Analyzed"

Soil	**MC**	K_P^{2h}	$K_{P,err}^{2h}$	K_P^{48h}	$K_{P,err}^{48h}$	K_P^{240h}	$K_{P,err}^{240h}$	K_P^{720h}	$K_{P,err}^{720h}$
AM	DNT	4.859	0.38699	6.614	0.23156	NA	NA	6.276	0.46931
B	DNT	NA	NA	0.700	0.06215	0.980	0.00938	0.775	0.08171
BA	DNT	0.674	0.00550	0.844	0.00916	0.998	0.06874	0.897	0.01139
BOX	DNT	NA	NA	3.142	0.41971	3.565	0.41971	3.416	0.09700
BT	DNT	0.602	0.01387	0.671	0.02925	0.688	0.02160	0.634	0.00495
BU	DNT	NA	NA	34.945	3.39496	61.315	4.97817	NA	NA
FT	DNT	NA	NA	1.069	0.06942	1.229	0.01732	0.940	0.02997
GUA	DNT	0.983	0.01367	1.394	0.18732	1.557	0.05137	NA	NA
H	DNT	4.066	1.51952	4.303	0.12523	4.891	0.12523	5.071	0.12523
J	DNT	14.675	1.37436	49.194	4.16529	95.804	11.59551	266.727	12.68221
KA	DNT	0.497	0.00727	0.525	0.01845	0.499	0.00750	0.447	0.01121
LCL	DNT	NA	NA	10.564	1.44066	16.785	0.93833	NA	NA
LCO	DNT	NA	NA	36.037	1.18998	56.493	6.32668	107.865	6.32668
MPK	DNT	1.763	0.04297	2.503	0.08825	3.097	0.21442	4.108	0.21442
P	DNT	50.102	8.17531	159.793	19.80582	NA	NA	NA	NA
PO	DNT	NA	NA	11.751	0.87309	14.227	1.60366	8.440	1.60366
R	DNT	13.207	0.71081	21.508	1.51801	25.129	1.51801	38.351	3.90402
S2	DNT	1.612	0.05613	2.175	0.32477	2.756	0.15649	2.147	0.07312
SAS	DNT	1.736	0.03445	2.300	0.03988	2.723	0.11162	2.258	0.10379
SOU	DNT	0.983	0.14989	1.584	0.07607	2.097	0.12991	1.905	0.12991
SSL	DNT	1.702	0.09796	2.072	0.06197	NA	NA	2.261	0.05271
ST	DNT	1.883	0.05691	2.299	0.07496	2.720	0.03475	2.242	0.03264
U	DNT	1.125	0.05805	1.728	0.07468	2.112	0.08661	NA	NA
W	DNT	NA	NA	3.497	0.24663	3.971	0.06422	3.783	0.13870
W1	DNT	1.285	0.03314	1.565	0.07652	1.648	0.09258	1.540	0.05964
W2	DNT	1.333	0.05058	1.639	0.07071	1.795	0.09409	1.482	0.05961
Z	DNT	18.853	0.01366	26.869	2.24549	32.716	1.75720	30.910	1.34350

Table A.1 – continued from previous page

Soil	MC	K_P^{2h}	$K_{P,err}^{2h}$	K_P^{48h}	$K_{P,err}^{48h}$	K_P^{240h}	$K_{P,err}^{240h}$	K_P^{720h}	$K_{P,err}^{720h}$
AM	HMX	2.701	0.25809	2.501	0.11080	1.435	0.46780	NA	NA
B	HMX	NA	NA	0.761	0.09234	0.852	0.12396	0.636	0.03596
BA	HMX	0.791	0.00869	0.827	0.01943	0.838	0.00581	0.729	0.09641
BOX	HMX	NA	NA	2.992	0.11023	3.162	0.11023	3.654	0.11023
BT	HMX	0.702	0.01698	0.694	0.03496	0.607	0.00418	0.842	0.00418
BU	HMX	NA	NA	8.009	0.58823	10.044	1.45003	NA	NA
FT	HMX	NA	NA	1.345	0.10011	1.504	0.02023	1.477	0.11721
GUA	HMX	1.076	0.01238	1.377	0.20942	1.178	0.08605	1.179	0.08605
H	HMX	1.548	0.35967	2.018	0.35967	1.935	0.35967	1.262	0.35967
J	HMX	3.315	0.14690	8.721	1.75698	6.822	0.76447	6.129	0.63250
KA	HMX	0.679	0.02391	0.673	0.03447	0.640	0.01761	0.527	0.01761
LCL	HMX	NA	NA	2.960	0.36758	3.959	0.16846	5.484	0.84307
LCO	HMX	NA	NA	6.391	0.78913	11.550	0.94224	14.190	0.27780
MPK	HMX	1.445	0.18702	1.756	0.19088	1.661	0.12572	NA	NA
P	HMX	48.455	5.34318	NA	NA	NA	NA	NA	NA
PO	HMX	NA	NA	4.858	1.54819	NA	NA	2.750	NA
R	HMX	5.485	0.41188	5.134	2.53700	6.988	1.69921	NA	NA
S2	HMX	2.215	0.52148	1.402	0.15776	1.106	0.26045	0.664	0.26045
SAS	HMX	1.280	0.22701	1.622	0.22701	1.279	0.11867	NA	NA
SOU	HMX	1.130	0.15116	1.726	0.17678	1.963	0.12831	1.268	0.03933
SSL	HMX	2.076	0.40861	1.531	0.01069	NA	NA	NA	NA
ST	HMX	1.934	0.04341	2.467	0.10236	3.028	0.07613	2.018	0.08578
U	HMX	0.982	0.05430	1.150	0.05379	1.142	0.03315	0.768	0.01584
W	HMX	NA	NA	2.042	0.68437	2.281	0.24483	2.828	0.21123
W1	HMX	1.496	0.06070	1.569	0.10095	1.482	0.12467	NA	NA
W2	HMX	1.487	0.09409	1.666	0.09902	1.441	0.02216	1.324	0.11112
Z	HMX	13.216	1.02029	NA	NA	11.068	2.98688	NA	NA

Table A.1 – continued from previous page

Soil	MC	K_P^{2h}	$K_{P,err}^{2h}$	K_P^{48h}	$K_{P,err}^{48h}$	K_P^{240h}	$K_{P,err}^{240h}$	K_P^{720h}	$K_{P,err}^{720h}$
AM	NG	1.222	0.13838	1.047	0.13838	NA	NA	NA	NA
B	NG	NA	NA	0.349	0.04526	0.439	0.00619	0.463	0.01626
BA	NG	0.413	0.00510	0.446	0.00504	0.450	0.00913	0.434	0.00874
BOX	NG	NA	NA	0.686	0.12914	1.055	0.07600	NA	NA
BT	NG	0.406	0.00754	0.367	0.00231	0.313	0.00769	0.441	0.13609
BU	NG	NA	NA	3.490	0.46348	5.555	0.59292	NA	NA
FT	NG	NA	NA	0.648	0.02032	0.697	0.00228	0.709	0.02396
GUA	NG	0.540	0.00681	0.730	0.04328	0.639	0.01943	NA	NA
H	NG	1.209	0.46434	NA	NA	NA	NA	NA	NA
J	NG	1.657	0.10631	2.746	0.11241	3.330	0.13934	NA	NA
KA	NG	0.467	0.00443	0.484	0.01292	0.464	0.00754	0.386	0.00372
LCL	NG	NA	NA	1.175	0.10982	2.180	0.03517	NA	NA
LCO	NG	NA	NA	2.056	0.57712	7.173	0.57712	NA	NA
MPK	NG	0.723	0.01753	0.765	0.03432	0.901	0.04175	NA	NA
P	NG	4.699	0.62476	16.625	2.18214	NA	NA	NA	NA
PO	NG	NA	NA	1.239	0.11390	3.813	0.61528	NA	NA
R	NG	3.980	0.11984	5.981	0.59882	NA	NA	NA	NA
S2	NG	0.615	0.01518	0.513	0.01518	NA	NA	NA	NA
SAS	NG	0.634	0.00549	NA	NA	NA	NA	NA	NA
SOU	NG	0.507	0.11097	0.666	0.03159	0.856	0.03824	0.476	0.03824
SSL	NG	0.622	0.00587	0.491	0.00587	NA	NA	NA	NA
ST	NG	0.773	0.03632	1.081	0.02356	1.096	0.02769	0.975	0.01587
U	NG	0.511	0.01195	0.574	0.01013	0.662	0.01869	NA	NA
W	NG	NA	NA	1.072	0.12194	1.397	0.09510	1.716	0.12364
W1	NG	0.500	0.00456	0.513	0.00932	0.410	0.00596	0.493	0.00831
W2	NG	0.529	0.00915	0.555	0.00406	0.417	0.00539	0.449	0.01395
Z	NG	4.245	0.21740	17.556	13.79197	NA	NA	NA	NA

Table A.1 – continued from previous page

Soil	MC	K_P^{2h}	$K_{P,err}^{2h}$	K_P^{48h}	$K_{P,err}^{48h}$	K_P^{240h}	$K_{P,err}^{240h}$	K_P^{720h}	$K_{P,err}^{720h}$
AM	RDX	1.403	0.07559	1.355	0.15565	1.247	0.15565	1.061	0.11833
B	RDX	NA	NA	0.456	0.04239	0.537	0.00575	0.613	0.05678
BA	RDX	0.518	0.00584	0.556	0.00539	0.607	0.02281	0.597	0.01129
BOX	RDX	NA	NA	1.503	0.54046	1.289	0.54046	1.215	0.06707
BT	RDX	0.475	0.00792	0.415	0.01787	0.401	0.00430	0.143	0.00904
BU	RDX	NA	NA	4.918	0.37078	5.040	0.29655	NA	NA
FT	RDX	NA	NA	0.895	0.01393	0.916	0.01404	0.838	0.02005
GUA	RDX	0.747	0.00656	0.900	0.02875	0.910	0.02282	0.897	0.00215
H	RDX	1.374	0.55130	1.406	0.07134	1.373	0.04338	1.510	0.21200
J	RDX	2.061	0.13906	3.340	0.25803	5.003	0.66555	6.077	0.50449
KA	RDX	0.536	0.00746	0.556	0.01510	0.520	0.00879	0.510	0.00781
LCL	RDX	NA	NA	1.745	0.03310	2.110	0.02767	2.806	0.00261
LCO	RDX	NA	NA	3.564	0.90183	4.888	0.47428	7.222	0.55206
MPK	RDX	0.885	0.01192	0.983	0.01646	1.028	0.02720	1.234	0.01873
P	RDX	13.911	1.37804	20.196	2.31031	NA	NA	35.816	NA
PO	RDX	NA	NA	2.114	0.21822	2.643	0.23198	2.113	0.81768
R	RDX	3.616	0.07308	4.771	0.22524	5.412	0.22524	6.007	0.03471
S2	RDX	0.840	0.02817	0.883	0.02817	1.042	0.04813	0.940	0.01865
SAS	RDX	0.922	0.00572	0.928	0.03931	1.008	0.01610	1.021	0.02597
SOU	RDX	0.757	0.13546	0.973	0.04380	1.299	0.04083	1.073	0.02228
SSL	RDX	0.886	0.02764	0.922	0.01649	NA	NA	1.029	0.05430
ST	RDX	1.641	0.06687	1.851	0.19234	2.218	0.02512	1.831	0.02512
U	RDX	0.602	0.01937	0.685	0.01593	0.722	0.01403	0.730	0.00838
W	RDX	NA	NA	1.289	0.12623	1.323	0.04049	1.530	0.02287
W1	RDX	0.857	0.01007	0.858	0.00834	0.748	0.00402	0.884	0.00553
W2	RDX	0.897	0.00642	0.937	0.01257	0.864	0.02661	0.860	0.01026
Z	RDX	6.269	0.44788	7.784	0.44662	8.961	0.25753	8.562	0.29074

Table A.1 – continued from previous page

Soil	MC	K_P^{2h}	$K_{P,err}^{2h}$	K_P^{48h}	$K_{P,err}^{48h}$	K_P^{240h}	$K_{P,err}^{240h}$	K_P^{720h}	$K_{P,err}^{720h}$
AM	TNT	2.778	0.15197	NA	NA	NA	NA	NA	NA
B	TNT	NA	NA	0.687	0.07509	0.992	0.00761	0.741	0.00761
BA	TNT	0.826	0.02563	1.113	0.02980	1.525	0.11275	1.149	0.02842
BOX	TNT	NA	NA	3.258	0.21686	4.573	0.52731	4.396	0.52731
BT	TNT	0.740	0.02947	0.841	0.05276	0.993	0.06730	0.821	0.07333
BU	TNT	NA	NA	16.923	0.83829	24.055	2.20175	NA	NA
FT	TNT	NA	NA	1.103	0.00832	1.215	0.02356	1.089	0.04091
GUA	TNT	0.685	0.03260	NA	NA	NA	NA	NA	NA
H	TNT	2.109	0.02570	3.159	0.08405	3.585	0.08405	NA	NA
J	TNT	7.490	1.07249	22.741	4.52804	NA	NA	NA	NA
KA	TNT	0.508	0.00606	0.530	0.01525	0.514	0.01060	0.436	0.00135
LCL	TNT	NA	NA	5.234	0.31118	7.749	0.20075	11.179	0.20075
LCO	TNT	NA	NA	10.924	3.26182	21.986	2.66405	NA	NA
MPK	TNT	1.634	0.08136	2.221	0.08136	NA	NA	NA	NA
P	TNT	29.471	3.53470	52.228	17.79729	NA	NA	NA	NA
PO	TNT	NA	NA	7.221	0.20978	9.911	0.78244	11.402	0.78244
R	TNT	8.928	0.47529	15.323	0.64789	NA	NA	25.798	1.82253
S2	TNT	1.552	0.06290	1.938	0.31188	2.574	0.39381	2.047	0.10475
SAS	TNT	1.586	0.02981	1.892	0.06200	2.887	0.18852	2.174	0.17435
SOU	TNT	0.893	0.14238	1.674	0.04774	NA	NA	NA	NA
SSL	TNT	1.564	0.06439	1.901	0.06110	NA	NA	2.311	0.07268
ST	TNT	2.274	0.04206	2.691	0.28753	3.129	0.04309	2.364	0.06371
U	TNT	0.715	0.02060	1.937	0.02060	NA	NA	NA	NA
W	TNT	NA	NA	3.231	0.09462	3.877	0.07426	4.348	0.07426
W1	TNT	1.653	0.09134	2.215	0.20621	2.638	0.29495	2.314	0.29495
W2	TNT	1.683	0.11256	2.232	0.24395	2.695	0.31016	1.988	0.31016
Z	TNT	16.472	0.60328	26.930	2.38738	27.239	1.21049	29.740	1.17207

A.2.4 Reversible model plots

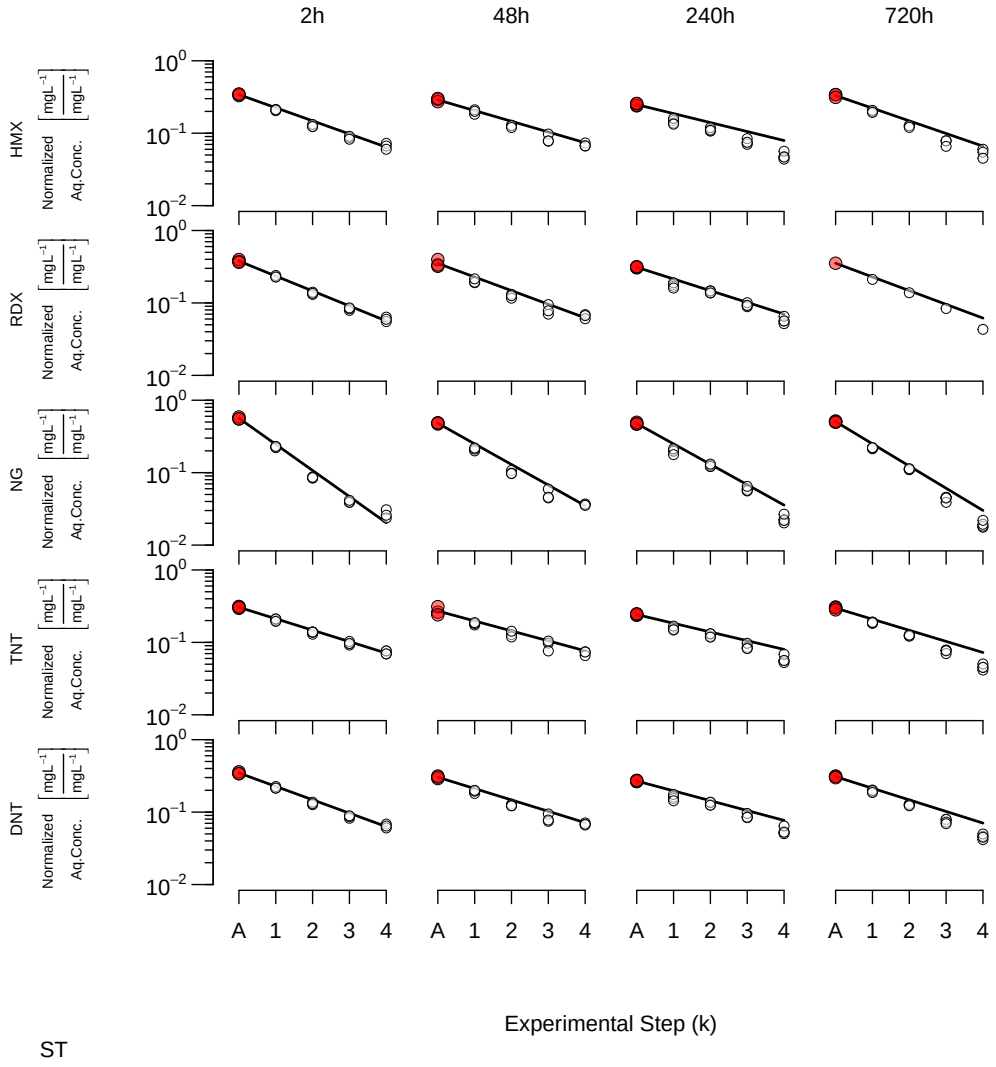
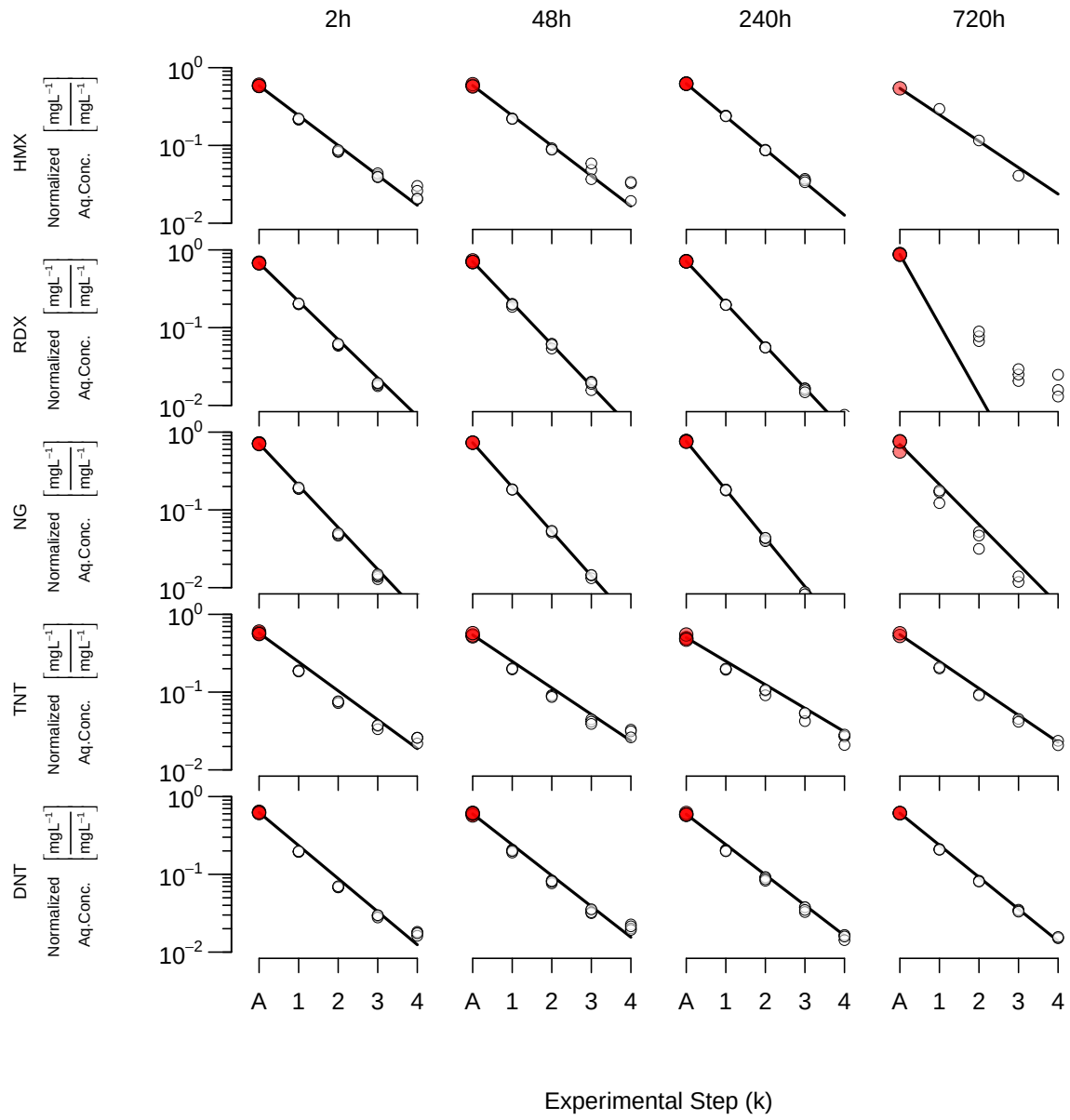
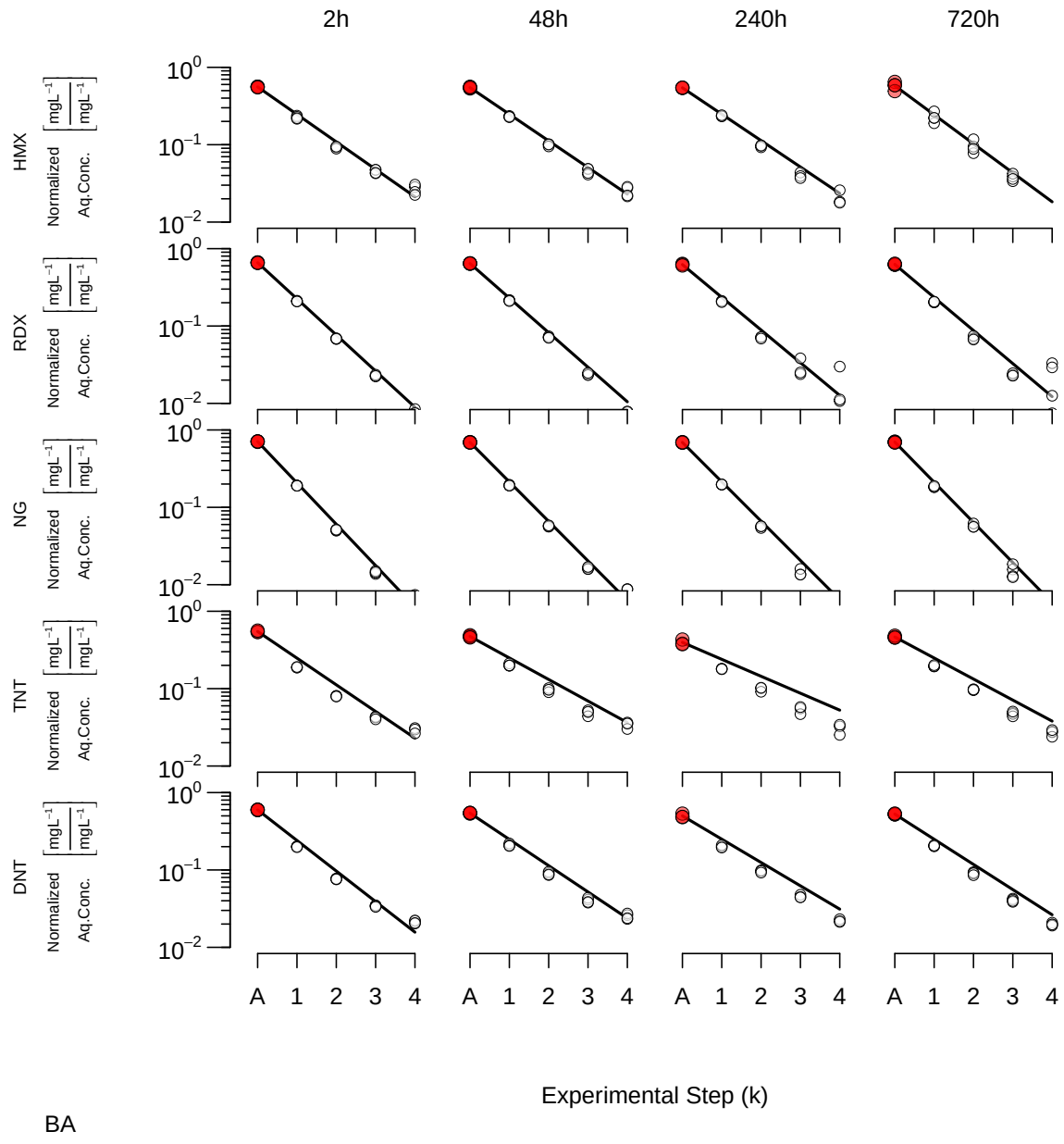


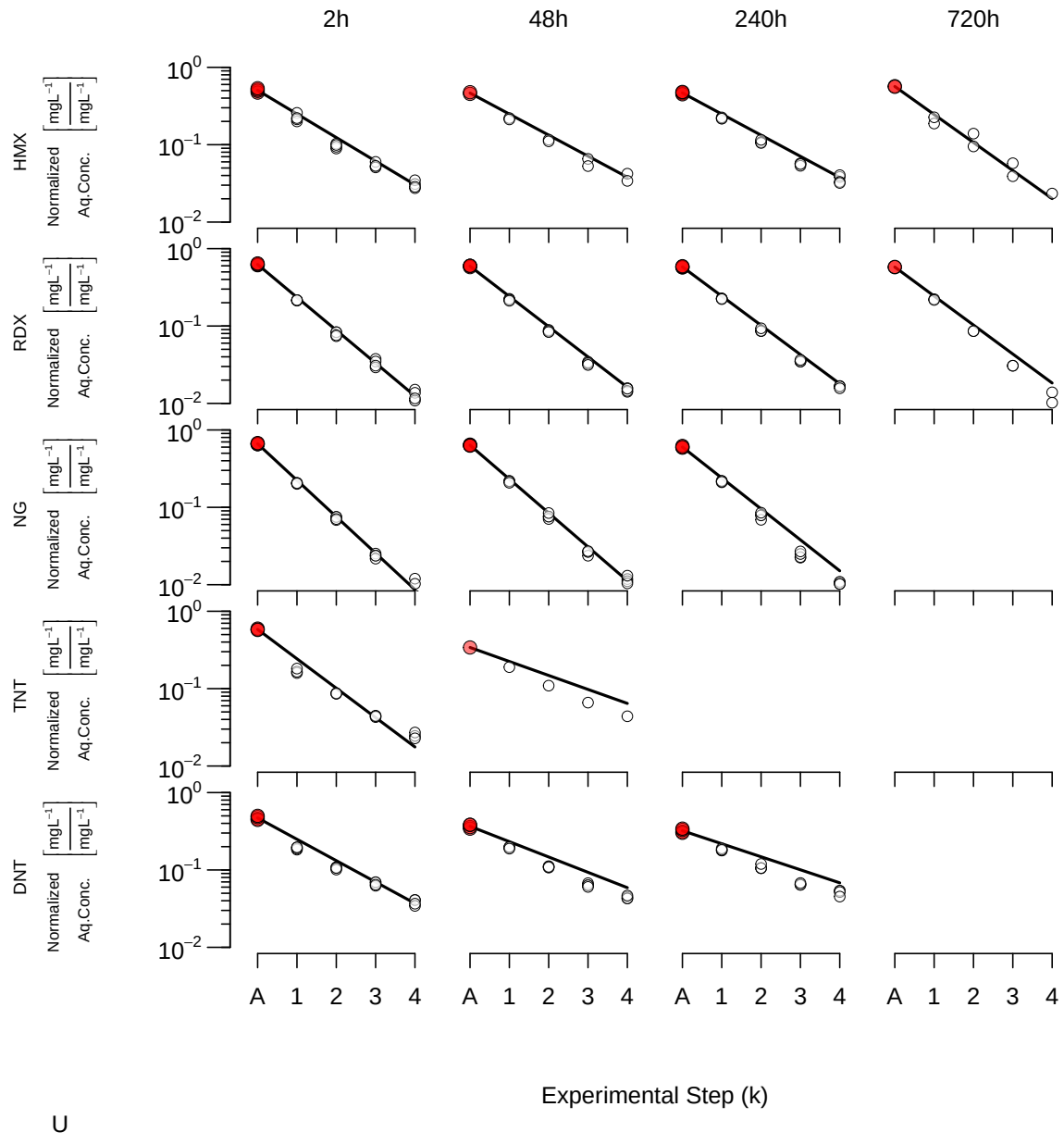
Figure A.2: Fit of reversible model (lines) to observed aqueous concentrations (points)


2h
48h
240h
720h
HMX
RDX
NG
TNT
DNT
Normalized Aq.Conc. [mgL⁻¹ / mgL⁻¹]
10^0
10^{-1}
10^{-2}
A 1 2 3 4
Experimental Step (k)

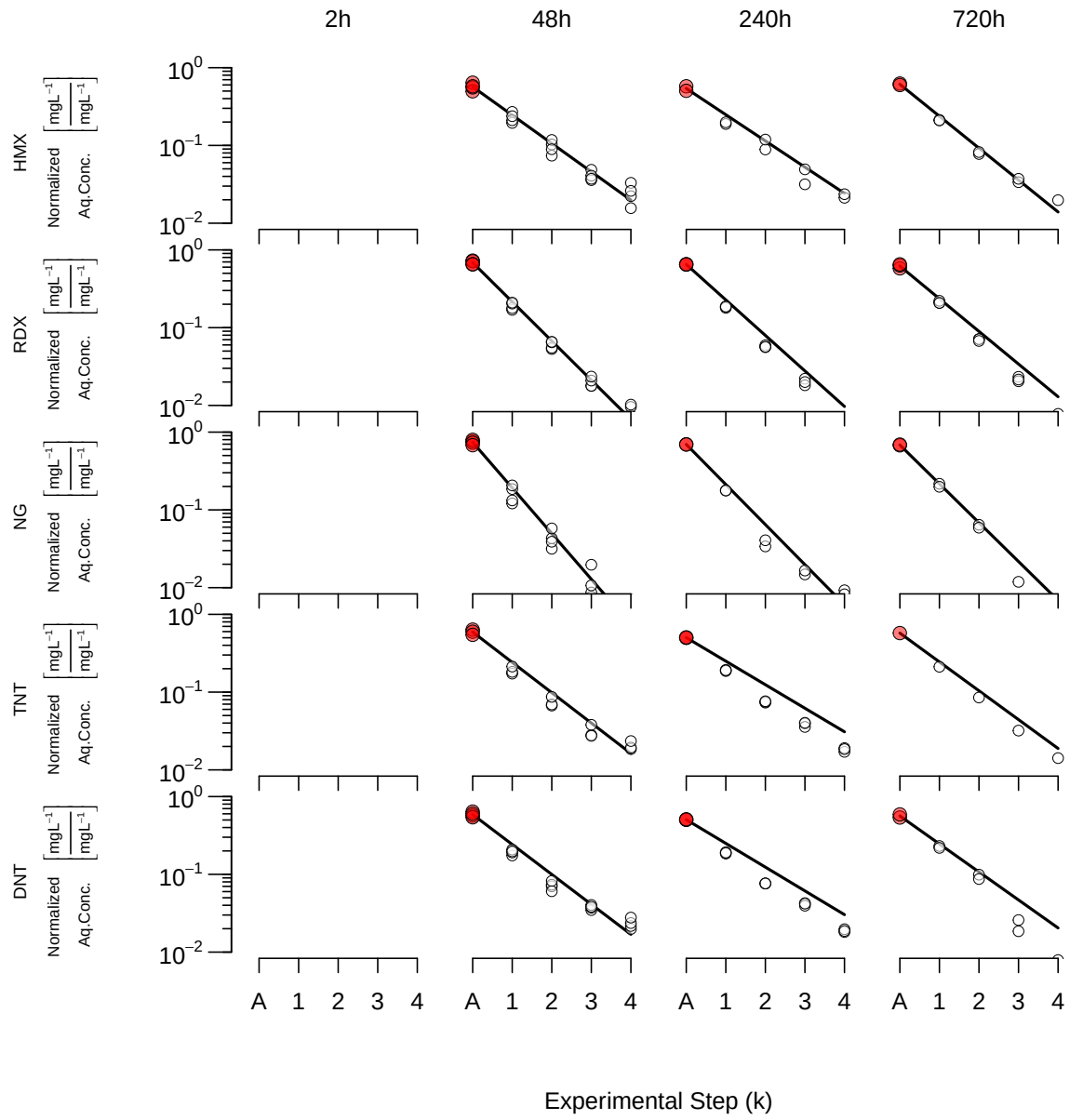
BT


2h
48h
240h
720h
HMX
RDX
NG
TNT
DNT
Normalized Aq.Conc. [mgL⁻¹ / mgL⁻¹]
10^0
10^{-1}
10^{-2}
A 1 2 3 4
Experimental Step (k)

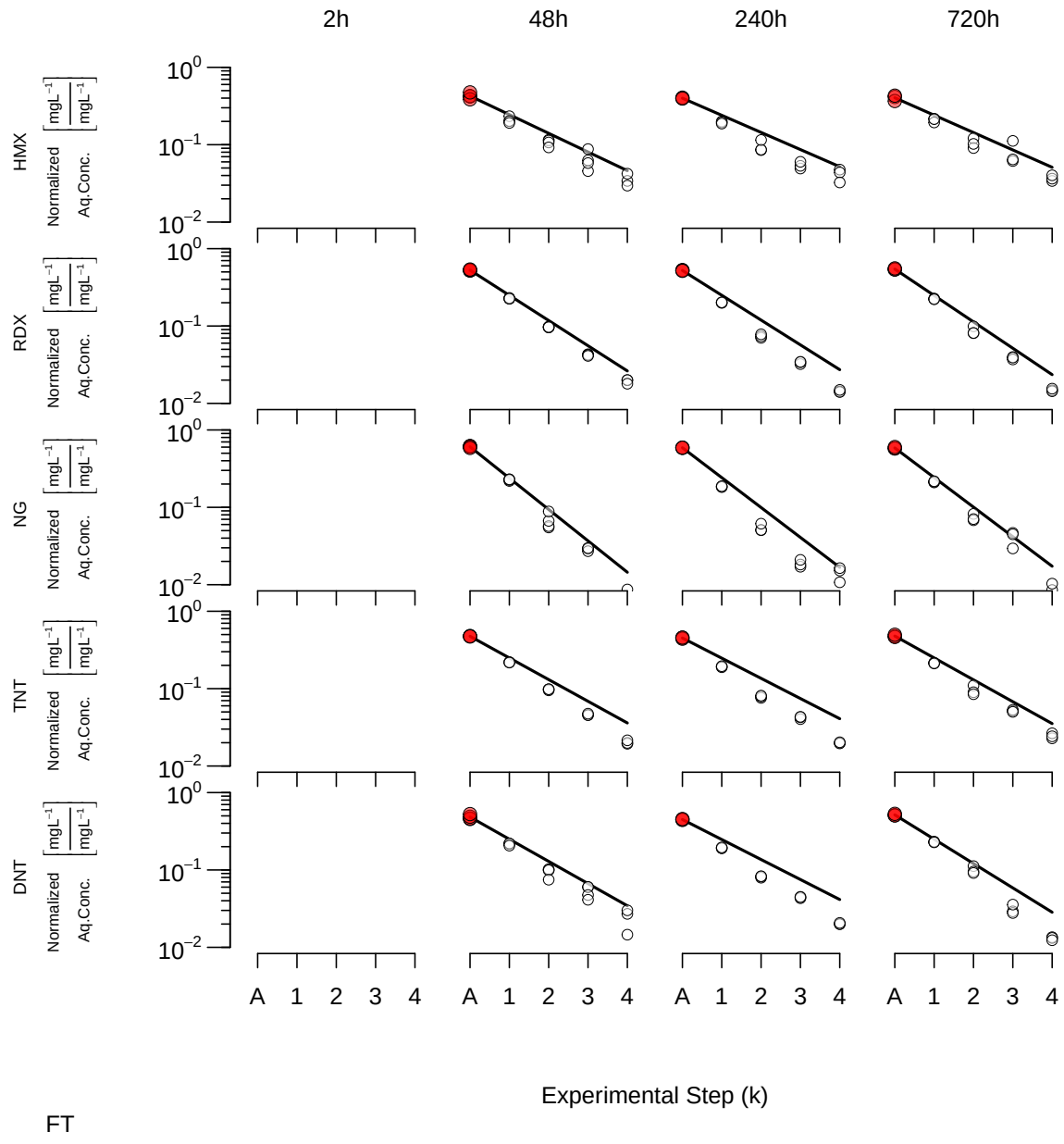
BA

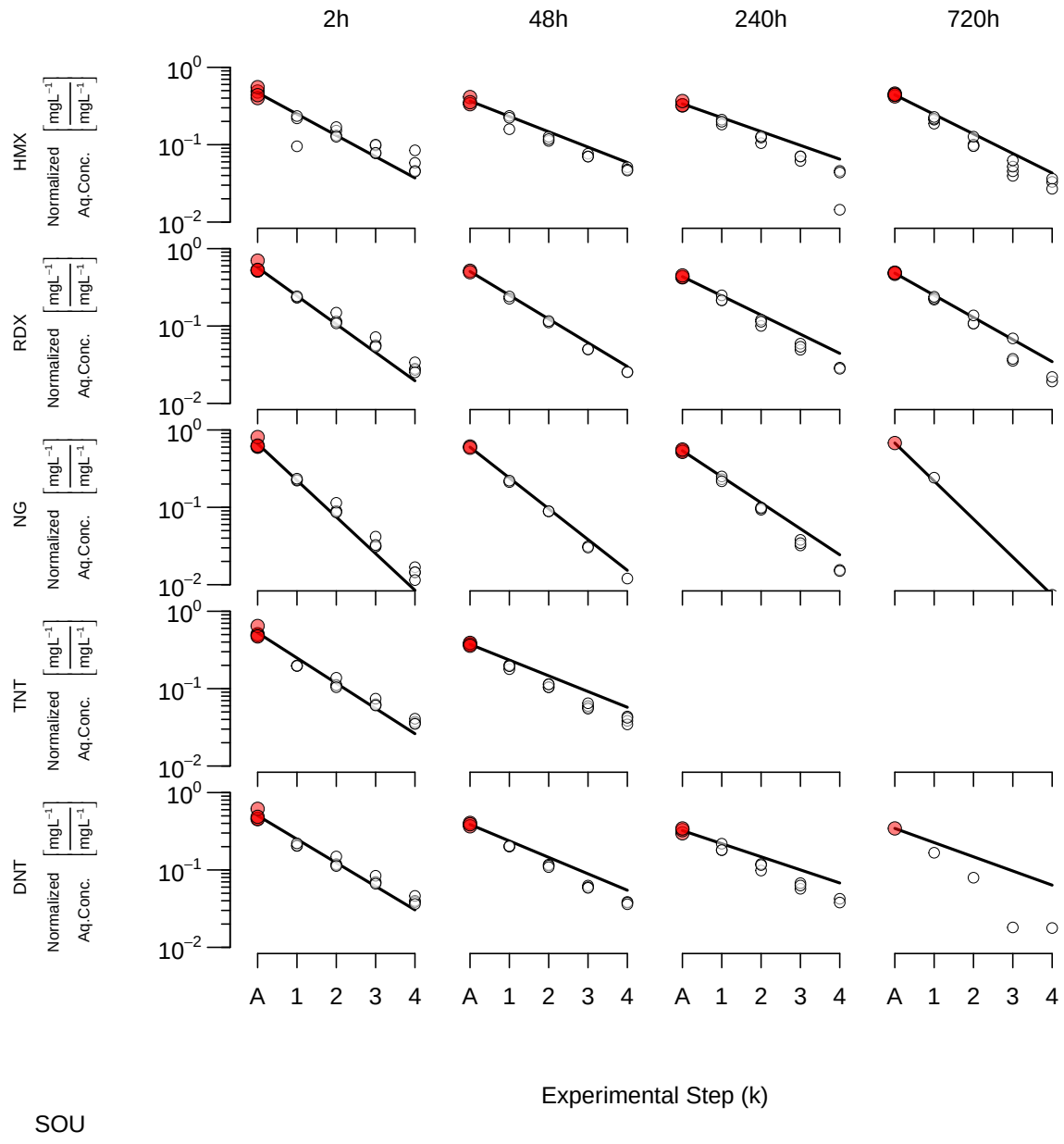

2h
48h
240h
720h
HMX
RDX
NG
TNT
DNT
Normalized Aq.Conc. [mgL⁻¹ / mgL⁻¹]
10^0
10^{-1}
10^{-2}
A 1 2 3 4
Experimental Step (k)

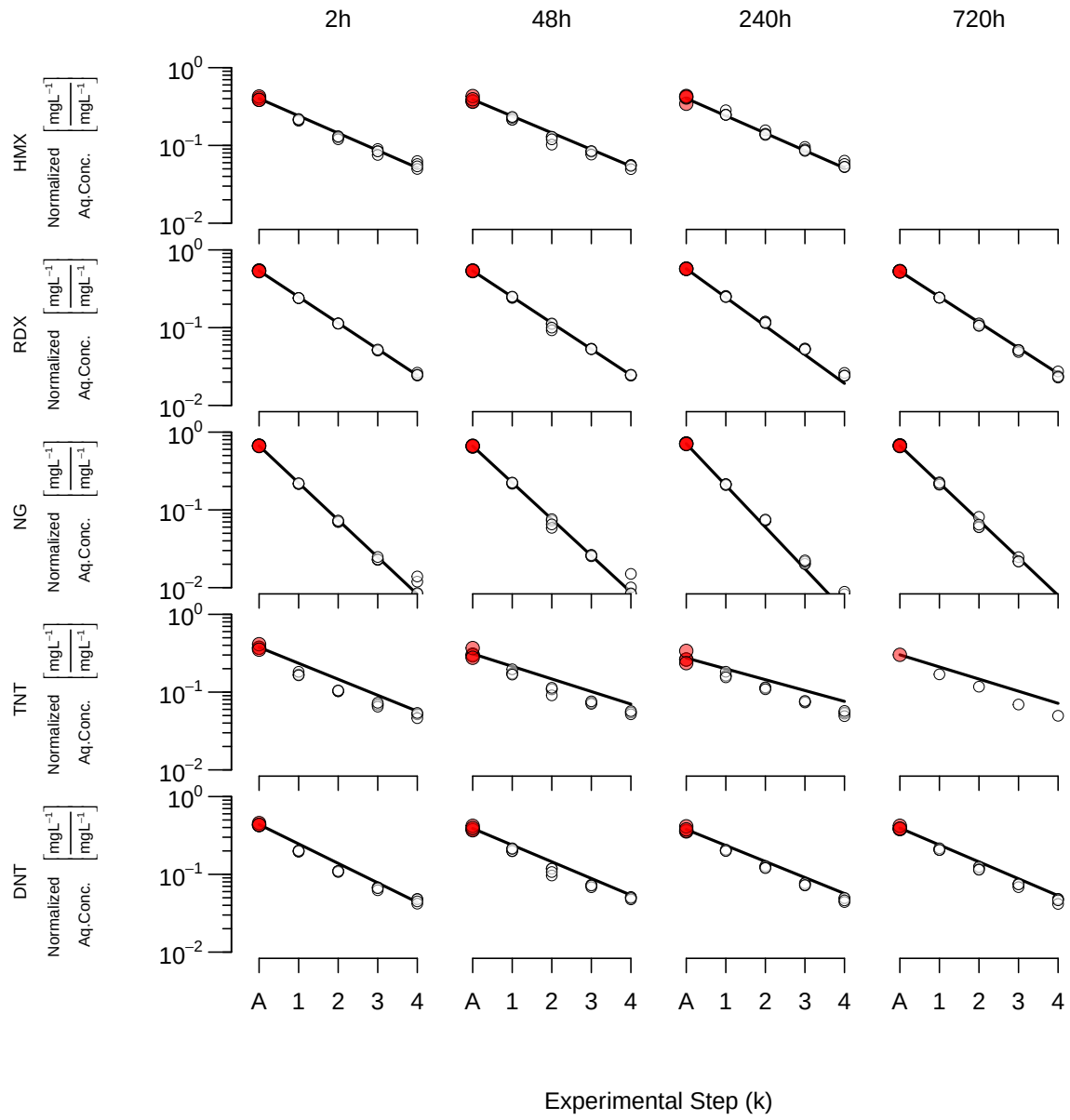
U


2h
48h
240h
720h
HMX
RDX
NG
TNT
DNT
Normalized Aq.Conc. [mgL⁻¹ / mgL⁻¹]
10^0
10^{-1}
10^{-2}
A 1 2 3 4
Experimental Step (k)

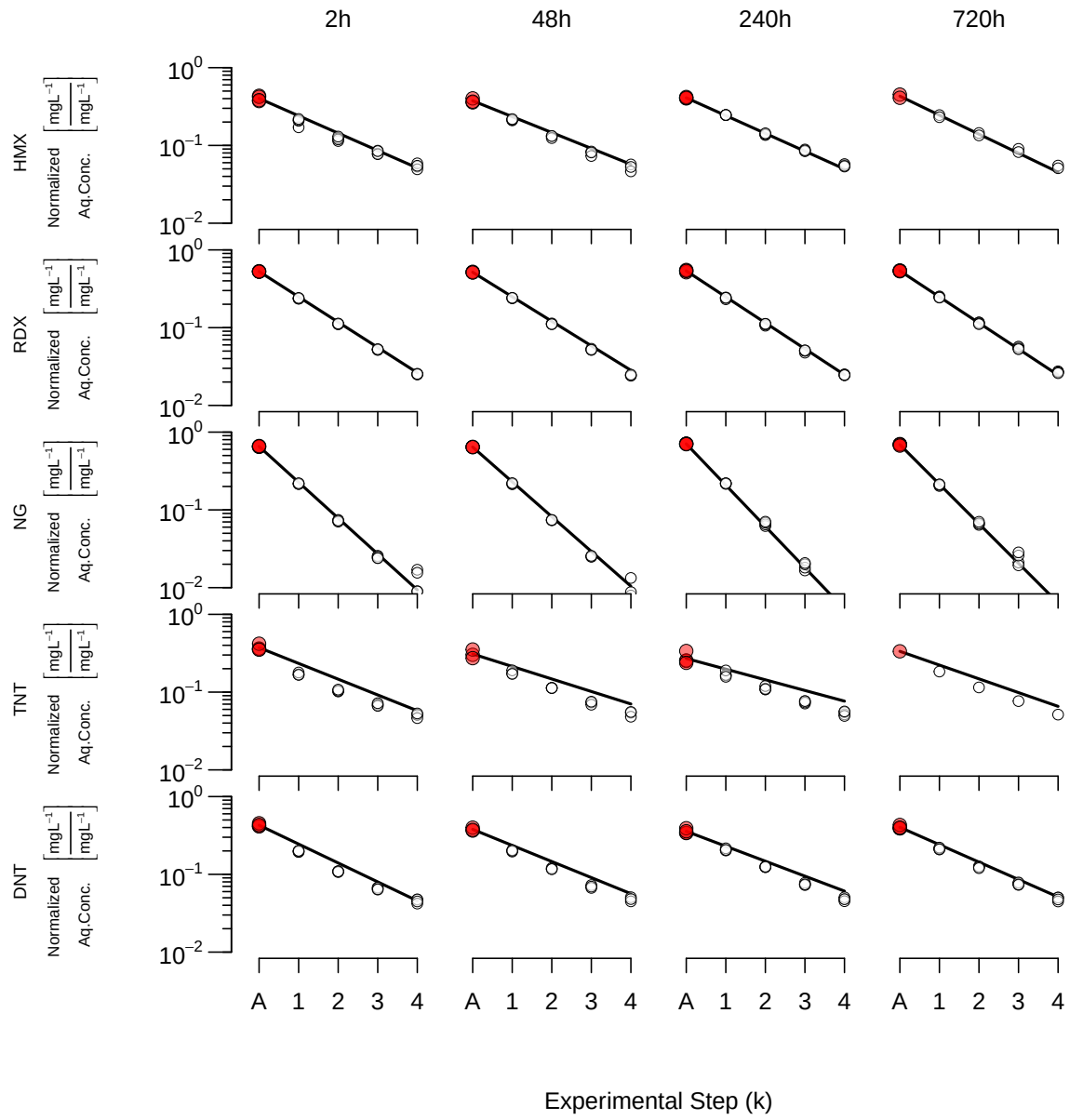
B


2h
48h
240h
720h
HMX
RDX
NG
TNT
DNT
Normalized Aq.Conc. [mgL⁻¹ / mgL⁻¹]
10^0
10^{-1}
10^{-2}
A 1 2 3 4
Experimental Step (k)
FT

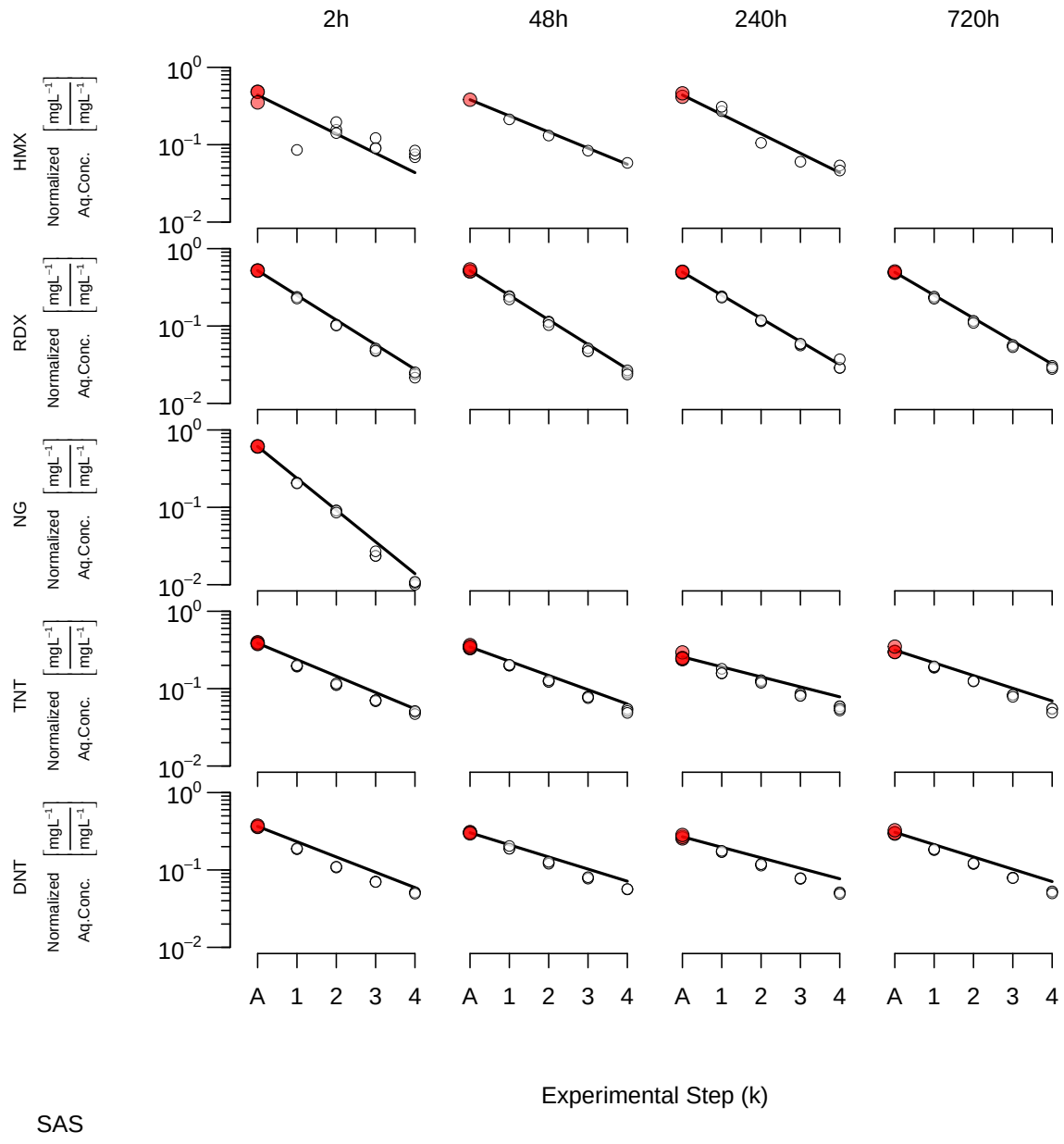

2h
48h
240h
720h
HMX
RDX
NG
TNT
DNT
Normalized Aq.Conc. [mgL⁻¹ / mgL⁻¹]
10^0
10^{-1}
10^{-2}
A 1 2 3 4
Experimental Step (k)
SOU


2h
48h
240h
720h
HMX
RDX
NG
TNT
DNT
Normalized Aq.Conc. [mgL⁻¹ / mgL⁻¹]
10^0
10^{-1}
10^{-2}
A 1 2 3 4
Experimental Step (k)

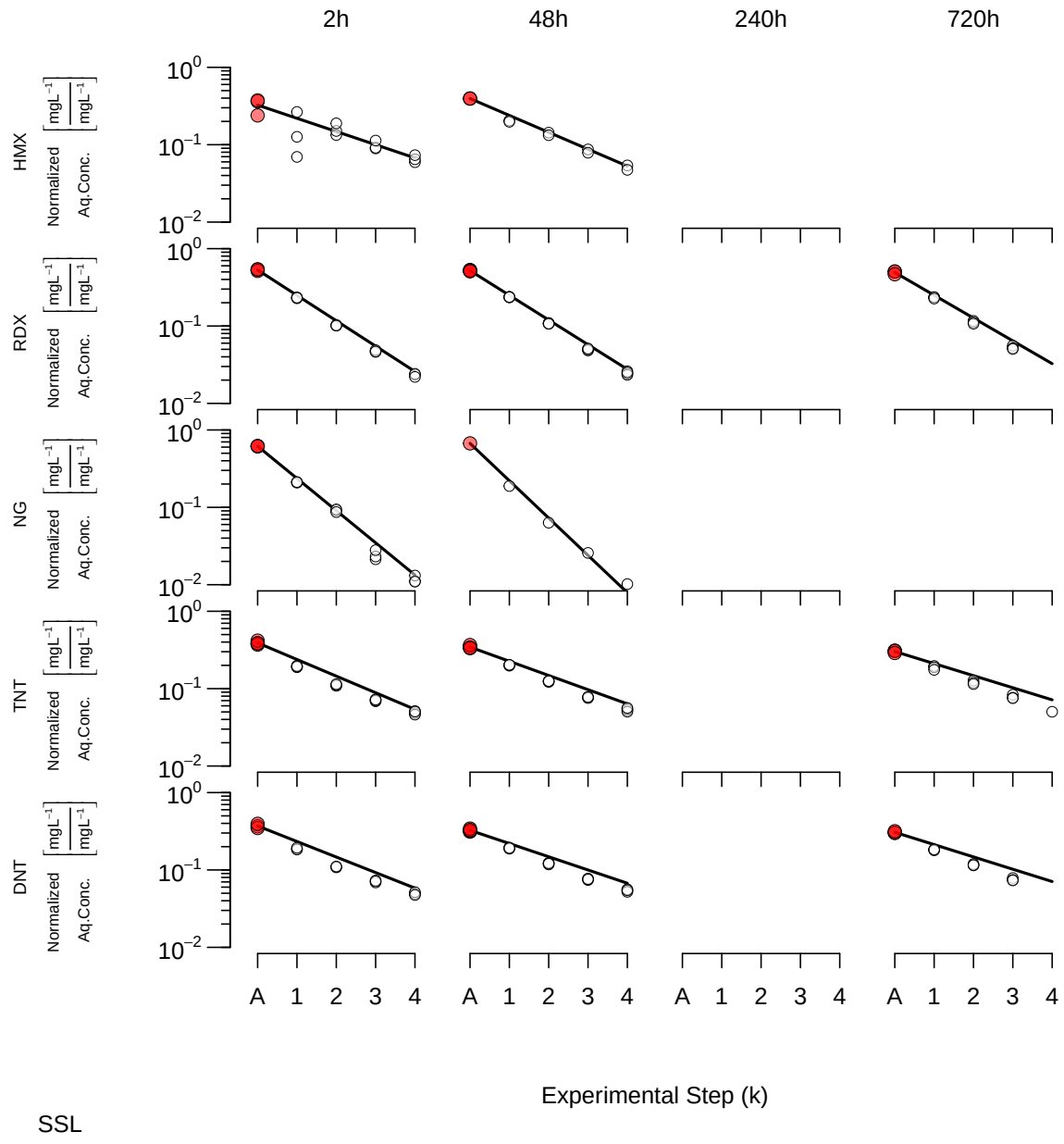
W1

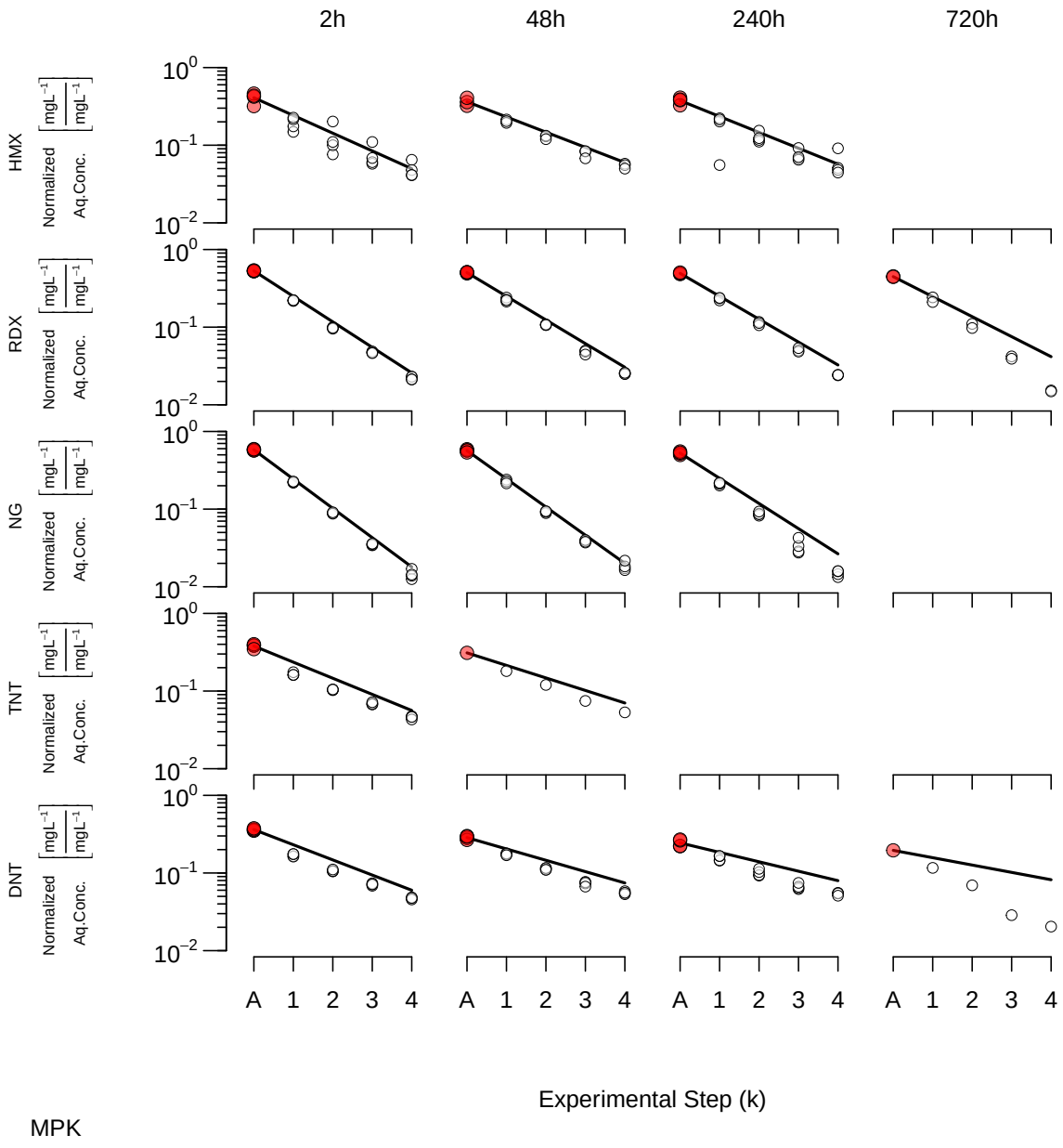

2h
48h
240h
720h
HMX
RDX
NG
TNT
DNT
Normalized Aq.Conc. [mgL⁻¹ / mgL⁻¹]
10^0
10^{-1}
10^{-2}
A 1 2 3 4
Experimental Step (k)

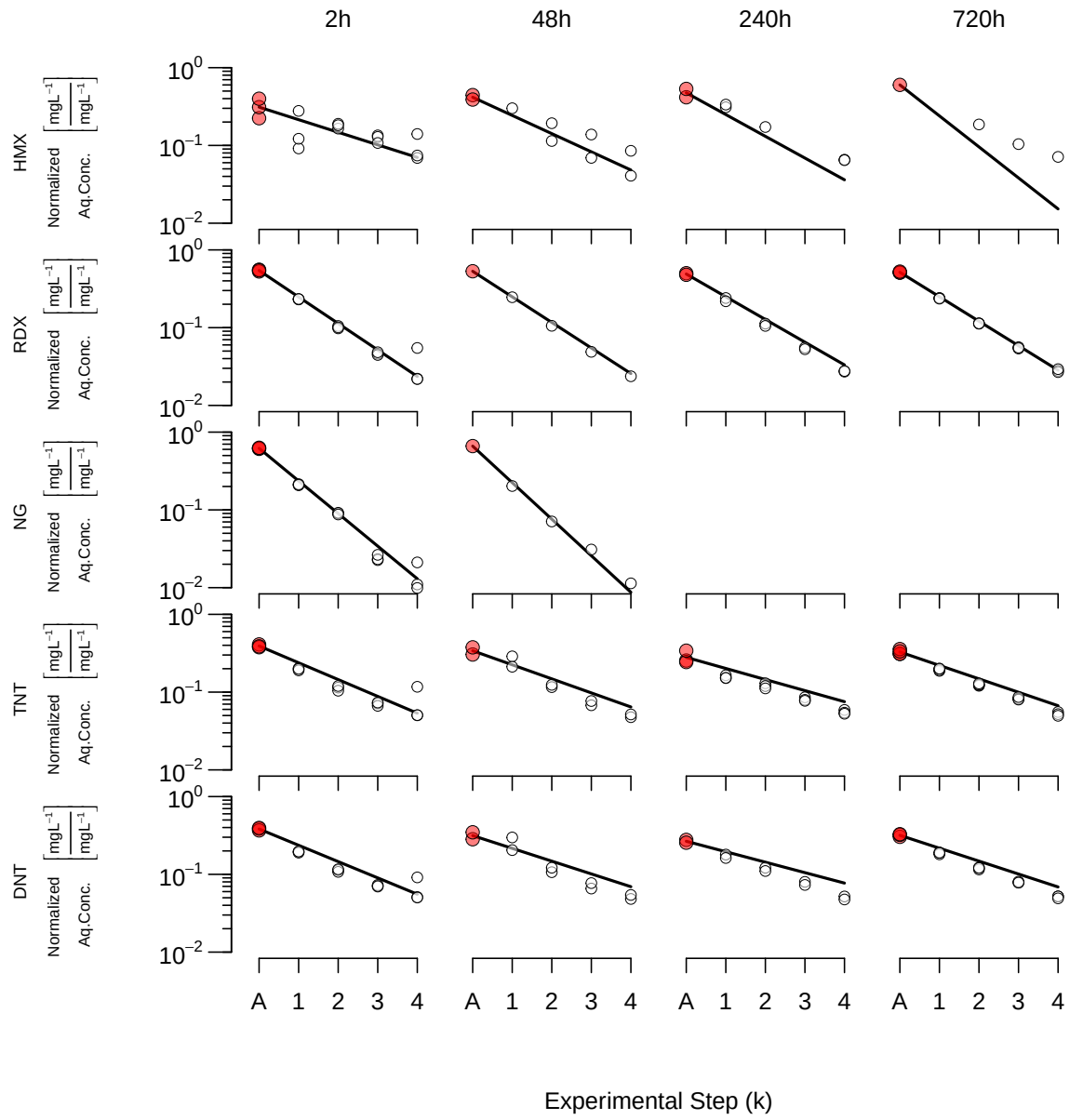
W2


2h
48h
240h
720h
HMX
RDX
NG
TNT
DNT
Normalized Aq.Conc. [mgL⁻¹ / mgL⁻¹]
10^0
10^{-1}
10^{-2}
A 1 2 3 4
Experimental Step (k)

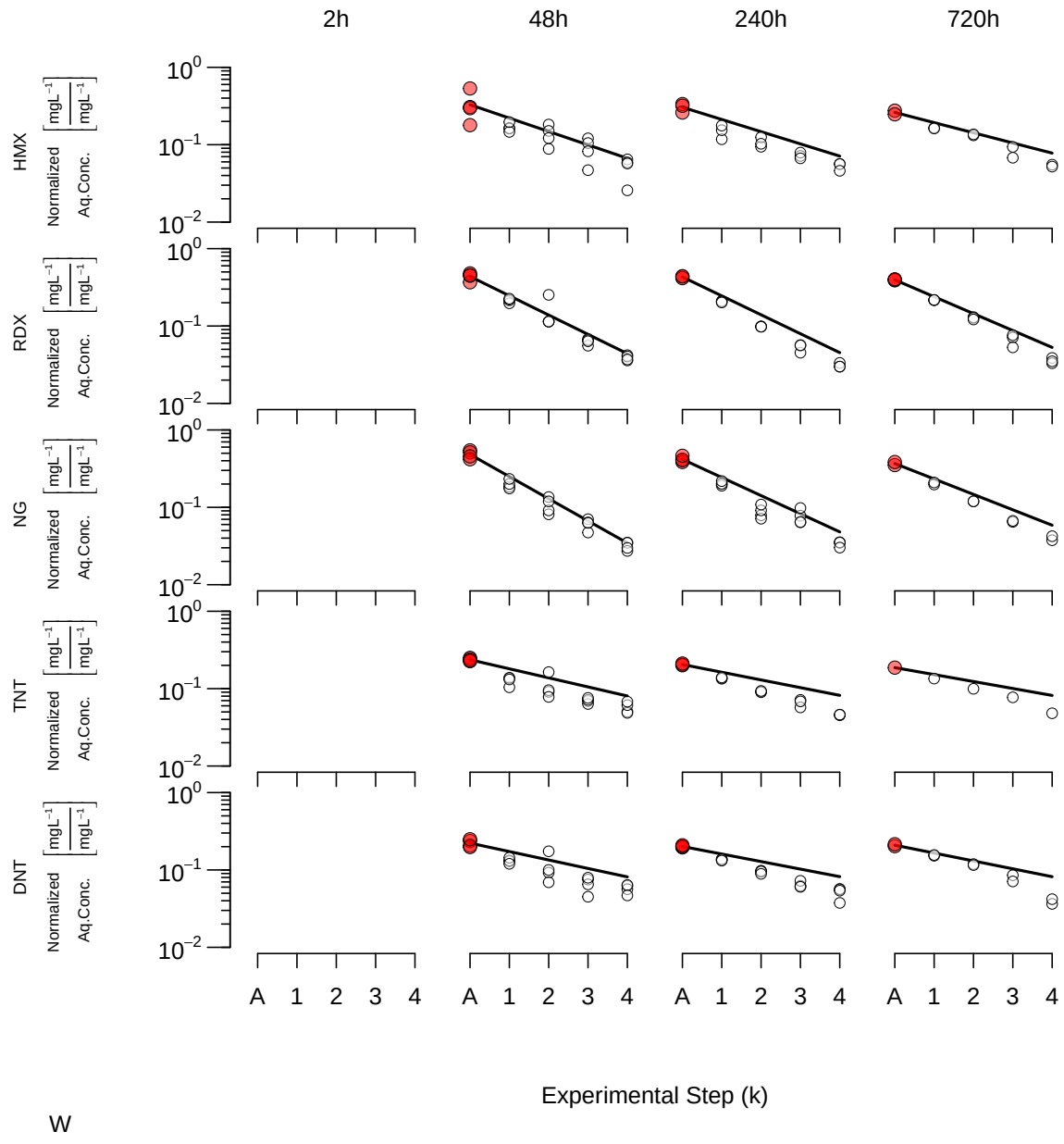
SAS


2h
48h
240h
720h
HMX
RDX
NG
TNT
DNT
Normalized Aq.Conc. [mgL⁻¹ / mgL⁻¹]
10^0
10^-1
10^-2
A 1 2 3 4
Experimental Step (k)
SSL

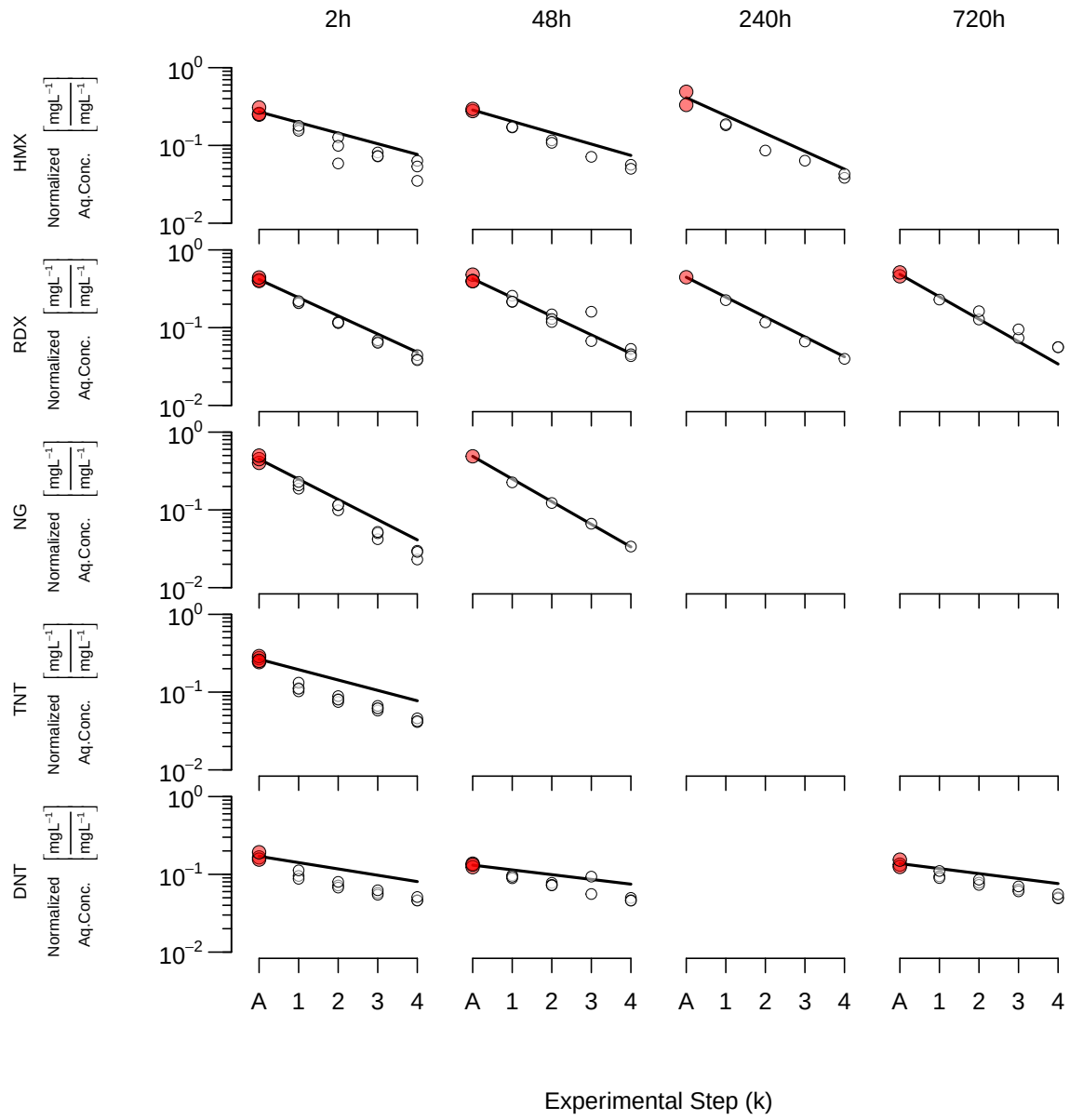

2h
48h
240h
720h
HMX
RDX
NG
TNT
DNT
Normalized Aq.Conc. [mgL⁻¹ / mgL⁻¹]
10^0
10^{-1}
10^{-2}
A 1 2 3 4
Experimental Step (k)
MPK


2h
48h
240h
720h
HMX
RDX
NG
TNT
DNT
Normalized Aq.Conc. [mgL⁻¹ / mgL⁻¹]
10^0
10^{-1}
10^{-2}
A 1 2 3 4
Experimental Step (k)

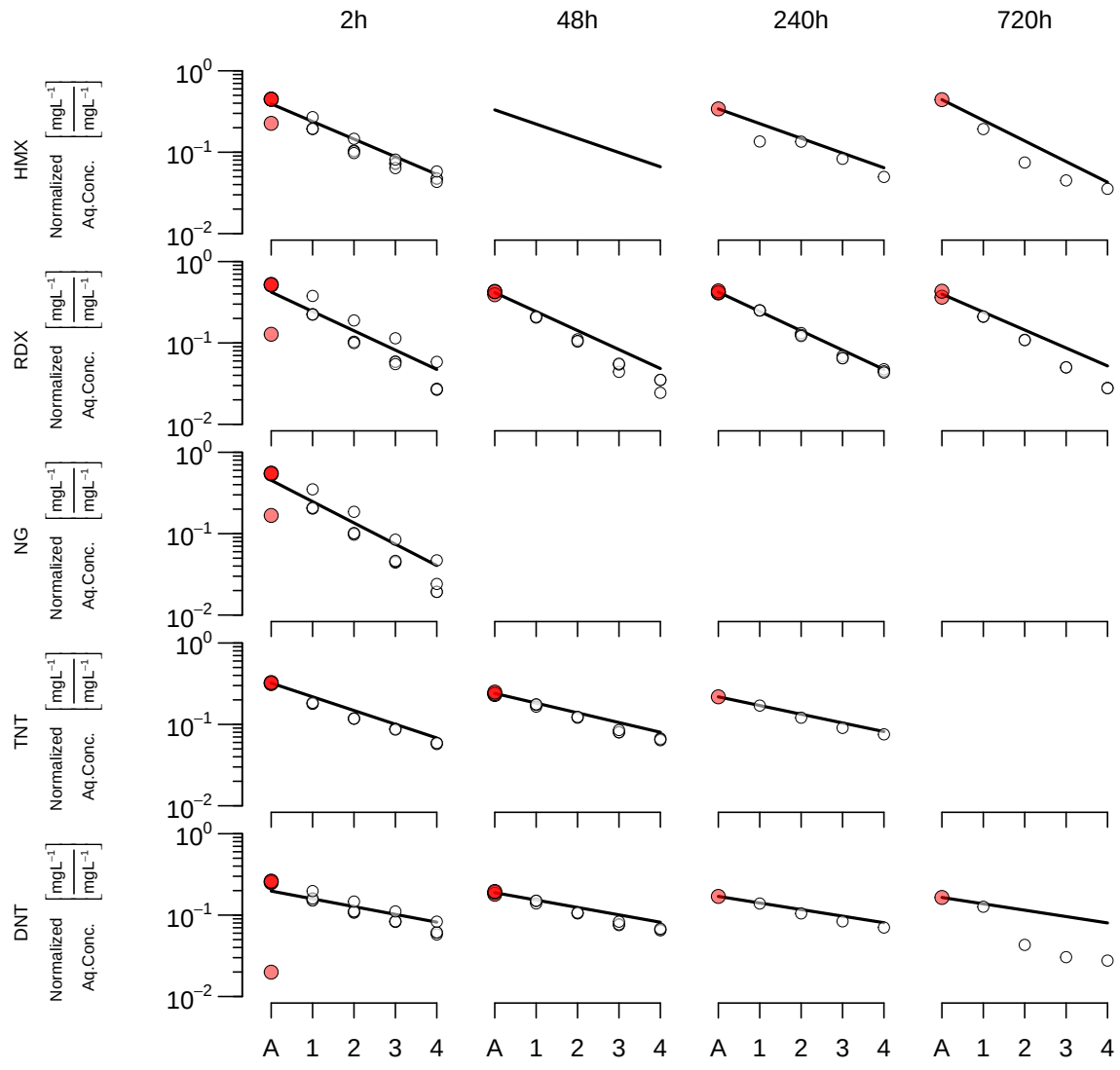
S2


2h
48h
240h
720h
HMX
RDX
NG
TNT
DNT
Normalized Aq.Conc. [mgL⁻¹ / mgL⁻¹]
10^0
10^{-1}
10^{-2}
A 1 2 3 4
Experimental Step (k)

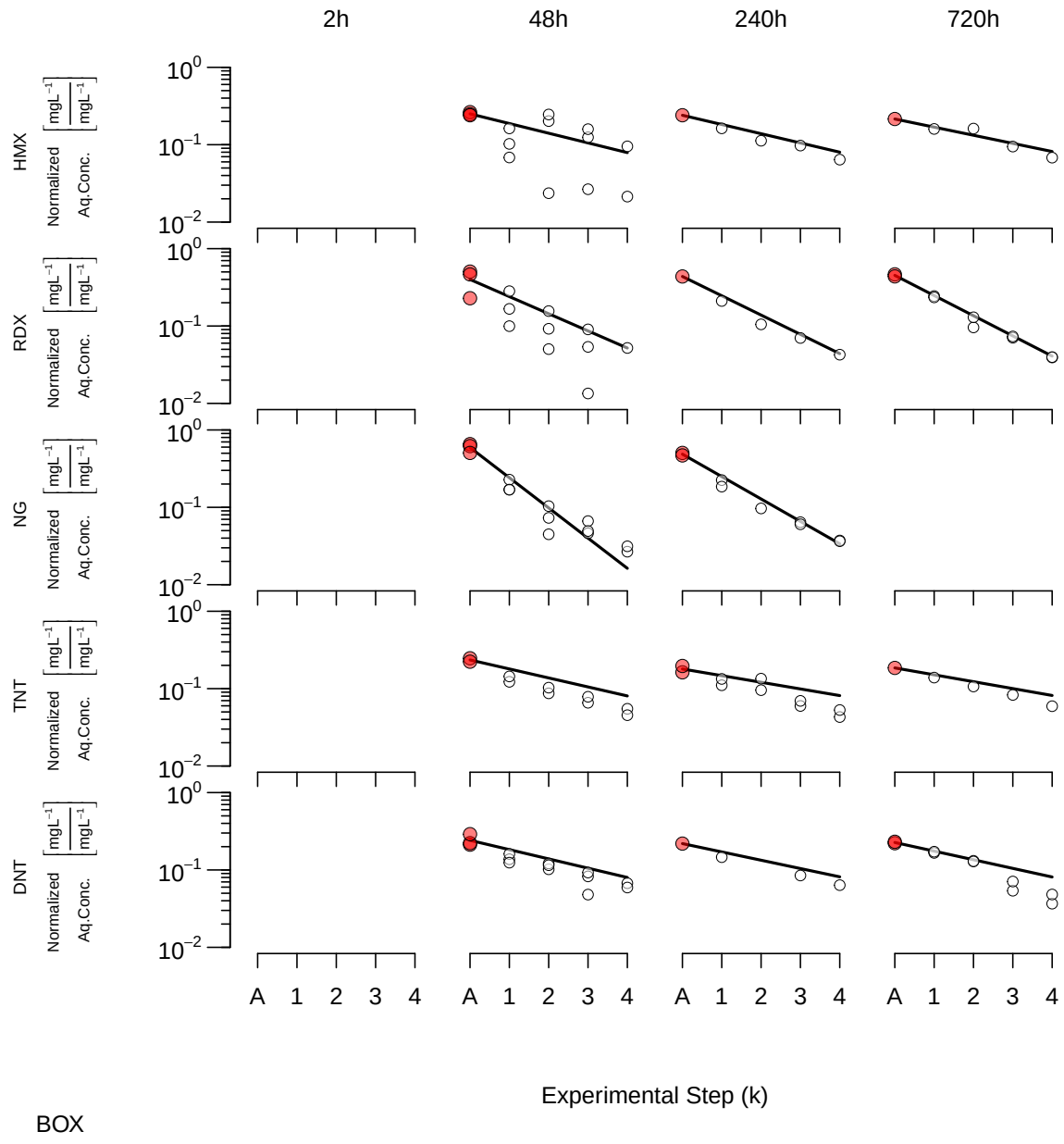
W

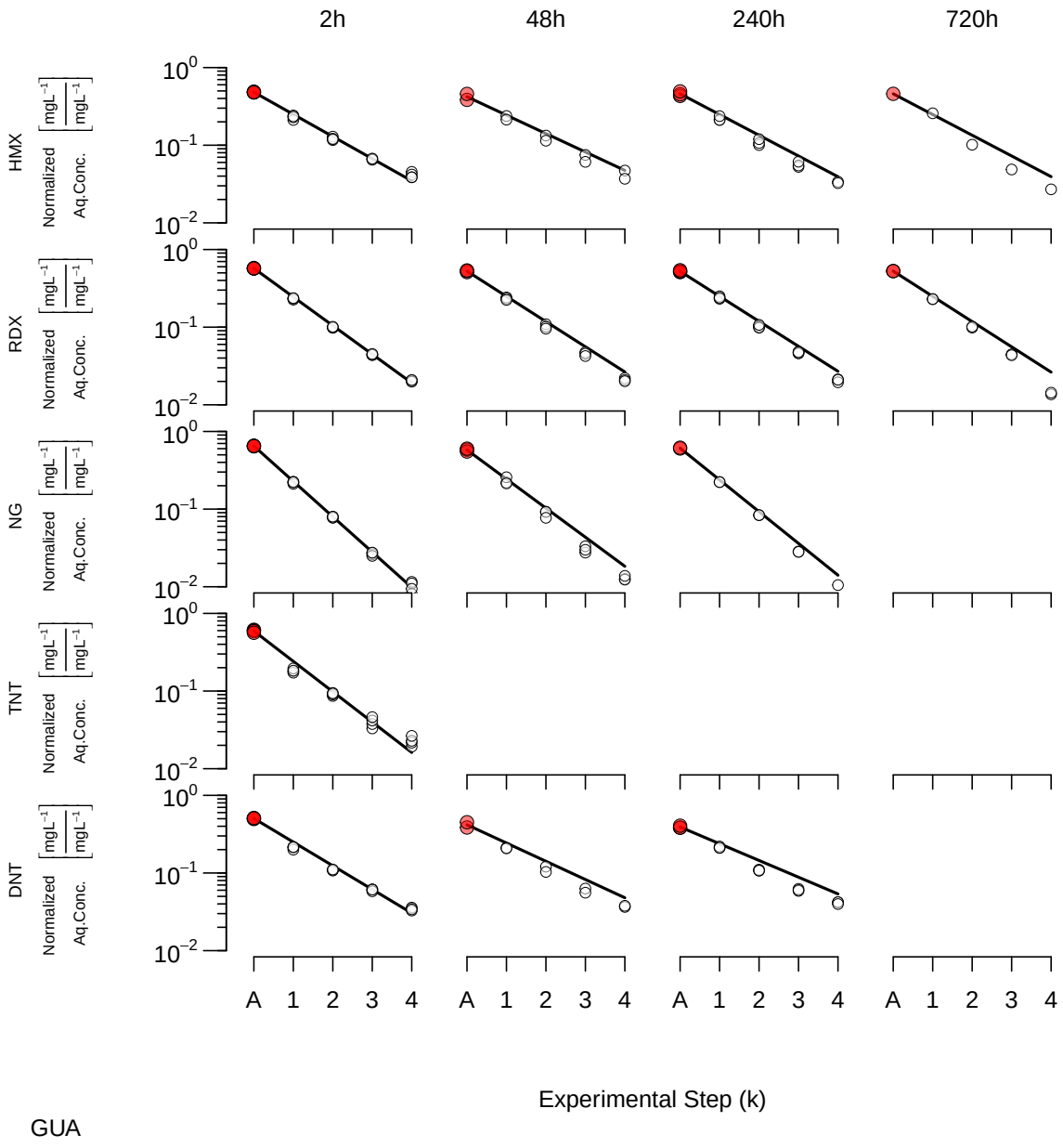

2h
48h
240h
720h
HMX
RDX
NG
TNT
DNT
Normalized Aq.Conc. [mgL⁻¹ / mgL⁻¹]
10^0
10^{-1}
10^{-2}
A 1 2 3 4
Experimental Step (k)

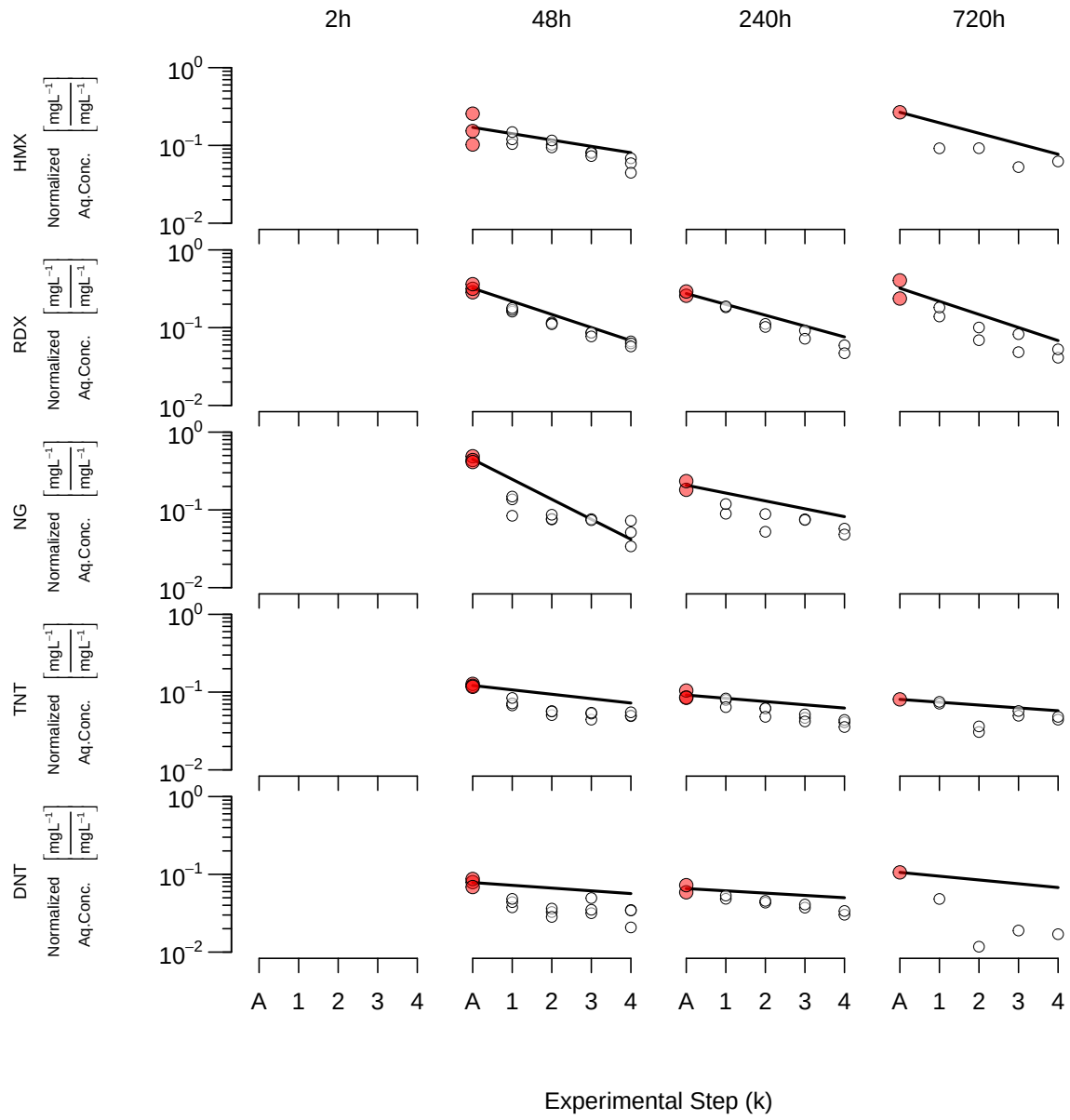
AM

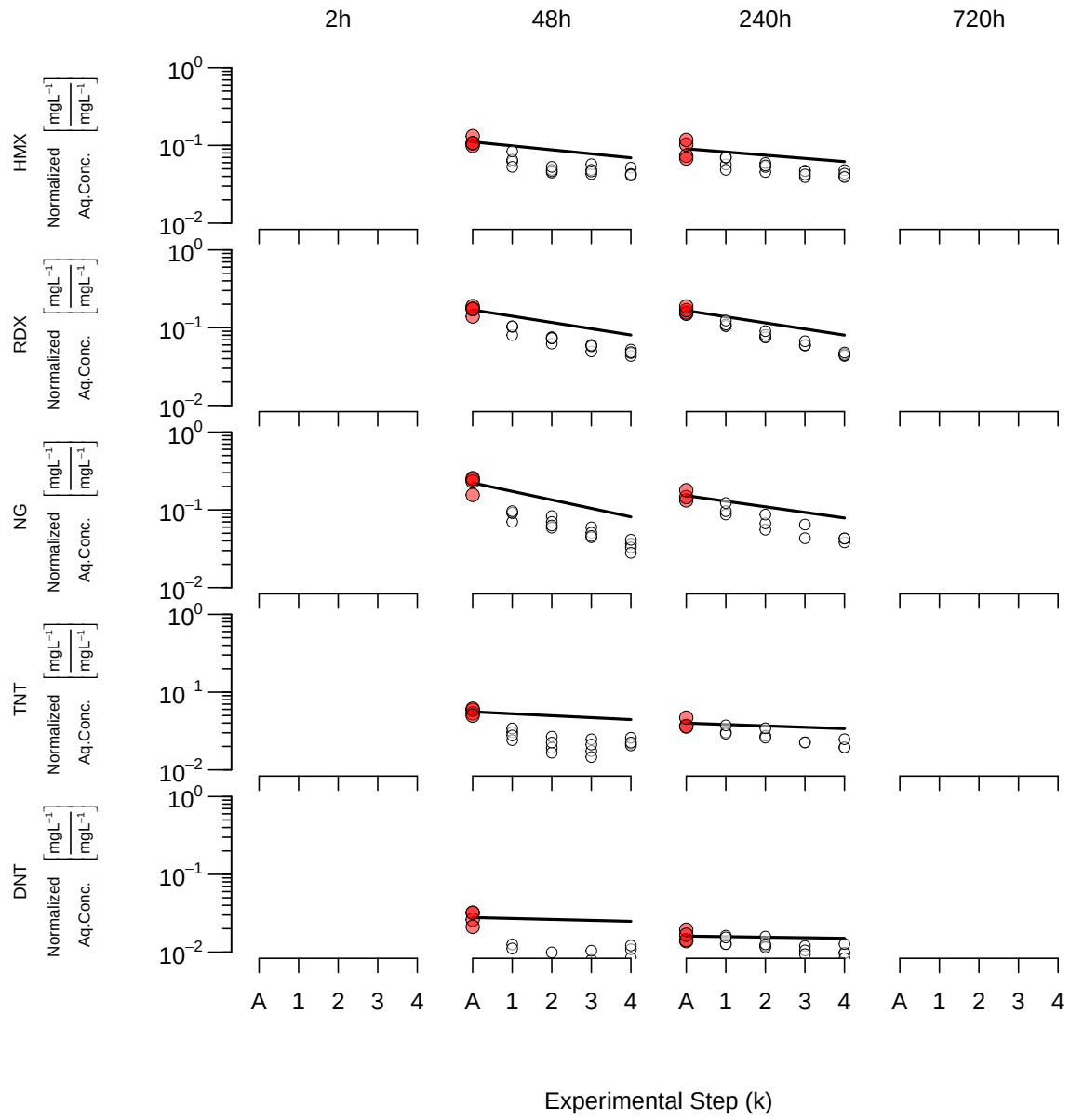

2h
48h
240h
720h
HMX
RDX
NG
TNT
DNT
Normalized Aq.Conc. [mgL⁻¹ / mgL⁻¹]
10^0
10^{-1}
10^{-2}
A 1 2 3 4
Experimental Step (k)

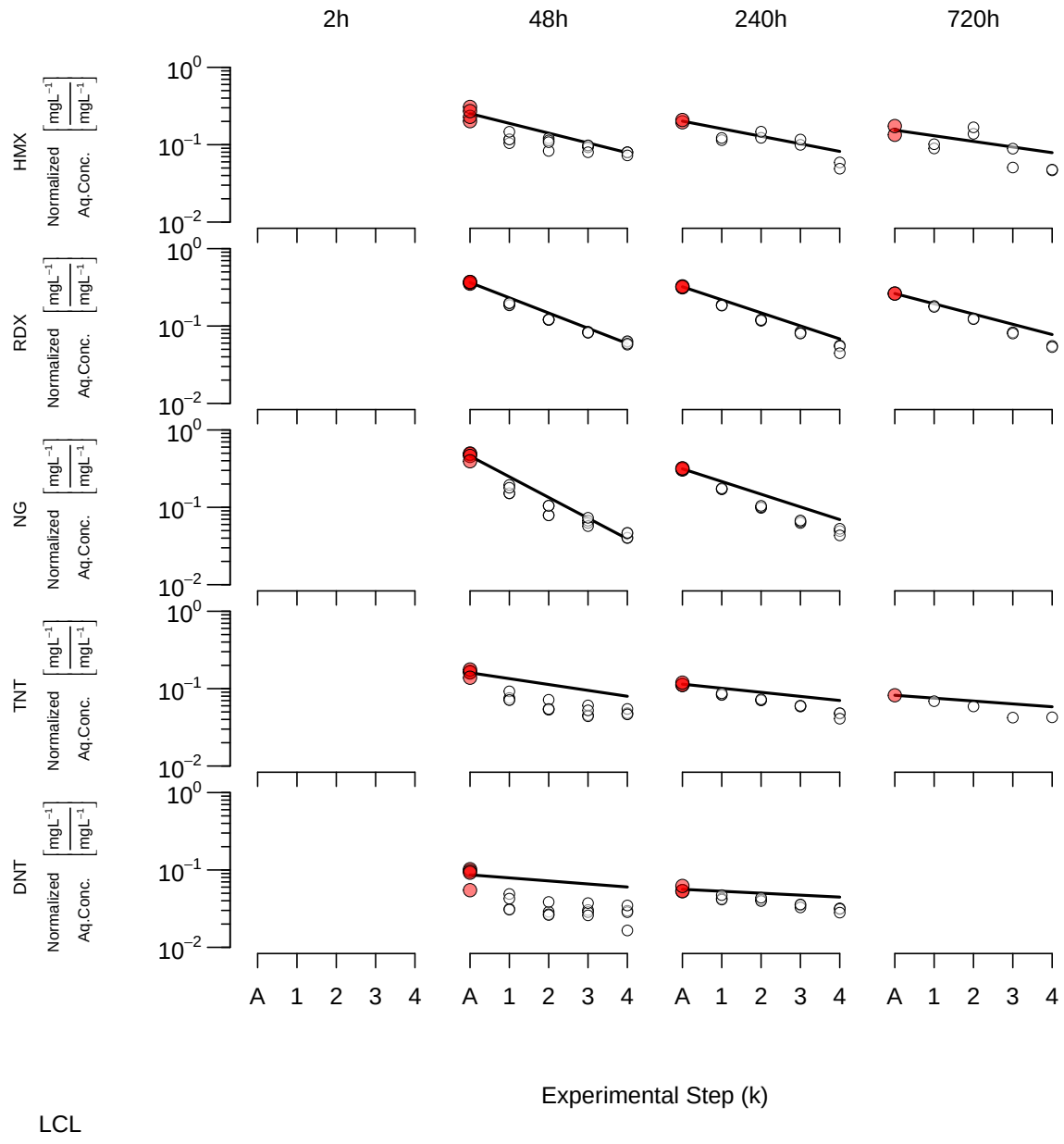
H

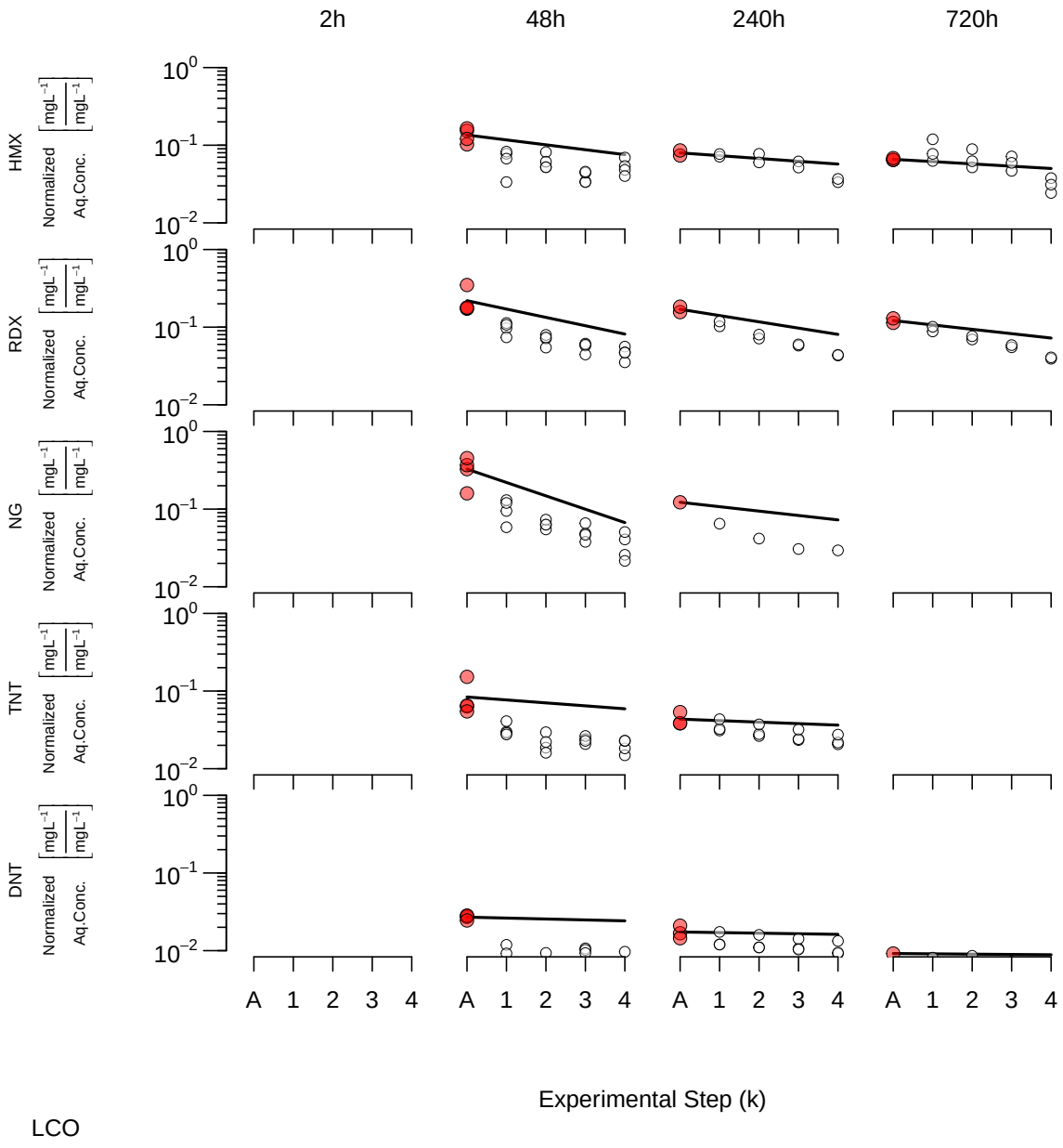

2h
48h
240h
720h
HMX
RDX
NG
TNT
DNT
Normalized Aq.Conc. [mgL⁻¹ / mgL⁻¹]
10^0
10^{-1}
10^{-2}
A 1 2 3 4
Experimental Step (k)
BOX

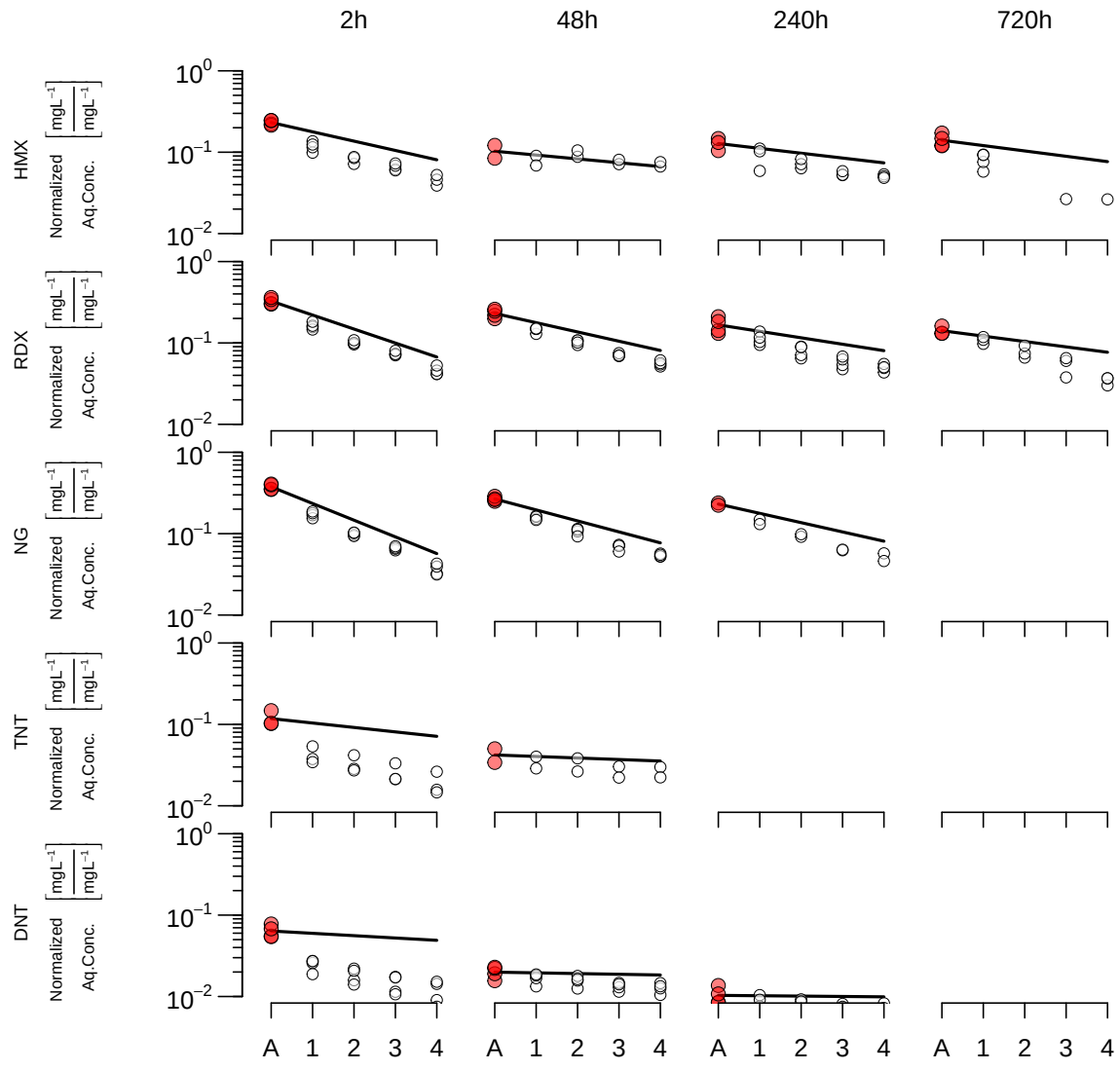

2h
48h
240h
720h
HMX
RDX
NG
TNT
DNT
Normalized Aq.Conc. [mgL⁻¹ / mgL⁻¹]
10^0
10^{-1}
10^{-2}
A 1 2 3 4
Experimental Step (k)
GUA


2h
48h
240h
720h
HMX
RDX
NG
TNT
DNT
Normalized Aq.Conc. [mgL⁻¹ / mgL⁻¹]
10^0
10^{-1}
10^{-2}
A 1 2 3 4
Experimental Step (k)
PO

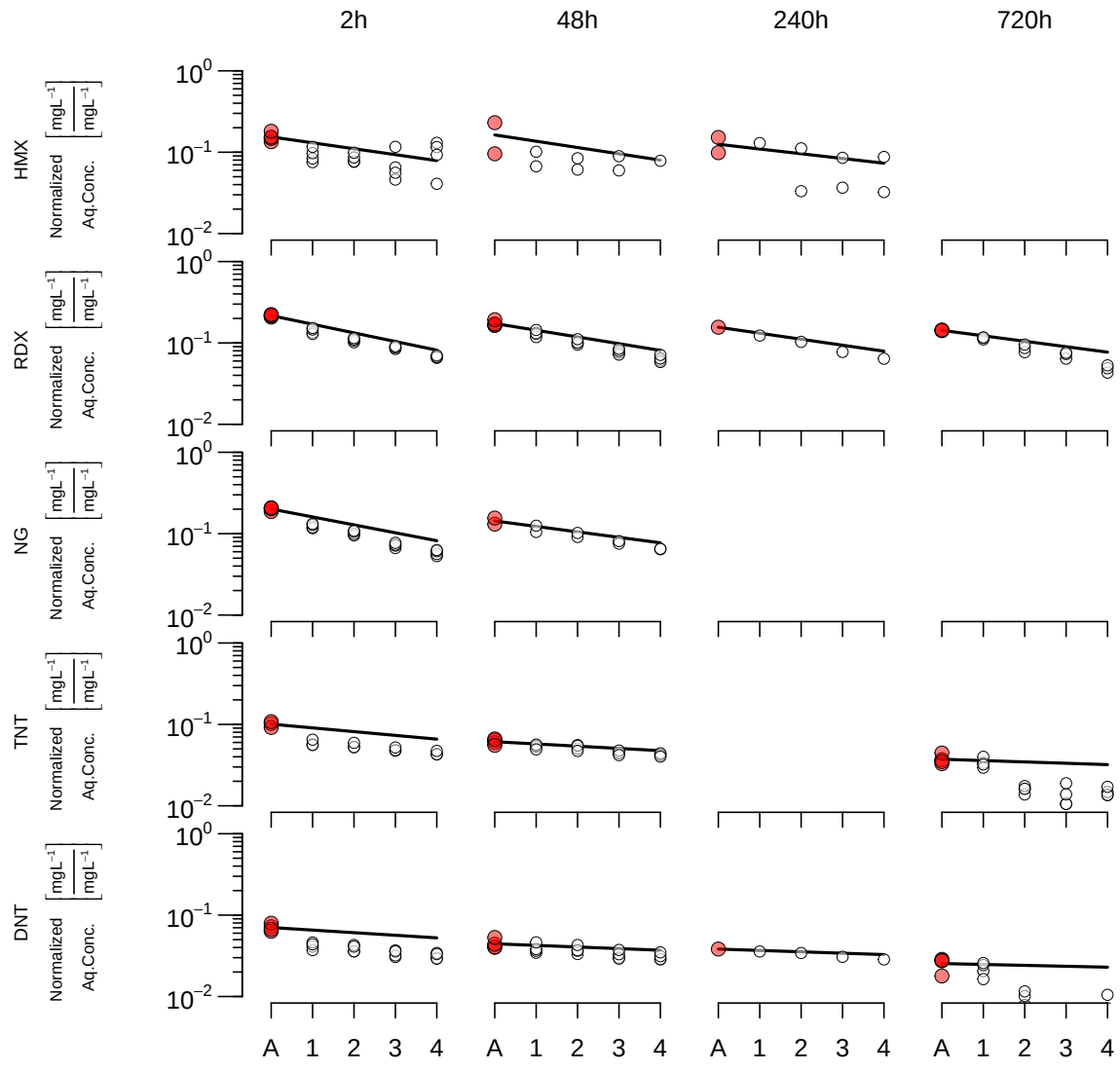

2h
48h
240h
720h
HMX
RDX
NG
TNT
DNT
Normalized Aq.Conc. [mgL⁻¹ / mgL⁻¹]
10^0
10^{-1}
10^{-2}
A 1 2 3 4
Experimental Step (k)
BU


2h
48h
240h
720h
HMX
RDX
NG
TNT
DNT
Normalized Aq.Conc. [mgL⁻¹ / mgL⁻¹]
10^0
10^{-1}
10^{-2}
A 1 2 3 4
Experimental Step (k)
LCL

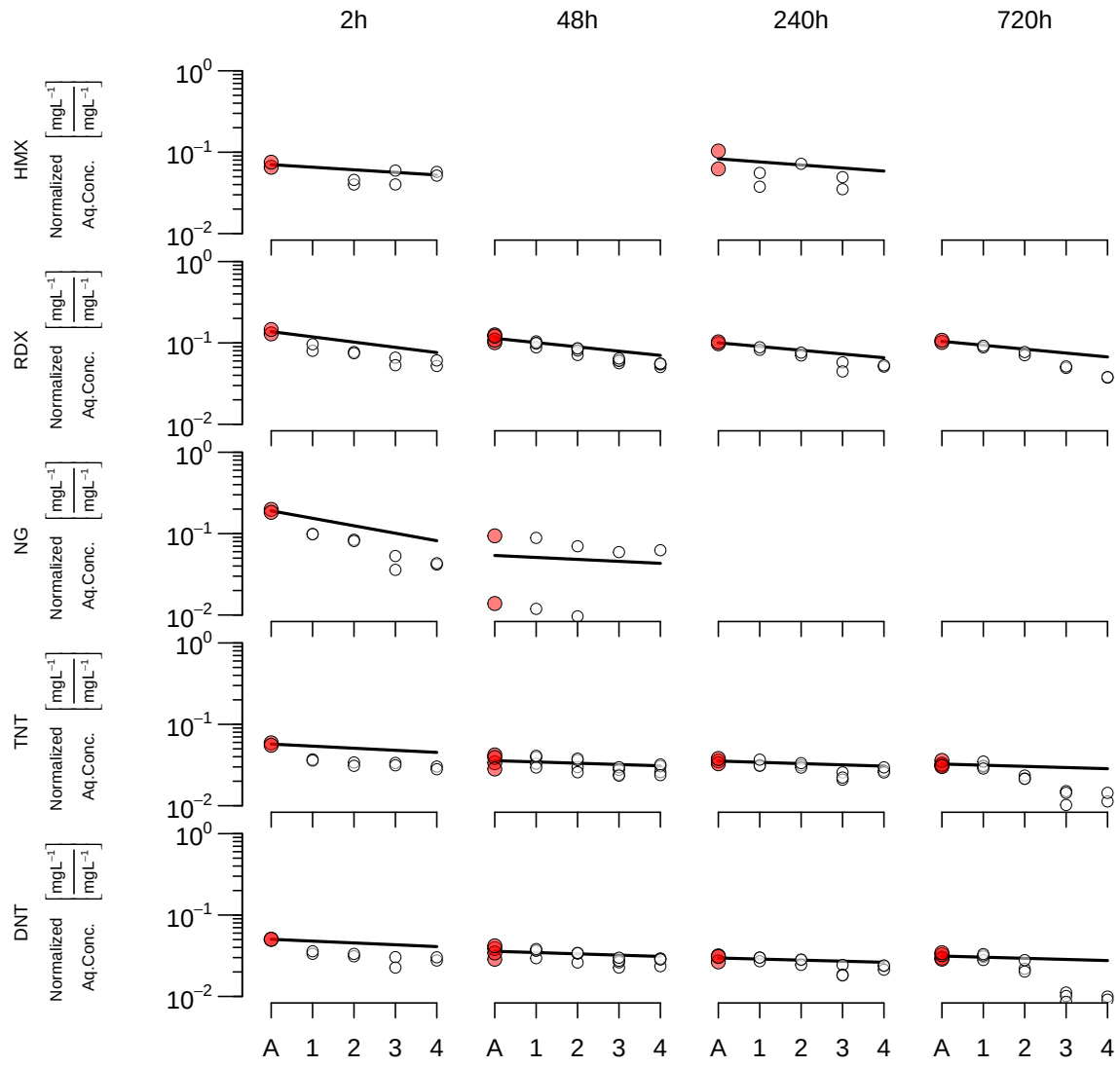

2h
48h
240h
720h
HMX
RDX
NG
TNT
DNT
Normalized Aq.Conc. [mgL⁻¹ / mgL⁻¹]
10^0
10^{-1}
10^{-2}
A 1 2 3 4
Experimental Step (k)
LCO


2h
48h
240h
720h
HMX
RDX
NG
TNT
DNT
Normalized Aq.Conc. [mgL⁻¹ / mgL⁻¹]
10^0
10^{-1}
10^{-2}
A 1 2 3 4
Experimental Step (k)

J


2h
48h
240h
720h
HMX
RDX
NG
TNT
DNT
Normalized Aq.Conc. [mgL⁻¹ / mgL⁻¹]
10^0
10^{-1}
10^{-2}
A 1 2 3 4
Experimental Step (k)

R


2h
48h
240h
720h
HMX
RDX
NG
TNT
DNT
Normalized Aq.Conc. [mgL⁻¹ / mgL⁻¹]
10^0
10^-1
10^-2
A 1 2 3 4
Experimental Step (k)
Z

A.2.5 Reversible model additional analysis

To better understand the shortcomings of the reversible model, RMSE were calculated for each sorbent and each munition using Eq 2.13 (Figure A.3A). The RMSE for all MC are < 0.2 for the majority of low f_{OC} sorbents ($f_{OC} < 0.02$), but there was a significant increase in RMSE for higher f_{OC} sorbents. This increase is especially evident for NG, TNT and DNT munitions. In addition, RMSE were determined for each adsorption contact time and each munition, Figure A.3B. There appears to be an increase in RMSE as adsorption time increases. To more accurately describe the observed partitioning, the data are analyzed next using the reversible resistant model.

The adsorption partition coefficient was analyzed by using a multilinear model [**?**]. The multilinear model decomposes a partition coefficient into multi-site partitioning to the sorbent matrix using sorbent specific partition coefficients. In this analysis, the sorbent properties were organic carbon (OC) content and clay sized particle fractions:

$$K_P(i,j) = f_{OC}(i)K_{OC}(j) + f_{clay}(i)K_{clay}(j) \tag{A.11}$$

where $f_{OC}(i)$ is the OC mass fraction of sorbent i $[g\ OC/g\ sorbent]$, $K_{OC}(j)$ is the partition coefficient for MC j binding to OC $[L/kg\ OC]$, $f_{clay}(i)$ is the clay sized particle mass fraction of sorbent i $[g\ clay/g\ sorbent]$, and $K_{clay}(j)$ is the partition coefficient for MC j binding to the clay sized particles $[L/kg\ clay]$. It has been previously observed by Gonzalez that using these two sites is sufficient to accurately model the adsorption partition coefficient.

The multilinear model parameters were estimated by minimizing the RMSE, Eq 2.13, between RR estimated K_P and multilinear regression predicted K_P using R and the *nls* package [**?**]. Figure A.4 shows the estimated partition coefficients for each MC (rows) and each adsorption contact time (columns) plotted against f_{OC} on log-log axes. The partition coefficients are shown as points with error bars of one standard error. The two reference sorbents are shown as squares. The multilinear model is shown as the solid red line. Sorbent specific partition coefficients K_{OC} and K_{clay} are shown in Tables 2.2 and 2.3. To evaluate the contribution of clay sized particle sorption with only a single sorption site, OC:

$$K_P(i,j) = f_{OC}(i)K_{OC}(j) \tag{A.12}$$

is shown as the dashed red line in Figure A.4.

The predicted and estimated partition coefficients are in close agreement. Behavior similar to the single sorption site partition coefficient (Eq A.12) is seen for $f_{OC} > 0.01$. Below this threshold, mutltilinear predicted partition coefficients deviate from a linear relationship with f_{OC}. This non-linearity is due to the increasing importance of binding to the clay size particle fraction as f_{OC} decreases.

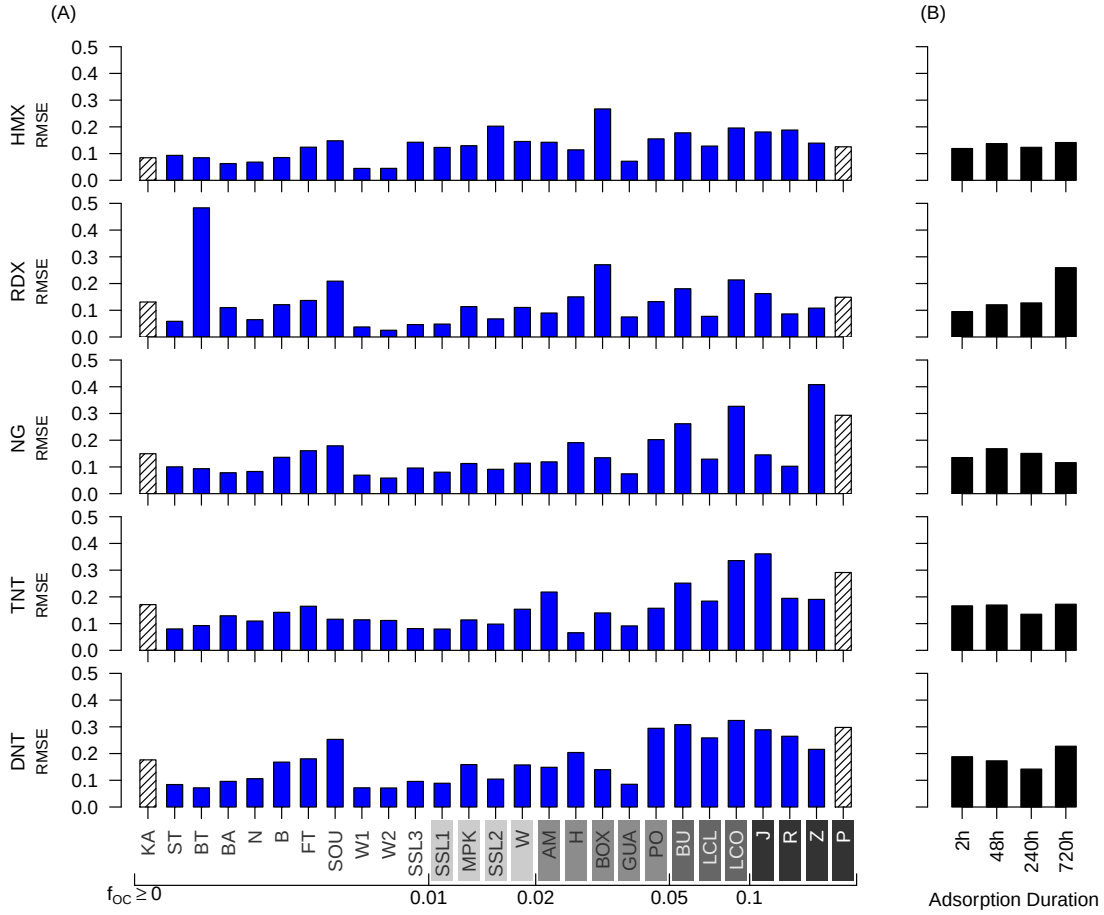


Figure A.3: RMSE, Eq 2.13, for the reversible partitioning model aqueous concentrations, C_{aq}^{N}. (A) RMSE determined for each soil and referece sorbent. Abbreviations are defined in Appendix E.2.1. Shading indicates increasing f_{OC}. Filled bars indicate soils, hashed bars indicate reference sorbents. (B) RMSE determined for each adsorption contact time.

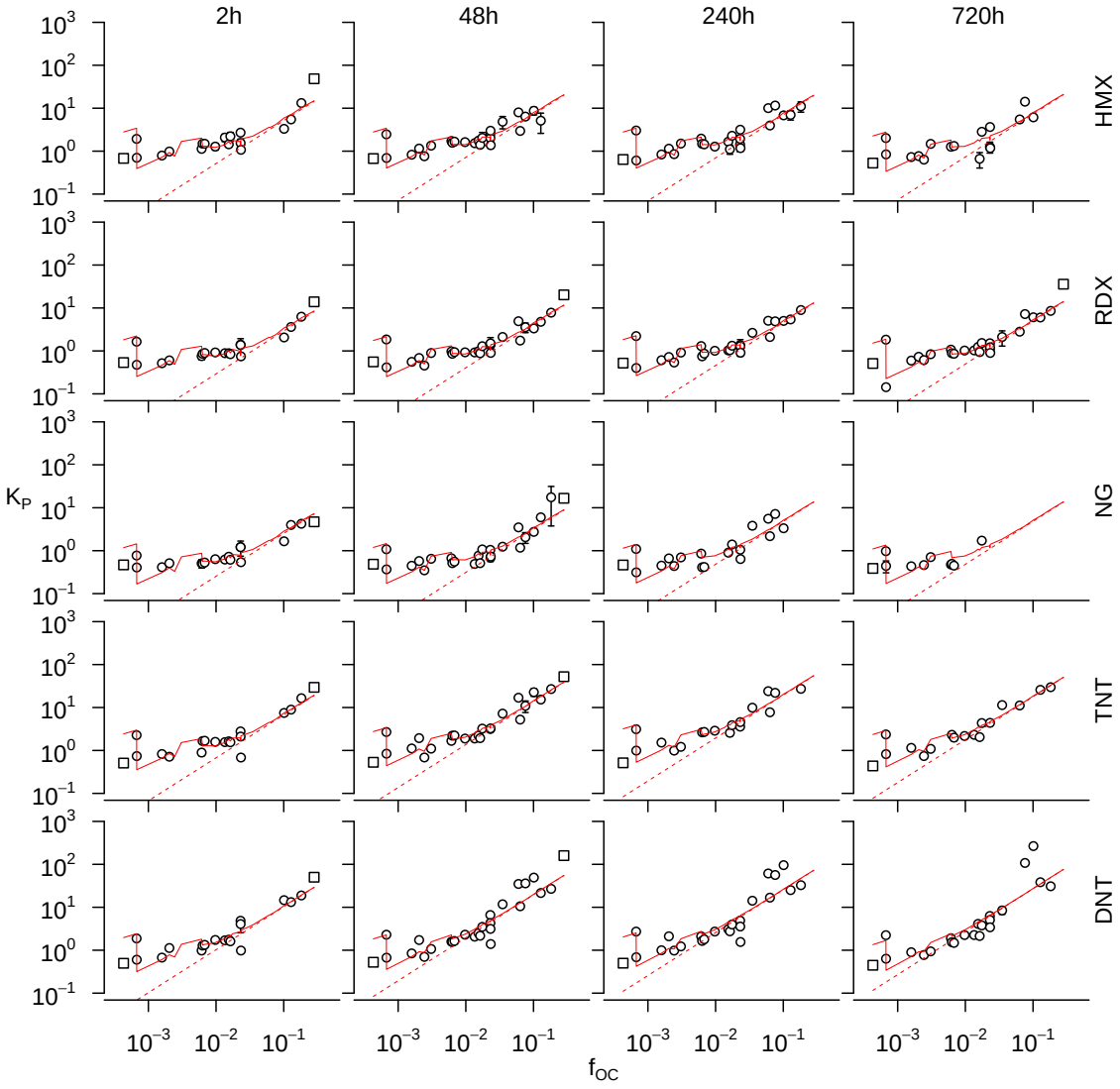


Figure A.4: Adsorption partition coefficients [L/kg] from RR model for soils are shown by mean (point) ± std. error (error bars) if the standard error is greater than the symbol. Red line shows K_P predicted by the two-site multilinear regression, Eq A.11. Dashed red line shows K_P predicted by the one-site regression, Eq A.12. Square points indicate reference sorbents not used in the multilinear regression.

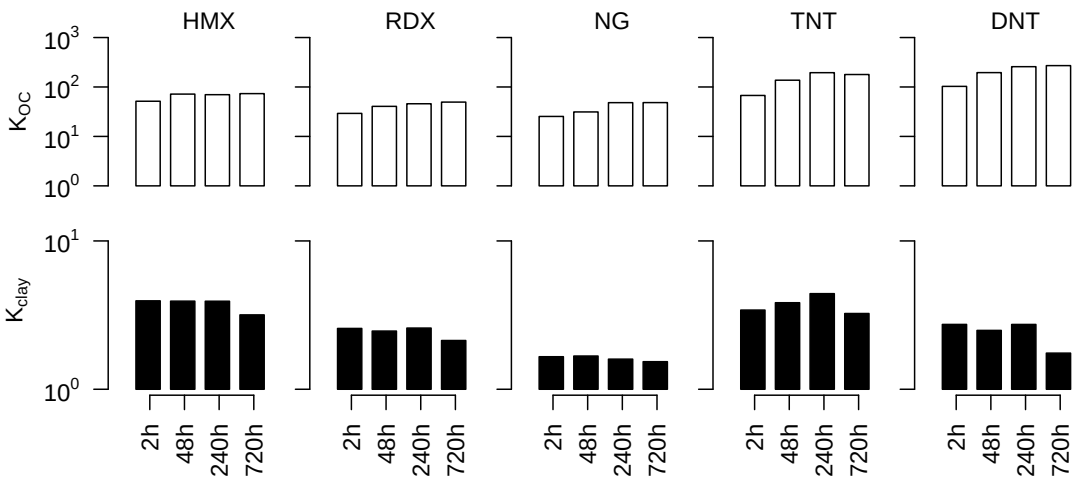


Figure A.5: Multilinear component partition coefficients, K_{OC} and K_{clay} [L/kg], for the adsorption partition coefficients versus adsorption contact time. Hollow bars show $K_{OC,x}(j)$, filled bars show $K_{clay,x}(j)$

The multilinear partition coefficients, Fig A.5, show that there is a time component to sorption to OC as K_{OC} increases with adsorption contact time. However K_{clay} does not show this relationship. This suggests that only the OC fraction of the sorbent is changing binding strength as the adsorption contact time increases.

A.2.5.1 Multilinear model of reversible resistant partition coefficients

To analyze the RR partition coefficients, a multilinear model for K_x and K_0 was needed, Eqs A.13 and A.14.

$$K_x(i,j) = f_{OC}(i)K_{OC,x}(j) + f_{clay}(i)K_{clay,x}(j) \tag{A.13}$$

$$K_0(i,j) = f_{OC}(i)K_{OC,0}(j) + f_{clay}(i)K_{clay,0}(j) \tag{A.14}$$

where $K_{OC,x}(j)$ and $K_{OC,0}(j)$ are the reversible and resistant partition coefficients associated with MC j binding to OC, $K_{clay,x}(j)$ and $K_{clay,0}(j)$ are the reversible and resistant partition coefficients associated with MC j binding to clay sized particles. Sorbent specific partition coefficients $K_{OC,x}$, $K_{OC,0}$, $K_{clay,x}$, and $K_{clay,0}$ are shown in Tables 2.2 and 2.3.

A.3 Reversible resistant model

A.3.1 Derivation of normalized reversible resistant isotherm

The RR model for adsorption is:

$$C_{tot} = C_d + C_x + C_0 \tag{A.15}$$
$$C_{tot} = C_d + mq_x + m_q 0 \tag{A.16}$$

To normalize, let $C^N = C/C_{tot}$ and $q^N = mq/C_{tot}$:

$$1 = C_d^N + mq_x^N + mq_0^N \tag{A.17}$$
$$1 = C_d^N + mK_x C_d^N + mK_0 C_d^N \tag{A.18}$$

The isotherm is defined as:

$$q^N = mK_x C_d^N + mK_0 C_d^N \tag{A.19}$$
$$q^N = (mK_x + mK_0)\, C_d^N q^N \qquad = mK_p C_d^N \tag{A.20}$$

which has slope mK_p and the intercept is the origin.

For the desorptions, $C_0 = mq_0 = mK_0 C_a$, where C_a is the adsorption dissolved concentration:

$$C_{tot} = C_d + mq_x + mq_0 \tag{A.21}$$
$$C_{tot} = C_d + mK_x C_d + mK_0 C_a \tag{A.22}$$

Let $C^N = C/C_{tot}$ and $q^N = mq/C_{tot}$:

$$1 = \frac{C_d}{C_{tot}} + mK_x \frac{C_d}{C_{tot}} + mK_0 \frac{C_a}{C_{tot}} \tag{A.23}$$
$$1 = C_d^N + mK_x C_d^N + mK_0 C_a^N \tag{A.24}$$
$$1 = C_d^N + mq_x^N + mq_0^N \tag{A.25}$$

Then the isotherm is defined as:

$$q^N = q_x^N + q_0^N \tag{A.26}$$
$$q^N = mK_x C_d^N + mK_0 C_a^N \tag{A.27}$$

Thus, the desorption isotherm is defined by slope mK_x and intercept $mK_0 C_a^N$

A.3.2 Derivation of normalized reversible resistant model

$$C_{tot} = C_d + C_x + C_0 \tag{A.28}$$
$$C_{tot} = C_d + K_x C_d + K_0 C_d \tag{A.29}$$
$$C_{tot} = C_d(1 + K_x + K_0) \tag{A.30}$$
$$f_0 = \frac{K_0}{1 + K_x + K_0} \tag{A.31}$$
$$C_{tot}(1 - f_0) = C'_{tot} = C_d + C_x \tag{A.32}$$
$$C'_{tot} = C_d + K_x C_d \tag{A.33}$$
$$f_d = \frac{1}{1 + K_x} \tag{A.34}$$
$$f_x = \frac{K_x}{1 + K_x} = 1 - f_d \tag{A.35}$$

where C'_{tot} is the reversible total concentration. then the aqueous concentration after adsorption is:

$$C_d(1) = f_d C'_{tot}(1) \tag{A.36}$$

Total reversible concentration after the supernatant is discarded is the fraction reversible:

$$C'_{tot}(2) = f_x C'_{tot}(1) \tag{A.37}$$

Following the method used previously for the reversible model, the aqueous concentration after k steps is:

$$C_d(k) = f_d(1 - f_d)^{k-1} C'_{tot}(1) \tag{A.38}$$

Which is equivalent to

$$C_d(k) = f_d(1 - f_d)^{k-1}(1 - f_0) C_{tot}(1) \tag{A.39}$$

which we can normalized by dividing by the initial total concentration, yielding the model

$$C_d^N(k) = \frac{C_d(k)}{C_{tot}(1)} = f_d(1 - f_d)^{k-1}(1 - f_0) \tag{A.40}$$

A.3.3 R code for reversible resistant fit

```
# Read HPLC data
hplc.raw     <-  read.table('../data/hplc_data.csv',header=TRUE,
    stringsAsFactor=FALSE,sep=',',as.is=TRUE)

# Read soil property data
prop.raw     <-  read.table('../data/soil_properties.csv',header=TRUE,
    stringsAsFactors=FALSE,sep=',',as.is=TRUE)

# Read mass balance check data (mbal = 0 ==> bad mass balance)
mbal.yesno  <-  read.table(file='../data/MB_yesno_v3.csv',sep=',',as.is=
    TRUE,stringsAsFactors=FALSE)

# Convert % to fraction
foc          <-  prop.raw$TOC/100
fclay        <-  prop.raw$Clay/100

# Order soils by foc content
soil_order  <-  prop.raw[prop.raw[,1] %in% unique(hplc.raw[,2]),]
soil_order  <-  soil_order[order(soil_order$TOC),]$SoilCode
nSoil        <-  length(soil_order)

mc_list      <-  c('HMX','RDX','NG','TNT','DNT')
nMC          <-  length(mc_list)

# Determine total mass
hplc.raw$MTOT   <-  hplc.raw$A.C*hplc.raw$V.A+
                    hplc.raw$D1.C*hplc.raw$V.D1+
                    hplc.raw$D2.C*hplc.raw$V.D2+
                    hplc.raw$D3.C*hplc.raw$V.D3+
                    hplc.raw$D4.C*hplc.raw$V.D4+
                    hplc.raw$E1.C*hplc.raw$V.E1+
                    hplc.raw$E2.C*hplc.raw$V.E2+
                    hplc.raw$E3.C*hplc.raw$V.E3

# Determine extracted mass
hplc.raw$M.EXT  <-  hplc.raw$E1.C*hplc.raw$V.E1+
                    hplc.raw$E2.C*hplc.raw$V.E2+
                    hplc.raw$E3.C*hplc.raw$V.E3



# Generate output matrix
fit.out <-  matrix(NA,nc=7,nr=nMC*4*nSoil)

# Reversible Resistant function for NLS fit
rr.nls  <-  function(logKX,logK0) {
     kx  <-  10^logKX
     k0  <-  10^logK0

```

```
47      #print(c(logKX,logK0))
48
49      fd  <-  1/(1+kx)
50      fx  <-  kx/(1+kx)
51      f0  <-  k0/(1+kx+k0)
52
53
54      ct  <-  (1-f0)*fx^seq(0,4,1)
55      cd  <-  fd*ct
56      cx  <-  fx*ct
57      cp  <-  cx+f0
58
59      mod.out <-  c(cd,cp)
60      lmod.out    <-  log10(mod.out)
61
62      #lmod.out    <-  log10(cd)
63      return(lmod.out)
64  }
65  # Set "last_kx" variable to -9999 to see if fit succeeded
66  last_kx=-9999
67  for (ii in 1:nSoil) {
68      for (jj in 1:nMC) {
69
70          dat.plt <-  matrix(NA,nrow=20,ncol=18)
71          # Generate fitting matrix of appropriate soil/MC normalized data
72          for (ij in 1:20){
73              dat.sub <-  subset(hplc.raw,MC==mc_list[jj] & SOILCODE==soil
                    _order[ii] & VIAL==ij)
74              dat.plt[ij,1]   <-  dat.sub[,'VIAL']
75              dat.plt[ij,2]   <-  dat.sub[,'A.C']/(dat.sub[,'MTOT']/dat.
                    sub[,'V.A'])
76              dat.plt[ij,3]   <-  dat.sub[,'D1.C']/(dat.sub[,'MTOT']/dat.
                    sub[,'V.A'])
77              dat.plt[ij,4]   <-  dat.sub[,'D2.C']/(dat.sub[,'MTOT']/dat.
                    sub[,'V.A'])
78              dat.plt[ij,5]   <-  dat.sub[,'D3.C']/(dat.sub[,'MTOT']/dat.
                    sub[,'V.A'])
79              dat.plt[ij,6]   <-  dat.sub[,'D4.C']/(dat.sub[,'MTOT']/dat.
                    sub[,'V.A'])
80              dat.plt[ij,7]   <-  dat.sub[,'M.EXT']/dat.sub[,'MTOT']
81
82              dat.plt[ij,8]    <-  1-dat.plt[ij,2]
83              dat.plt[ij,9]    <-  1-dat.plt[ij,3]-dat.plt[ij,2]
84              dat.plt[ij,10]   <-  1-dat.plt[ij,4]-dat.plt[ij,2]-dat.plt[
                    ij,3]
85              dat.plt[ij,11]   <-  1-dat.plt[ij,5]-dat.plt[ij,2]-dat.plt[
                    ij,3]-dat.plt[ij,4]
86              dat.plt[ij,12]   <-  1-dat.plt[ij,6]-dat.plt[ij,2]-dat.plt[
                    ij,3]-dat.plt[ij,4]-dat.plt[ij,5]
87
88              dat.plt[ij,13]   <-  dat.sub[,'A.C']*dat.sub[,'V.A']
```

```
89              dat.plt[ij,14]   <-  dat.sub[,'D1.C']*dat.sub[,'V.D1']
90              dat.plt[ij,15]   <-  dat.sub[,'D2.C']*dat.sub[,'V.D2']
91              dat.plt[ij,16]   <-  dat.sub[,'D3.C']*dat.sub[,'V.D3']
92              dat.plt[ij,17]   <-  dat.sub[,'D4.C']*dat.sub[,'V.D4']
93              dat.plt[ij,18]   <-  dat.sub[,'M.EXT']
94
95              # NA for sets that are outside MB check
96              is.na(dat.plt[ij,2:18]) <-  is.nan(dat.plt[ij,2:18])
97              is.na(dat.plt[ij,2:18]) <-  ifelse(mbal.yesno[mbal.yesno
                    [,1]==soil_order[ii] & mbal.yesno[,2]==ij & mbal.yesno
                    [,3]==mc_list[jj],4]==1,FALSE,TRUE)
98          }
99
100         for (ij in 1:4) {
101             # Vial number 1:5, 6:10, 11:15, 16:20 correspond to 2, 48,
                    240, 720 hr adsorption
102             vlo         <-  1+5*(ij-1)
103             vhi         <-  5*ij
104
105              # Select data for correct adsorption time
106             dat.tads    <-  dat.plt[vlo:vhi,]
107
108             fit.out[ij+4*(jj-1)+4*nMC*(ii-1),1]  <-  mc_list[jj]
109             fit.out[ij+4*(jj-1)+4*nMC*(ii-1),2]  <-  soil_order[ii]
110             fit.out[ij+4*(jj-1)+4*nMC*(ii-1),3]  <-  c(2,48,240,720)[ij]
111
112             # Fit to C and Q, fit in logspace
113             cd.obs          <-  log10(dat.tads[,2:6])
114             qs.obs          <-  log10(dat.tads[,8:12])
115
116             # Get rid of values R can't handle (infinite, nan)
117             is.na(cd.obs[,1:5]) <-  cd.obs[,1]==0 | !is.finite(cd.obs
                    [,1])
118             is.na(qs.obs[,1:5]) <-  is.na(cd.obs[,1]) |  !is.finite(cd.
                    obs[,1])
119
120             is.na(cd.obs)       <-  !is.finite(cd.obs)
121             is.na(qs.obs)       <-  !is.finite(qs.obs)
122
123             # See if there are any non-NA rows
124             if (any(!is.na(cd.obs[,1]))) {
125                 # See if there are more than 1 non-NA (colmeans fails on
                        dim[1]=1)
126                 if (sum(!is.na(cd.obs[,1]))>1) {
127                     cd.fit  <-  colMeans(cd.obs,na.rm=T)
128                     qs.fit  <-  colMeans(qs.obs,na.rm=T)
129                 }   else {
130                     cd.fit  <-  cd.obs
131                     qs.fit  <-  qs.obs
132                 }
133                 df.fit  <-  c(cd.fit,qs.fit)
```

```
134                 #fit.nls2     <-  -9999
135                 # Attempt to catch singular gradient (and other) errors
136                 #nls.control(warnOnly=TRUE, maxiter = 500)
137                 try(fit.nls2<-  nls(df.fit~rr.nls(logKX,logK0),control =
                        list(maxiter = 500,algorithm = 'plinear')))
138                 if (summary(fit.nls2)$parameters[1]==last_kx) {
139                     # NLS didn't converge, or other error
140                     fd.fit  <-  'ERR'
141                     fd.ser  <-  'ERR'
142                     f0.fit  <-  'ERR'
143                     f0.ser  <-  'ERR'
144                 } else {
145                     # Success, record value
146                     fd.fit  <-  summary(fit.nls2)$parameters[1]
147                     fd.ser  <-  summary(fit.nls2)$parameters[3]
148                     f0.fit  <-  summary(fit.nls2)$parameters[2]
149                     f0.ser  <-  summary(fit.nls2)$parameters[4]
150                     last_kx <-  summary(fit.nls2)$parameters[1]
151                 }
152             } else {
153                 # If there's no data to fit, set fit values to NA
154                 fd.fit  <-  NA
155                 fd.ser  <-  NA
156                 f0.fit  <-  NA
157                 f0.ser  <-  NA
158             }
159             # Write data to output matrix
160             fit.out[ij+4*(jj-1)+4*nMC*(ii-1),4]  <-  fd.fit
161             fit.out[ij+4*(jj-1)+4*nMC*(ii-1),5]  <-  fd.ser
162             fit.out[ij+4*(jj-1)+4*nMC*(ii-1),6]  <-  f0.fit
163             fit.out[ij+4*(jj-1)+4*nMC*(ii-1),7]  <-  f0.ser
164         }
165     }
166
167 }
168 # Write output file
169 write.table(x=fit.out,file=paste('../data/RR_Norm_nls_v7.csv',sep=''),
        col.names=c('mc','soil','tads','kx','se.kx','k0','se.k0'),sep=',')
```

A.3.4 Reversible resistant model parameters

A.3.4.1 Reversible resistant model K_x

Table A.2: Parameters for reversible resistant model derived desorption partition coefficient K_x. * Indicates noncoverged model. NA indicates "Not Analyzed"

MC	**Soil**	$log_{10}K_x^{2h}$	$log_{10}K_{x,err}^{2h}$	$log_{10}K_x^{48h}$	$log_{10}K_{x,err}^{48h}$	$log_{10}K_x^{240h}$	$log_{10}K_{x,err}^{240h}$	$log_{10}K_x^{720h}$	$log_{10}K_{x,err}^{720h}$
DNT	AM	0.44239	3.87e-02	0.59258	4.28e-02	NA	NA	0.57160	1.77e-02
DNT	B	NA	NA	-0.12990	2.82e-02	-0.10921	1.45e-02	-0.28474	1.74e-02
DNT	BA	-0.14934	2.36e-02	-0.08996	1.85e-02	-0.07457	7.93e-03	-0.11169	8.66e-03
DNT	BOX	NA	NA	0.39728	3.19e-02	*	*	0.26399	3.15e-02
DNT	BT	-0.19818	2.38e-02	-0.15164	2.17e-02	-0.17341	8.81e-03	-0.19068	1.01e-02
DNT	BU	NA	NA	0.63174	2.19e-01	0.88824	2.50e-02	NA	NA
DNT	FT	NA	NA	-0.05646	8.49e-03	-0.06883	9.59e-03	-0.18197	1.16e-02
DNT	GUA	0.01436	1.48e-02	0.06876	1.05e-02	0.10181	1.46e-02	NA	NA
DNT	H	0.58243	8.19e-02	0.50619	1.57e-02	0.59475	1.17e-02	0.18309	5.83e-02
DNT	J	0.29887	6.48e-02	0.93141	2.97e-02	0.91477	4.50e-02	*	*
DNT	KA	-0.37109	2.86e-03	-0.36722	3.80e-03	-0.36340	5.93e-03	-0.52693	2.32e-02
DNT	LCL	NA	NA	0.53754	1.04e-01	0.80314	2.89e-02	NA	NA
DNT	LCO	NA	NA	0.53789	1.89e-01	0.91437	4.24e-02	*	*
DNT	MPK	0.18357	2.31e-02	0.28542	1.52e-02	0.32222	2.00e-02	0.09280	2.28e-02
DNT	P	0.49587	1.09e-01	1.25882	1.65e-01	NA	NA	NA	NA
DNT	PO	NA	NA	0.63125	1.01e-01	0.73406	2.03e-02	0.23057	1.37e-01
DNT	R	0.69934	7.59e-02	1.02526	2.99e-02	1.11643	2.06e-02	0.32060	9.12e-02
DNT	S2	0.21142	3.35e-02	0.19637	2.51e-02	0.28680	3.16e-03	0.24057	7.69e-03
DNT	SAS	0.18507	2.15e-02	0.27242	8.15e-03	0.28928	3.02e-03	0.25451	6.54e-03
DNT	SOU	0.07789	1.93e-02	0.09314	7.80e-03	0.00432	3.82e-02	-0.10447	4.11e-02
DNT	SSL	0.17779	2.01e-02	0.24019	1.21e-02	NA	NA	*	*
DNT	ST	0.26424	1.45e-02	0.32560	2.18e-02	0.33807	2.03e-02	0.21438	5.15e-03
DNT	U	0.06090	2.13e-02	0.14376	1.51e-02	0.21447	2.02e-02	NA	NA
DNT	W	NA	NA	0.38159	3.05e-02	0.37389	1.35e-02	0.30787	3.44e-02
DNT	W1	0.10749	2.24e-02	0.15776	1.98e-02	0.16606	8.83e-03	0.14519	1.06e-02
DNT	W2	0.11133	2.18e-02	0.15975	1.39e-02	0.18081	5.51e-03	0.15104	1.08e-02
DNT	Z	0.82691	9.00e-02	1.07908	6.48e-02	1.03932	1.04e-01	0.35229	7.41e-02

Table A.2 – continued from previous page

MC	Soil	$log_{10}K_x^{2h}$	$log_{10}K_{x,err}^{2h}$	$log_{10}K_x^{48h}$	$log_{10}K_{x,err}^{48h}$	$log_{10}K_x^{240h}$	$log_{10}K_{x,err}^{240h}$	$log_{10}K_x^{720h}$	$log_{10}K_{x,err}^{720h}$
HMX	AM	0.27522	2.58e-02	0.28062	1.82e-02	0.11472	3.64e-02	NA	NA
HMX	B	NA	NA	-0.11124	1.41e-02	-0.09707	1.51e-02	-0.16542	1.96e-02
HMX	BA	-0.08194	1.66e-02	-0.08439	1.06e-02	-0.12092	7.58e-03	0.12943	3.13e-01
HMX	BOX	NA	NA	0.29507	6.92e-02	0.42958	2.13e-02	0.48759	4.50e-02
HMX	BT	-0.11546	1.98e-02	-0.08240	2.03e-02	-0.07362	2.98e-01	-0.12215	3.16e-01
HMX	BU	NA	NA	0.62297	8.38e-02	0.70696	5.37e-02	NA	NA
HMX	FT	NA	NA	0.05688	9.90e-03	0.08610	2.51e-02	0.09922	1.73e-02
HMX	GUA	0.05726	1.46e-02	0.09788	7.12e-03	0.01692	1.11e-02	-0.03605	1.23e-02
HMX	H	0.15138	1.74e-02	*	*	0.25450	4.36e-02	0.01400	3.58e-02
HMX	J	0.32970	3.63e-02	*	*	0.58374	3.53e-02	*	*
HMX	KA	-0.18828	1.56e-02	-0.18576	1.67e-02	-0.17707	2.36e-02	0.14099	3.70e-01
HMX	LCL	NA	NA	0.51021	6.94e-02	0.50081	7.73e-02	0.50141	1.10e-01
HMX	LCO	NA	NA	0.57091	1.20e-01	0.67808	7.18e-02	0.67897	1.29e-01
HMX	MPK	0.14338	2.12e-02	0.20909	1.19e-02	0.21288	3.80e-02	NA	NA
HMX	P	1.48620	1.08e+00	NA	NA	NA	NA	NA	NA
HMX	PO	NA	NA	0.53053	2.04e-02	NA	NA	0.36209	9.31e-02
HMX	R	0.79510	1.39e-01	0.80619	1.48e-01	0.55587	8.49e-02	NA	NA
HMX	S2	*	*	0.23563	3.15e-02	*	*	*	*
HMX	SAS	0.36768	1.33e-01	0.21675	1.34e-02	0.08788	4.35e-02	NA	NA
HMX	SOU	0.19404	3.82e-02	0.17266	1.13e-02	0.10296	1.50e-02	0.01082	1.38e-02
HMX	SSL	0.35375	5.85e-02	0.18371	1.24e-02	NA	NA	NA	NA
HMX	ST	0.28134	1.84e-02	0.34255	1.88e-02	0.31807	1.60e-02	0.22268	1.05e-02
HMX	U	-0.02275	1.52e-02	0.04504	1.42e-02	0.02719	1.41e-02	-0.09077	1.48e-02
HMX	W	NA	NA	0.23793	2.22e-02	0.26907	2.87e-02	0.32428	1.83e-02
HMX	W1	0.19326	1.54e-02	0.18581	1.56e-02	*	*	NA	NA
HMX	W2	0.18635	1.90e-02	0.18966	7.88e-03	*	*	*	*
HMX	Z	*	*	NA	NA	*	*	NA	NA

Table A.2 – continued from previous page

MC	Soil	$log_{10}K_x^{2h}$	$log_{10}K_{x,err}^{2h}$	$log_{10}K_x^{48h}$	$log_{10}K_{x,err}^{48h}$	$log_{10}K_x^{240h}$	$log_{10}K_{x,err}^{240h}$	$log_{10}K_x^{720h}$	$log_{10}K_{x,err}^{720h}$
NG	AM	-0.01930	8.81e-03	0.02835	6.63e-03	NA	NA	NA	NA
NG	B	NA	NA	-0.43102	2.31e-02	-0.35737	3.21e-02	-0.09959	2.75e-01
NG	BA	-0.38094	1.66e-02	-0.35157	1.48e-02	-0.08311	2.74e-01	-0.07478	2.72e-01
NG	BOX	NA	NA	*	*	0.04414	2.74e-02	NA	NA
NG	BT	-0.39244	1.65e-02	-0.40410	1.16e-02	-0.29458	2.77e-01	-0.18742	2.72e-01
NG	BU	NA	NA	0.26507	4.90e-02	0.41610	2.05e-02	NA	NA
NG	FT	NA	NA	-0.28545	1.07e-02	-0.25070	3.10e-02	-0.22875	1.76e-02
NG	GUA	-0.27048	2.67e-03	-0.20987	4.94e-03	-0.24828	4.84e-03	NA	NA
NG	H	-0.02720	1.14e-02	NA	NA	NA	NA	NA	NA
NG	J	0.11116	1.81e-02	0.30125	2.02e-02	0.33102	2.24e-02	NA	NA
NG	KA	-0.40216	6.30e-03	-0.39577	7.11e-03	-0.39494	2.17e-03	-0.17487	2.70e-01
NG	LCL	NA	NA	0.08816	3.73e-02	0.21212	2.04e-02	NA	NA
NG	LCO	NA	NA	0.13029	5.73e-02	0.36047	5.57e-02	NA	NA
NG	MPK	-0.18475	2.06e-03	-0.14434	6.48e-03	-0.16726	4.93e-03	NA	NA
NG	P	0.22985	5.35e-02	0.64777	5.27e-02	NA	NA	NA	NA
NG	PO	NA	NA	0.15911	7.15e-02	0.43607	7.19e-02	NA	NA
NG	R	0.45008	2.48e-02	0.66272	5.31e-03	NA	NA	NA	NA
NG	S2	-0.23273	1.54e-02	-0.24998	1.08e-02	NA	NA	NA	NA
NG	SAS	-0.25222	9.92e-03	NA	NA	NA	NA	NA	NA
NG	SOU	-0.19963	1.12e-02	-0.22138	5.57e-03	-0.22494	1.97e-02	0.03471	3.39e-01
NG	SSL	-0.24471	1.29e-02	-0.28074	1.40e-02	NA	NA	NA	NA
NG	ST	-0.09814	2.26e-02	0.01073	2.27e-02	-0.02720	1.73e-02	-0.09707	7.34e-03
NG	U	-0.29631	4.69e-03	-0.25321	8.30e-03	-0.25707	7.16e-03	NA	NA
NG	W	NA	NA	0.01307	1.53e-02	0.07084	2.83e-02	0.12547	4.36e-03
NG	W1	-0.28322	9.72e-03	-0.27939	8.31e-03	-0.37273	2.00e-01	-0.07762	2.83e-01
NG	W2	-0.26081	1.25e-02	-0.27599	4.24e-03	0.02262	3.47e-01	-0.17758	2.88e-01
NG	Z	0.32803	4.63e-02	0.75007	6.64e-02	NA	NA	NA	NA

Table A.2 – continued from previous page

MC	Soil	$log_{10}K_x^{2h}$	$log_{10}K_{x,err}^{2h}$	$log_{10}K_x^{48h}$	$log_{10}K_{x,err}^{48h}$	$log_{10}K_x^{240h}$	$log_{10}K_{x,err}^{240h}$	$log_{10}K_x^{720h}$	$log_{10}K_{x,err}^{720h}$
RDX	AM	0.09587	9.56e-03	0.16107	2.19e-02	0.07330	9.42e-03	0.18373	2.78e-02
RDX	B	NA	NA	-0.32449	1.36e-02	-0.33686	6.89e-03	-0.31528	3.54e-03
RDX	BA	-0.31175	2.21e-03	-0.30253	8.80e-04	-0.21438	1.78e-02	-0.21709	2.79e-02
RDX	BOX	NA	NA	-0.09153	4.90e-02	0.09679	1.91e-02	0.07102	1.23e-02
RDX	BT	-0.36158	1.83e-03	-0.37454	3.29e-03	-0.38250	8.84e-03	-0.27824	2.56e-01
RDX	BU	NA	NA	0.44137	4.10e-02	0.42613	1.30e-02	NA	NA
RDX	FT	NA	NA	-0.11489	3.45e-03	-0.16935	7.89e-03	-0.16177	3.57e-03
RDX	GUA	-0.11958	4.96e-03	-0.09676	2.30e-03	-0.09778	3.97e-03	-0.14782	1.20e-02
RDX	H	0.04548	1.75e-02	0.02607	9.14e-03	0.10069	1.31e-02	0.01564	6.16e-03
RDX	J	0.20854	2.27e-02	0.36859	1.74e-02	0.44038	2.56e-02	0.37276	1.53e-02
RDX	KA	-0.34897	1.85e-03	-0.33088	3.51e-03	-0.35280	1.96e-03	-0.42383	1.25e-02
RDX	LCL	NA	NA	0.24429	2.24e-02	0.24453	1.01e-02	0.31713	3.84e-03
RDX	LCO	NA	NA	0.34975	5.55e-02	0.39913	1.80e-02	0.50382	1.20e-02
RDX	MPK	-0.08636	6.37e-03	-0.05487	6.20e-03	-0.05163	1.89e-03	-0.11522	1.36e-02
RDX	P	0.75206	9.60e-02	0.93583	4.54e-02	NA	NA	1.02830	3.21e-01
RDX	PO	NA	NA	0.29876	2.75e-02	0.29036	1.43e-02	0.19851	3.41e-02
RDX	R	0.48913	2.33e-02	0.54136	7.99e-03	0.59890	1.06e-02	0.51829	1.81e-02
RDX	S2	-0.05500	1.70e-02	-0.07788	3.97e-03	-0.02727	4.07e-03	-0.03449	4.08e-03
RDX	SAS	-0.07288	4.04e-03	-0.06171	4.95e-03	-0.00519	5.38e-03	-0.01861	4.63e-03
RDX	SOU	-0.02795	1.22e-02	-0.05167	4.02e-03	-0.11647	3.41e-02	-0.07832	1.02e-02
RDX	SSL	-0.08114	5.25e-03	-0.06414	3.58e-03	NA	NA	*	*
RDX	ST	0.21264	1.19e-02	0.26425	2.38e-02	0.30564	2.01e-02	0.17790	1.24e-02
RDX	U	-0.21989	6.43e-03	-0.19046	6.69e-03	-0.17052	6.65e-03	-0.21540	2.29e-03
RDX	W	NA	NA	0.07477	1.31e-02	0.01856	1.14e-02	0.08617	4.75e-03
RDX	W1	-0.06506	2.75e-03	-0.06908	5.64e-03	-0.14964	1.65e-01	-0.06920	2.75e-03
RDX	W2	-0.05801	2.55e-03	-0.05819	3.64e-04	-0.06834	4.11e-03	*	*
RDX	Z	0.61212	4.94e-02	0.66262	2.06e-02	0.69647	4.59e-02	0.52438	2.90e-02

Table A.2 – continued from previous page

MC	Soil	$log_{10}K_x^{2h}$	$log_{10}K_{x,err}^{2h}$	$log_{10}K_x^{48h}$	$log_{10}K_{x,err}^{48h}$	$log_{10}K_x^{240h}$	$log_{10}K_{x,err}^{240h}$	$log_{10}K_x^{720h}$	$log_{10}K_{x,err}^{720h}$
TNT	AM	0.26525	4.20e-02	NA	NA	NA	NA	NA	NA
TNT	B	NA	NA	-0.16072	2.59e-02	-0.11955	1.36e-02	-0.19083	5.51e-03
TNT	BA	-0.06887	3.00e-02	0.00590	2.21e-02	0.04468	1.10e-02	-0.02558	1.21e-02
TNT	BOX	NA	NA	0.34329	2.30e-02	0.41054	3.36e-02	0.49163	7.69e-03
TNT	BT	-0.11572	2.99e-02	-0.06176	2.66e-02	-0.04197	1.14e-02	-0.09992	1.25e-02
TNT	BU	NA	NA	0.60494	1.22e-01	0.75709	2.71e-02	NA	NA
TNT	FT	NA	NA	-0.07761	2.23e-03	-0.07742	1.06e-02	-0.04383	8.58e-03
TNT	GUA	-0.11972	2.13e-02	NA	NA	NA	NA	NA	NA
TNT	H	0.28464	1.83e-02	0.40005	1.25e-02	0.49763	1.47e-02	NA	NA
TNT	J	0.27742	6.70e-02	0.89047	4.26e-02	NA	NA	NA	NA
TNT	KA	-0.36370	1.56e-03	-0.35451	3.45e-03	-0.32305	1.54e-02	-0.51104	1.32e-02
TNT	LCL	NA	NA	0.48521	8.18e-02	0.61012	1.72e-02	0.70474	4.14e-02
TNT	LCO	NA	NA	0.44728	1.07e-01	0.77906	1.50e-02	NA	NA
TNT	MPK	0.16261	2.70e-02	0.25220	1.17e-02	NA	NA	NA	NA
TNT	P	0.59884	1.33e-01	1.06630	1.26e-01	NA	NA	NA	NA
TNT	PO	NA	NA	0.62527	8.37e-02	0.62519	1.59e-02	0.85358	2.00e-01
TNT	R	0.69938	7.82e-02	1.01647	2.97e-02	NA	NA	0.49040	8.73e-02
TNT	S2	0.21931	4.01e-02	0.17553	1.86e-02	0.31872	1.78e-02	0.23978	7.85e-03
TNT	SAS	0.16285	1.92e-02	0.21495	8.54e-03	0.34612	1.00e-02	0.25360	5.39e-03
TNT	SOU	0.04360	2.33e-02	0.11012	1.25e-02	NA	NA	NA	NA
TNT	SSL	0.16002	2.02e-02	0.21890	1.03e-02	NA	NA	0.25104	1.11e-02
TNT	ST	0.35842	1.09e-02	0.39718	1.13e-02	0.38670	1.54e-02	0.22786	6.28e-03
TNT	U	-0.09230	2.73e-02	0.16692	1.09e-02	NA	NA	NA	NA
TNT	W	NA	NA	0.37633	3.29e-02	0.34320	6.79e-03	0.41263	1.71e-02
TNT	W1	0.18248	3.03e-02	0.25326	2.17e-02	0.29618	1.10e-02	0.24151	1.40e-02
TNT	W2	0.18304	2.86e-02	0.24689	1.46e-02	0.29492	9.17e-03	0.22544	1.44e-02
TNT	Z	0.80122	9.05e-02	1.09011	8.06e-02	1.03501	1.18e-01	0.47486	8.54e-02

A.3.4.2 Reversible resistant model K_0

Table A.3: Parameters for reversible resistant model derived desorption partition coefficient K_0 * Indicates noncoverged model. NA indicates "Not Analyzed"

MC	**Soil**	$log_{10}K_x^{2h}$	$log_{10}K_{x,err}^{2h}$	$log_{10}K_x^{48h}$	$log_{10}K_{x,err}^{48h}$	$log_{10}K_x^{240h}$	$log_{10}K_{x,err}^{240h}$	$log_{10}K_x^{720h}$	$log_{10}K_{x,err}^{720h}$
DNT	AM	0.46371	3.13e-02	0.49905	3.17e-02	NA	NA	0.46670	1.36e-02
DNT	B	NA	NA	-0.86583	6.82e-02	-0.48088	2.92e-02	-0.85209	3.98e-02
DNT	BA	-0.96239	6.05e-02	-0.82998	4.50e-02	-0.62342	1.69e-02	-0.69219	1.90e-02
DNT	BOX	NA	NA	0.03300	4.45e-02	*	*	0.06092	4.15e-02
DNT	BT	-1.01169	6.06e-02	-1.02532	5.86e-02	-1.00632	2.29e-02	-1.17653	2.98e-02
DNT	BU	NA	NA	1.74558	9.79e-02	1.73172	5.61e-03	NA	NA
DNT	FT	NA	NA	-0.61544	1.81e-02	-0.34340	1.84e-02	-0.72332	2.55e-02
DNT	GUA	-0.98187	5.23e-02	-0.51229	2.21e-02	-0.43722	2.94e-02	NA	NA
DNT	H	-0.22190	3.17e-01	0.05338	2.54e-02	-0.01781	2.87e-02	0.54963	7.06e-02
DNT	J	1.25462	5.59e-02	1.63020	5.63e-03	1.97784	1.02e-02	*	*
DNT	KA	-1.12323	7.13e-03	-1.15737	9.62e-03	-1.18492	1.52e-02	-1.10360	5.73e-02
DNT	LCL	NA	NA	1.06105	5.60e-02	1.04727	9.81e-03	NA	NA
DNT	LCO	NA	NA	1.74339	1.03e-01	1.72040	8.71e-03	*	*
DNT	MPK	-0.25863	4.08e-02	-0.13318	2.47e-02	0.07554	2.54e-02	0.42988	3.26e-02
DNT	P	1.84333	6.46e-02	2.13817	1.40e-02	NA	NA	NA	NA
DNT	PO	NA	NA	1.02555	4.30e-02	0.97412	7.52e-03	1.04426	1.36e-01
DNT	R	1.03277	2.78e-02	1.05680	1.89e-02	1.07300	1.70e-02	1.57930	7.40e-02
DNT	S2	-0.54903	9.39e-02	-0.44246	5.71e-02	-0.07373	4.76e-03	-0.28529	1.48e-02
DNT	SAS	-0.35016	4.22e-02	-0.31548	1.72e-02	-0.09331	4.67e-03	-0.24967	1.21e-02
DNT	SOU	-0.89312	6.99e-02	-0.38386	1.49e-02	-0.13761	6.73e-02	0.01485	7.94e-02
DNT	SSL	-0.36814	4.01e-02	-0.33532	2.51e-02	NA	NA	*	*
DNT	ST	-0.87579	9.28e-02	-0.45119	6.76e-02	-0.17425	3.75e-02	-0.25580	9.25e-03
DNT	U	-0.68046	5.38e-02	-0.31953	2.79e-02	-0.18670	3.35e-02	NA	NA
DNT	W	NA	NA	0.15792	3.50e-02	0.24404	1.41e-02	0.12928	4.19e-02
DNT	W1	-0.63053	5.75e-02	-0.52253	4.75e-02	-0.53075	2.18e-02	-0.58057	2.71e-02
DNT	W2	-0.57459	5.22e-02	-0.46909	3.09e-02	-0.48047	1.29e-02	-0.73132	3.60e-02
DNT	Z	1.17182	2.55e-02	1.16076	3.73e-02	1.32355	3.30e-02	1.42079	5.75e-02

Table A.3 – continued from previous page

MC	Soil	$log_{10}K_x^{2h}$	$log_{10}K_{x,err}^{2h}$	$log_{10}K_x^{48h}$	$log_{10}K_{x,err}^{48h}$	$log_{10}K_x^{240h}$	$log_{10}K_{x,err}^{240h}$	$log_{10}K_x^{720h}$	$log_{10}K_{x,err}^{720h}$
HMX	AM	0.00256	3.56e-02	-0.05711	2.68e-02	-0.17804	6.04e-02	NA	NA
HMX	B	NA	NA	-1.29048	5.58e-02	-0.78097	3.51e-02	-1.18176	6.02e-02
HMX	BA	-1.21509	6.41e-02	-1.18627	3.89e-02	-1.03479	2.15e-02	-0.91823	1.39e+00
HMX	BOX	NA	NA	-0.00789	9.65e-02	-0.19055	4.94e-02	-0.48273	2.43e-01
HMX	BT	-1.24998	7.35e-02	-2.08349	3.93e-01	-1.18423	1.12e+00	-1.43911	1.51e+00
HMX	BU	NA	NA	0.75978	4.22e-02	0.81132	2.52e-02	NA	NA
HMX	FT	NA	NA	-0.51693	2.08e-02	-0.32182	4.57e-02	-0.51064	3.76e-02
HMX	GUA	-1.13601	7.69e-02	-0.76281	2.19e-02	-0.68946	2.65e-02	-0.75785	2.96e-02
HMX	H	-0.58723	4.55e-02	*	*	-0.24487	8.04e-02	-0.33432	6.61e-02
HMX	J	0.28717	3.85e-02	*	*	0.56194	2.33e-02	*	*
HMX	KA	-1.04418	4.10e-02	-1.08370	4.56e-02	-1.10342	6.61e-02	-0.84265	1.47e+00
HMX	LCL	NA	NA	-0.20029	2.06e-01	-0.04471	1.55e-01	0.29028	1.09e-01
HMX	LCO	NA	NA	0.70343	6.71e-02	0.74579	3.69e-02	0.77948	6.29e-02
HMX	MPK	-0.59395	5.51e-02	-0.57941	3.50e-02	-0.46525	9.24e-02	NA	NA
HMX	P	1.25682	1.66e+00	NA	NA	NA	NA	NA	NA
HMX	PO	NA	NA	0.21009	2.47e-02	NA	NA	0.24037	9.89e-02
HMX	R	-0.15594	8.85e-01	0.05135	5.90e-01	0.52281	5.92e-02	NA	NA
HMX	S2	*	*	-1.78271	1.40e+00	*	*	*	*
HMX	SAS	-0.90201	1.29e+00	-0.90832	7.79e-02	-0.70482	1.20e-01	NA	NA
HMX	SOU	-1.31072	4.93e-01	-0.46184	2.55e-02	-0.24340	2.58e-02	-0.49933	2.79e-02
HMX	SSL	-0.72494	3.62e-01	-0.82571	5.45e-02	NA	NA	NA	NA
HMX	ST	-0.75904	9.66e-02	-0.45897	6.22e-02	0.05246	2.09e-02	-0.38809	2.30e-02
HMX	U	-0.86864	4.21e-02	-0.79322	4.07e-02	-0.75379	3.70e-02	-1.28500	6.19e-02
HMX	W	NA	NA	-0.35920	4.76e-02	-0.07405	4.29e-02	-0.13410	3.10e-02
HMX	W1	-0.98932	9.82e-02	-0.82388	6.88e-02	*	*	NA	NA
HMX	W2	-0.76771	7.50e-02	-0.69175	2.72e-02	*	*	*	*
HMX	Z	*	*	NA	NA	*	*	NA	NA

Table A.3 – continued from previous page

MC	Soil	$log_{10}K_x^{2h}$	$log_{10}K_{x,err}^{2h}$	$log_{10}K_x^{48h}$	$log_{10}K_{x,err}^{48h}$	$log_{10}K_x^{240h}$	$log_{10}K_{x,err}^{240h}$	$log_{10}K_x^{720h}$	$log_{10}K_{x,err}^{720h}$
NG	AM	-0.57312	1.85e-02	-1.23435	3.79e-02	NA	NA	NA	NA
NG	B	NA	NA	-1.33736	6.18e-02	-1.01670	7.74e-02	-0.88214	6.95e-01
NG	BA	-1.40328	4.70e-02	-1.31890	4.08e-02	-0.86368	6.93e-01	-0.83980	6.80e-01
NG	BOX	NA	NA	*	*	-0.53679	5.81e-02	NA	NA
NG	BT	-1.37360	4.56e-02	-1.77575	4.12e-02	-1.26491	7.76e-01	-1.12847	7.69e-01
NG	BU	NA	NA	0.43980	5.37e-02	0.53311	1.65e-02	NA	NA
NG	FT	NA	NA	-1.00644	2.60e-02	-0.62070	6.71e-02	-0.90085	4.14e-02
NG	GUA	-1.81048	1.35e-02	-1.04144	1.27e-02	-1.17583	1.33e-02	NA	NA
NG	H	-0.82387	2.98e-02	NA	NA	NA	NA	NA	NA
NG	J	-0.23235	3.10e-02	0.00057	2.80e-02	0.17415	2.58e-02	NA	NA
NG	KA	-1.17173	1.59e-02	-1.20629	1.82e-02	-1.20942	5.56e-03	-0.85829	6.33e-01
NG	LCL	NA	NA	-0.48318	7.77e-02	-0.10652	3.14e-02	NA	NA
NG	LCO	NA	NA	0.20767	8.23e-02	0.81102	4.60e-02	NA	NA
NG	MPK	-1.06861	5.57e-03	-1.11769	1.93e-02	-0.66339	1.06e-02	NA	NA
NG	P	0.65215	5.84e-02	1.02721	2.16e-02	NA	NA	NA	NA
NG	PO	NA	NA	-0.24208	1.23e-01	0.33930	6.57e-02	NA	NA
NG	R	0.19059	2.79e-02	0.16083	1.03e-02	NA	NA	NA	NA
NG	S2	-1.24566	4.55e-02	-1.56111	4.25e-02	NA	NA	NA	NA
NG	SAS	-1.06992	2.53e-02	NA	NA	NA	NA	NA	NA
NG	SOU	-1.72808	6.40e-02	-1.10149	1.48e-02	-0.85098	4.53e-02	-0.54803	7.19e-01
NG	SSL	-1.18128	3.55e-02	-1.22967	3.87e-02	NA	NA	NA	NA
NG	ST	-1.11778	7.36e-02	-0.68075	5.35e-02	-0.70493	4.01e-02	-0.77912	1.71e-02
NG	U	-1.43944	1.49e-02	-1.32469	2.55e-02	-0.98563	1.74e-02	NA	NA
NG	W	NA	NA	-0.74388	3.88e-02	-0.44735	5.64e-02	-0.38332	8.45e-03
NG	W1	-2.02456	6.34e-02	-1.83754	4.22e-02	-0.97117	4.74e-01	-0.98934	8.23e-01
NG	W2	-1.66347	5.37e-02	-1.39210	1.34e-02	-1.03560	1.36e+00	-1.25512	9.35e-01
NG	Z	0.44415	4.55e-02	1.31303	2.04e-02	NA	NA	NA	NA

Table A.3 – continued from previous page

MC	Soil	$log_{10}K_x^{2h}$	$log_{10}K_{x,err}^{2h}$	$log_{10}K_x^{48h}$	$log_{10}K_{x,err}^{48h}$	$log_{10}K_x^{240h}$	$log_{10}K_{x,err}^{240h}$	$log_{10}K_x^{720h}$	$log_{10}K_{x,err}^{720h}$
RDX	AM	-0.59755	2.30e-02	-1.81587	7.67e-01	-0.83588	3.07e-02	-1.27239	3.17e-01
RDX	B	NA	NA	-1.33985	3.88e-02	-0.90905	1.61e-02	-1.02172	8.60e-03
RDX	BA	-1.36532	6.51e-03	-1.24461	2.41e-03	-1.10946	4.82e-02	-1.06506	7.27e-02
RDX	BOX	NA	NA	-0.77922	1.15e-01	-0.66507	5.05e-02	-1.02635	5.55e-02
RDX	BT	-1.31841	5.03e-03	-1.81894	1.28e-02	-1.87438	3.57e-02	-1.26340	7.27e-01
RDX	BU	NA	NA	0.47993	3.28e-02	0.42411	1.10e-02	NA	NA
RDX	FT	NA	NA	-0.84530	8.34e-03	-0.54228	1.64e-02	-0.82781	8.28e-03
RDX	GUA	-1.53648	2.80e-02	-0.97132	6.36e-03	-0.99343	1.12e-02	-0.86595	2.87e-02
RDX	H	-1.01088	7.07e-02	-0.41811	1.76e-02	-1.04222	6.69e-02	-0.36786	1.15e-02
RDX	J	-0.12782	3.56e-02	0.10264	2.15e-02	0.42452	2.14e-02	0.52628	1.34e-02
RDX	KA	-1.08772	4.57e-03	-1.13857	8.91e-03	-1.17683	5.01e-03	-1.12071	3.09e-02
RDX	LCL	NA	NA	-0.59511	7.45e-02	-0.30670	2.02e-02	-0.15857	6.69e-03
RDX	LCO	NA	NA	0.40455	5.35e-02	0.43815	1.58e-02	0.59025	8.11e-03
RDX	MPK	-0.90146	1.66e-02	-0.86202	1.62e-02	-0.87455	5.04e-03	-0.49911	2.76e-02
RDX	P	1.05996	3.20e-02	1.06984	2.03e-02	NA	NA	1.43252	7.34e-02
RDX	PO	NA	NA	-0.31433	6.11e-02	-0.13720	2.35e-02	-0.03038	4.99e-02
RDX	R	-0.05284	4.61e-02	0.14130	1.15e-02	0.15572	1.72e-02	0.40166	1.50e-02
RDX	S2	-1.35059	8.86e-02	-1.31693	1.81e-02	-0.89345	1.15e-02	-1.31648	2.15e-02
RDX	SAS	-0.99695	1.19e-02	-1.07527	1.65e-02	-1.23652	2.73e-02	-1.00890	1.56e-02
RDX	SOU	-1.45056	8.43e-02	-1.00760	1.25e-02	-0.52100	6.96e-02	-0.77031	2.40e-02
RDX	SSL	-1.03964	1.61e-02	-1.10611	1.24e-02	NA	NA	*	*
RDX	ST	-1.25243	1.45e-01	-0.63727	9.14e-02	-0.47131	6.17e-02	-0.55836	3.29e-02
RDX	U	-1.33715	2.11e-02	-1.11310	1.86e-02	-1.12227	1.91e-02	-0.94099	5.52e-03
RDX	W	NA	NA	-0.89920	4.75e-02	-0.43500	2.22e-02	-0.53953	1.05e-02
RDX	W1	-1.70247	2.64e-02	-1.61079	4.46e-02	-0.96350	4.24e-01	-1.38611	1.45e-02
RDX	W2	-1.32956	1.27e-02	-1.18788	1.44e-03	-1.54768	2.90e-02	*	*
RDX	Z	0.48863	3.84e-02	0.48249	1.81e-02	0.59780	3.33e-02	0.65663	1.80e-02

Table A.3 – continued from previous page

MC	Soil	$log_{10}K_x^{2h}$	$log_{10}K_{x,err}^{2h}$	$log_{10}K_x^{48h}$	$log_{10}K_{x,err}^{48h}$	$log_{10}K_x^{240h}$	$log_{10}K_{x,err}^{240h}$	$log_{10}K_x^{720h}$	$log_{10}K_{x,err}^{720h}$
TNT	AM	0.22346	5.01e-02	NA	NA	NA	NA	NA	NA
TNT	B	NA	NA	-0.82483	5.99e-02	-0.46072	2.74e-02	-0.88069	1.30e-02
TNT	BA	-0.71005	6.76e-02	-0.57237	4.70e-02	-0.24862	1.93e-02	-0.48315	2.40e-02
TNT	BOX	NA	NA	0.16243	2.65e-02	0.27813	3.32e-02	0.10870	1.07e-02
TNT	BT	-0.76407	6.83e-02	-0.80928	6.56e-02	-0.67273	2.53e-02	-0.86370	3.10e-02
TNT	BU	NA	NA	1.27116	5.58e-02	1.27997	8.15e-03	NA	NA
TNT	FT	NA	NA	-0.58146	4.63e-03	-0.33681	2.04e-02	-0.60547	1.82e-02
TNT	GUA	-0.98107	5.74e-02	NA	NA	NA	NA	NA	NA
TNT	H	-0.37083	4.39e-02	-0.17019	2.58e-02	-0.34264	5.89e-02	NA	NA
TNT	J	0.93795	6.29e-02	1.21248	1.18e-02	NA	NA	NA	NA
TNT	KA	-1.08729	3.85e-03	-1.17238	8.83e-03	-1.13234	3.91e-02	-1.13103	3.26e-02
TNT	LCL	NA	NA	0.59354	5.66e-02	0.59619	1.09e-02	0.79098	2.02e-02
TNT	LCO	NA	NA	1.15995	7.02e-02	1.22727	4.33e-03	NA	NA
TNT	MPK	-0.27143	4.80e-02	-0.23584	2.13e-02	NA	NA	NA	NA
TNT	P	1.58719	6.34e-02	1.75538	1.73e-02	NA	NA	NA	NA
TNT	PO	NA	NA	0.66655	4.76e-02	0.76500	7.93e-03	0.72749	1.69e-01
TNT	R	0.76188	3.99e-02	0.71544	4.45e-02	NA	NA	1.37132	5.22e-02
TNT	S2	-0.67544	1.46e-01	-0.56536	4.94e-02	-0.12794	2.97e-02	-0.37591	1.73e-02
TNT	SAS	-0.46888	4.31e-02	-0.45260	2.04e-02	-0.12484	1.72e-02	-0.33708	1.14e-02
TNT	SOU	-0.81518	6.85e-02	-0.30202	2.25e-02	NA	NA	NA	NA
TNT	SSL	-0.46147	4.47e-02	-0.45400	2.49e-02	NA	NA	-0.19611	1.91e-02
TNT	ST	-1.05073	1.43e-01	-0.48422	4.64e-02	-0.10605	2.72e-02	-0.19989	1.07e-02
TNT	U	-0.81882	6.57e-02	-0.23356	1.87e-02	NA	NA	NA	NA
TNT	W	NA	NA	0.12877	3.92e-02	0.25068	7.28e-03	0.22825	1.80e-02
TNT	W1	-0.30546	5.62e-02	-0.18271	3.67e-02	-0.08608	1.69e-02	-0.13169	2.21e-02
TNT	W2	-0.29396	5.26e-02	-0.19610	2.49e-02	-0.08247	1.40e-02	-0.29684	2.75e-02
TNT	Z	1.11865	2.75e-02	1.15123	4.95e-02	1.21635	4.97e-02	1.42347	5.27e-02

A.3.5 Reversible resistant model multilinear parameters

Table A.4: Multilinear parameters for reversible resistant model derived desorption partition coefficients K_x and K_0

	MC	K_{OC}^{2h}	K_{clay}^{2h}	K_{OC}^{48h}	K_{clay}^{48h}	K_{OC}^{240h}	K_{clay}^{240h}	K_{OC}^{720h}	K_{clay}^{720h}
K_x	HMX	3.81e+01	4.67e+00	5.45e+01	4.06e+00	4.79e+01	3.79e+00	5.23e+01	3.52e+00
	RDX	2.26e+01	2.72e+00	2.89e+01	2.54e+00	3.18e+01	2.46e+00	2.88e+01	2.53e+00
	NG	1.71e+01	1.88e+00	2.33e+01	1.78e+00	2.94e+01	2.04e+00	6.22e+01	2.12e+00
	TNT	3.37e+01	4.28e+00	6.56e+01	4.15e+00	8.50e+01	4.29e+00	5.46e+01	4.35e+00
	DNT	4.58e+01	3.85e+00	7.50e+01	3.55e+00	9.51e+01	3.23e+00	3.69e+01	3.49e+00
K_0	HMX	1.03e+01	2.45e-01	1.71e+01	2.36e-01	2.64e+01	6.74e-01	2.48e+01	3.06e-01
	RDX	5.22e+00	1.02e-01	7.61e+00	1.54e-01	1.07e+01	2.50e-01	1.14e+01	2.70e-01
	NG	4.64e+00	7.73e-02	8.19e+00	1.12e-01	1.85e+01	2.59e-01	1.19e+01	3.40e-01
	TNT	3.45e+01	2.40e-01	6.62e+01	4.55e-01	8.82e+01	1.01e+00	7.45e+01	5.06e-01
	DNT	4.09e+01	1.59e-01	8.73e+01	2.12e-01	1.19e+02	4.17e-01	8.63e+01	2.80e-01

A.3.6 Reversible resistant model plots

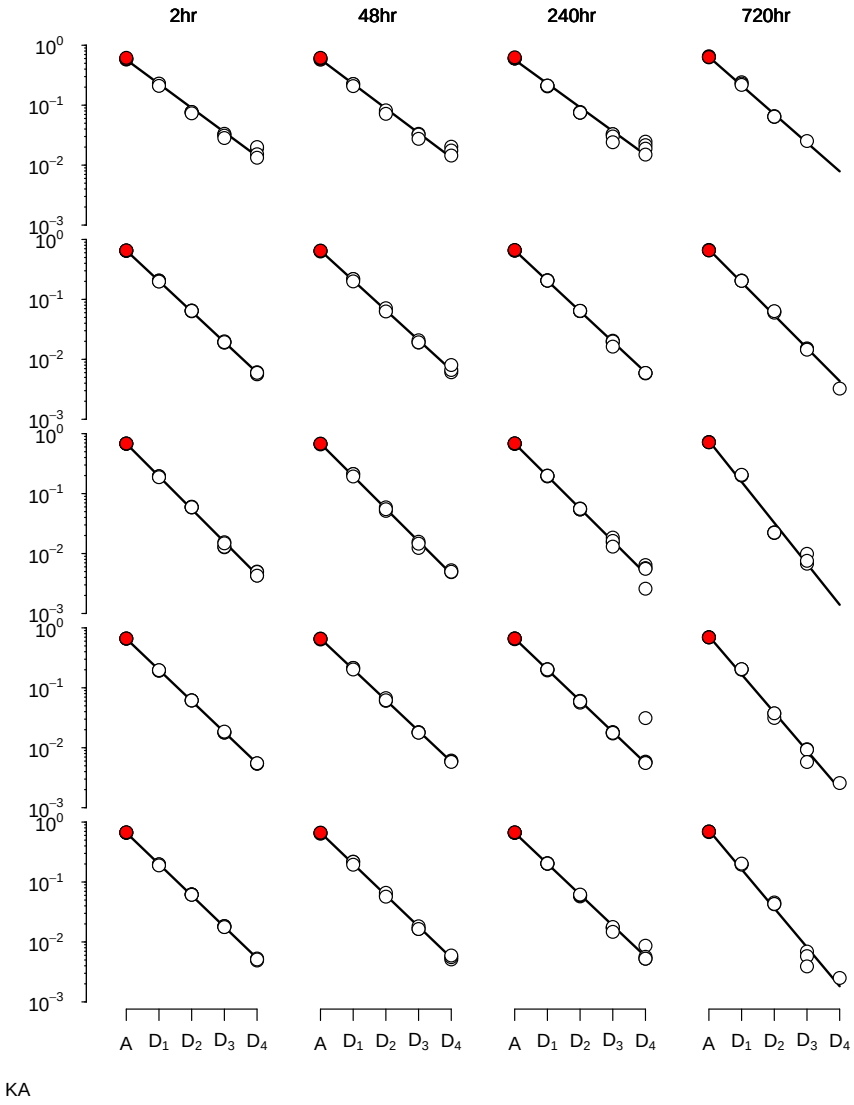
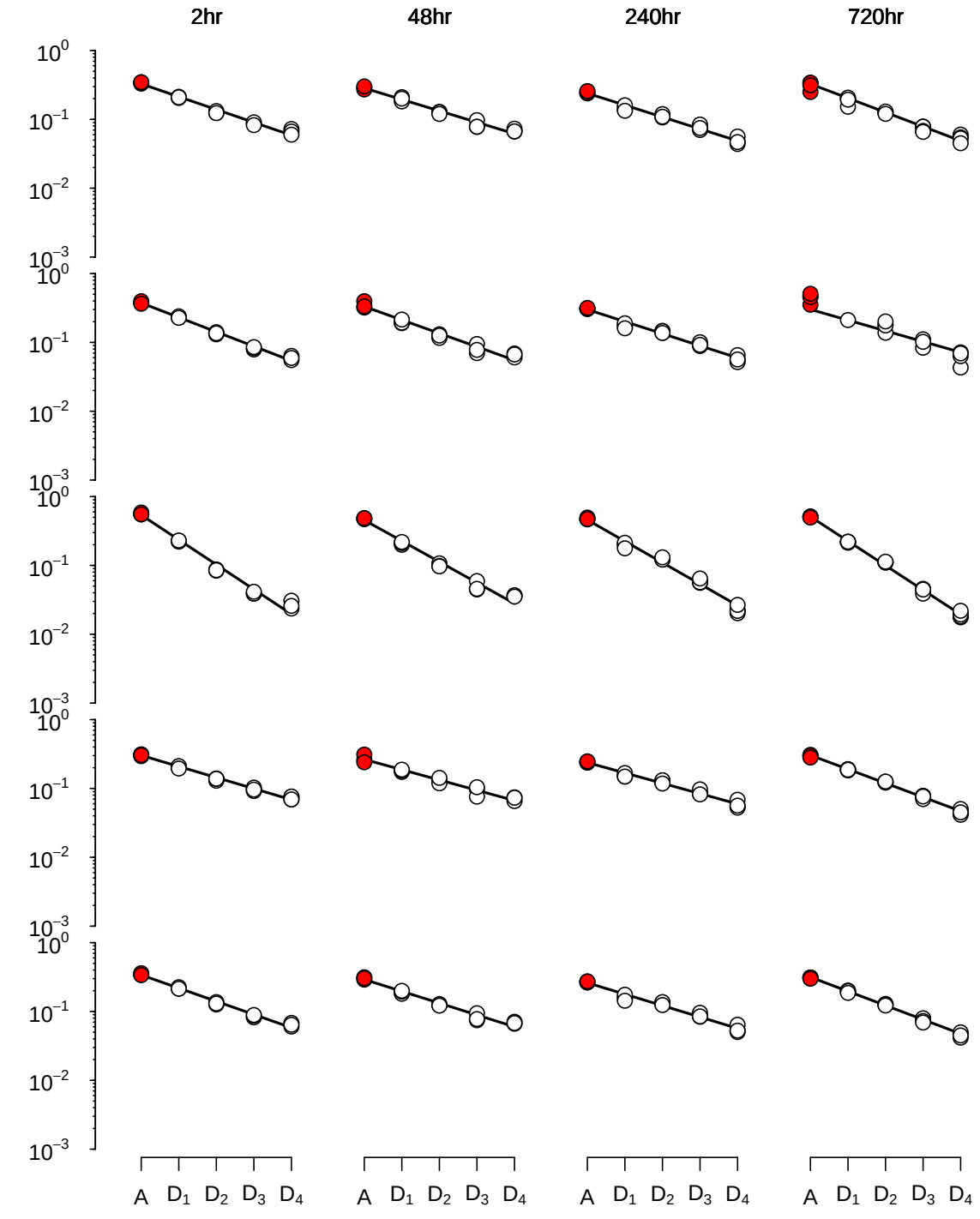
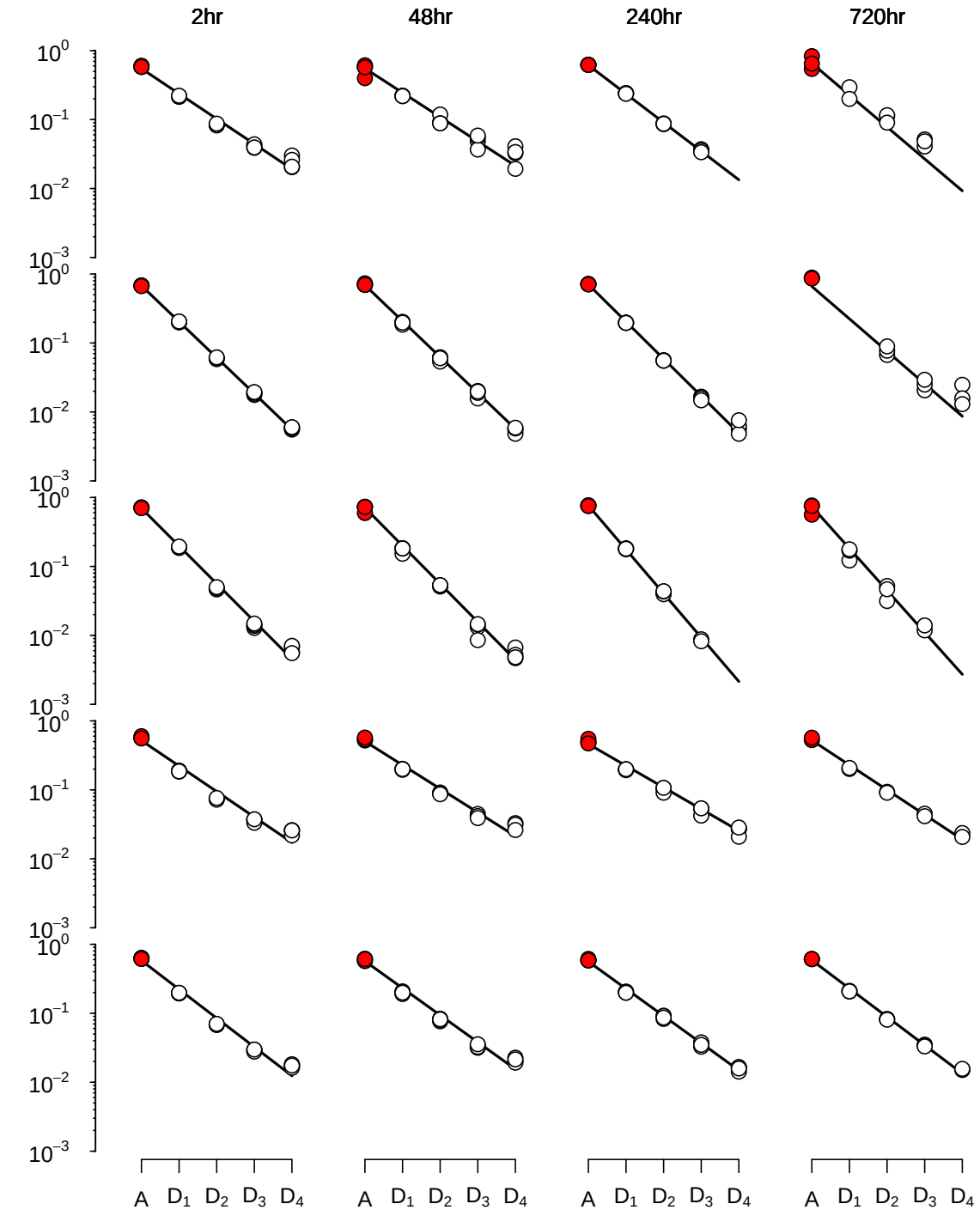
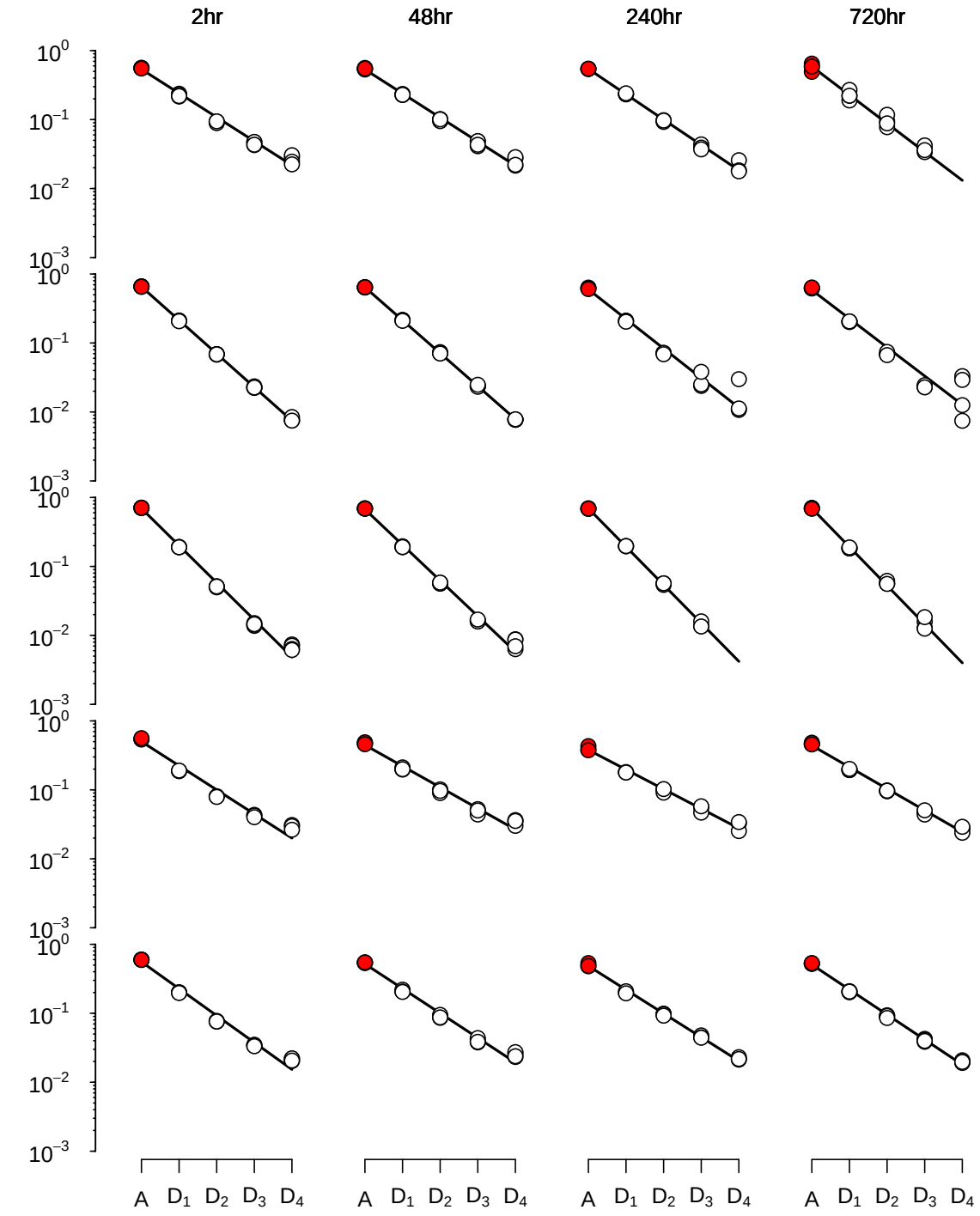


Figure A.6: Fit of RR model (lines) to observed aqueous concentrations (points)

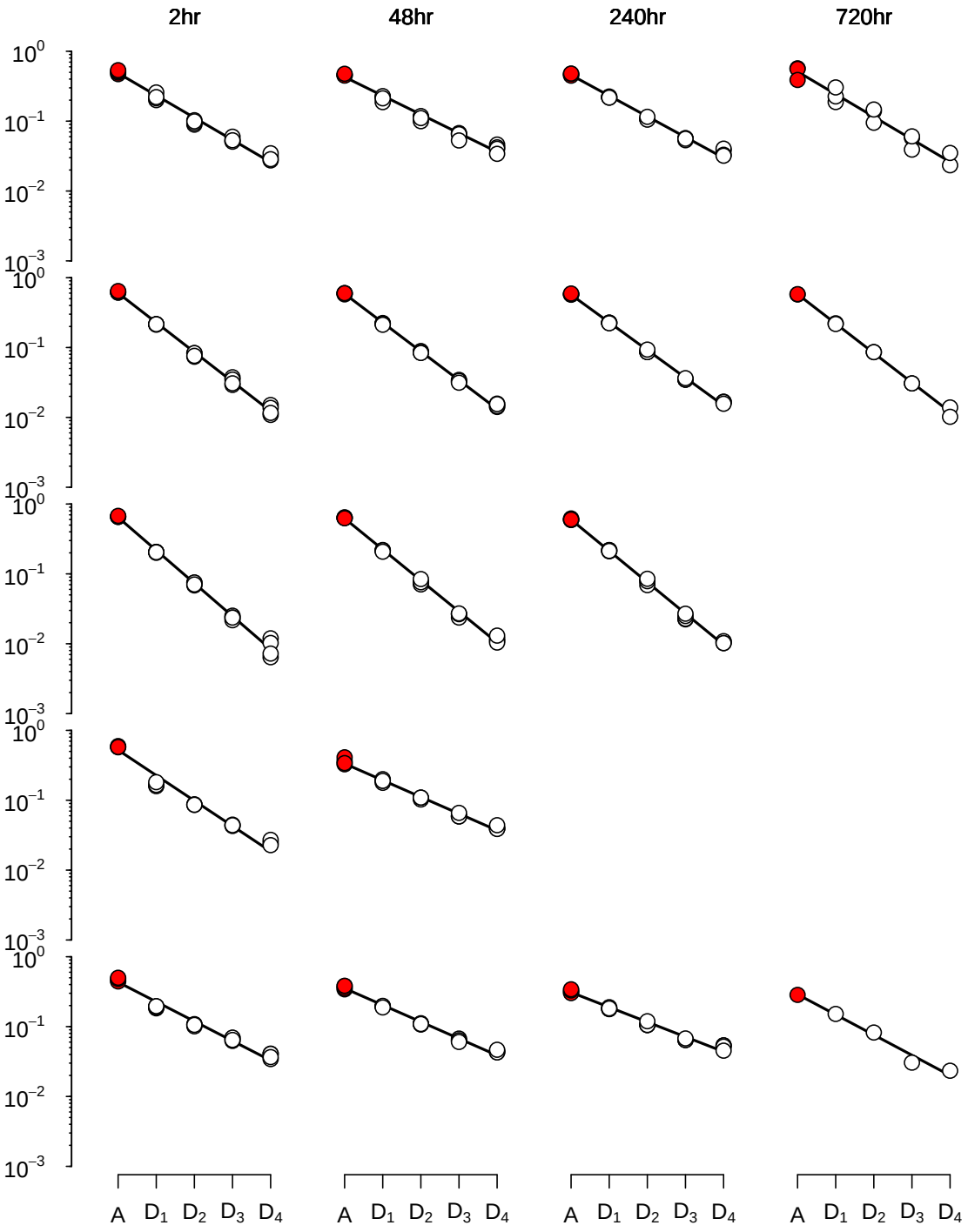

2hr
48hr
240hr
720hr
10^{0}
10^{-1}
10^{-2}
10^{-3}
A
D_1
D_2
D_3
D_4
ST



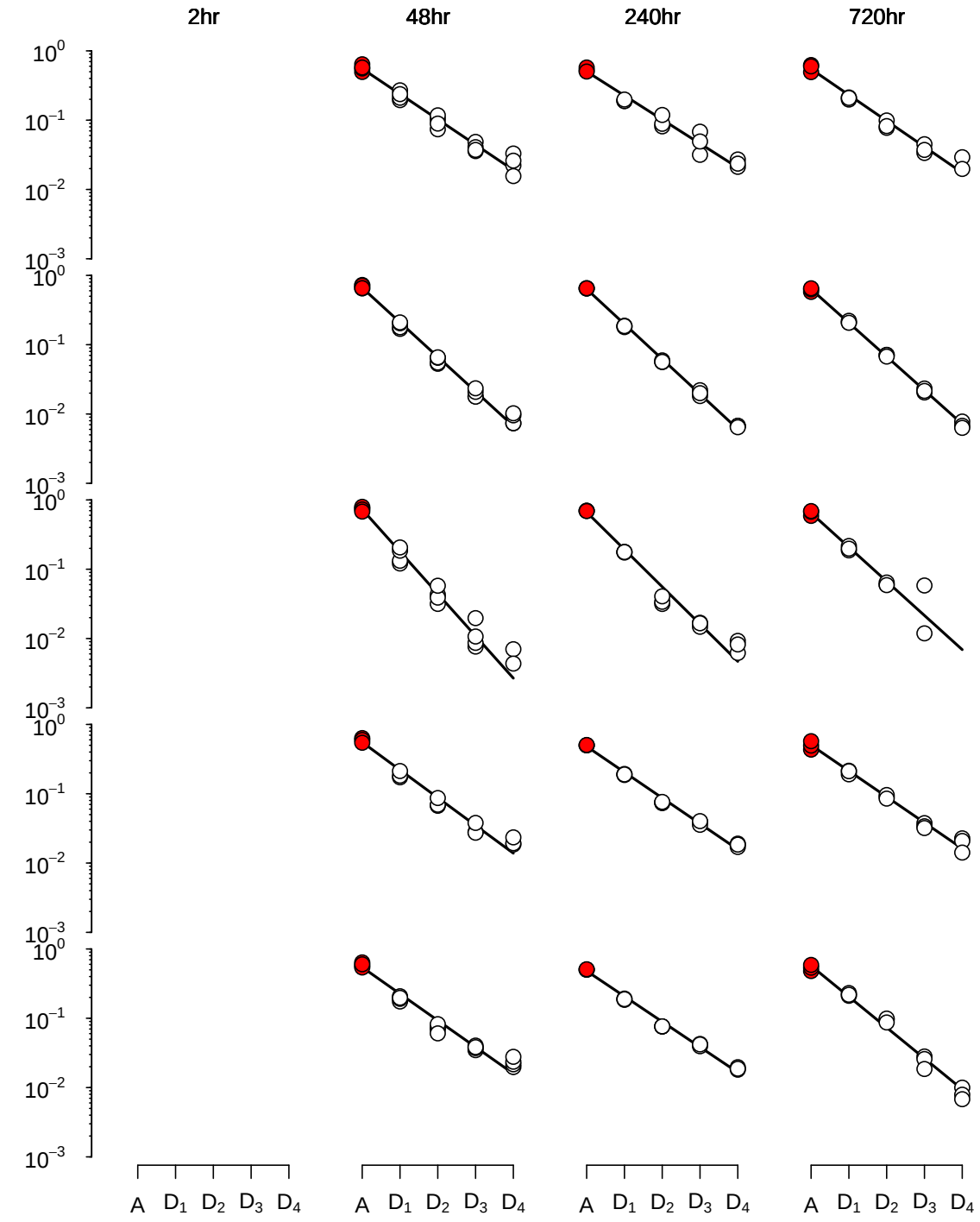
BT



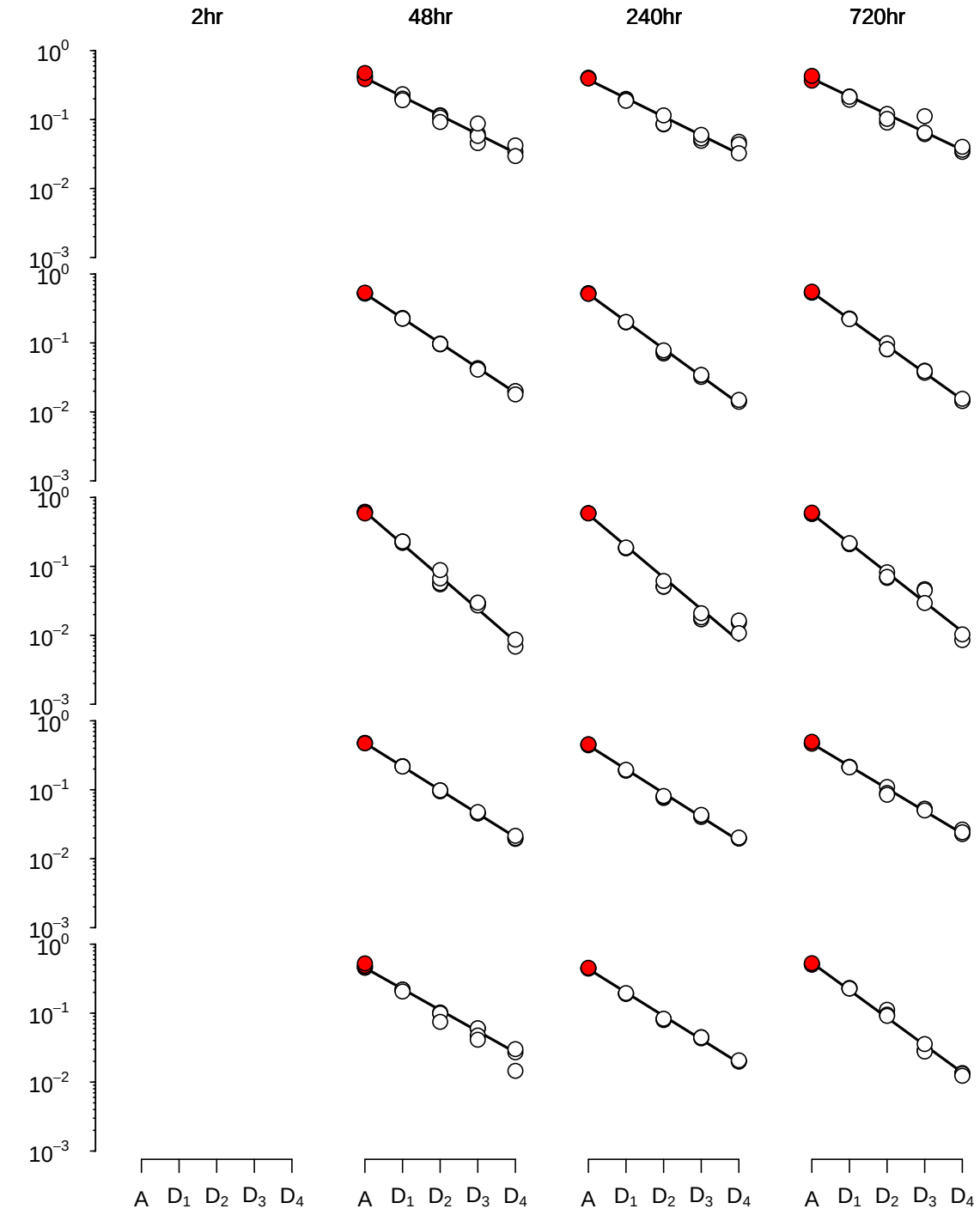
BA

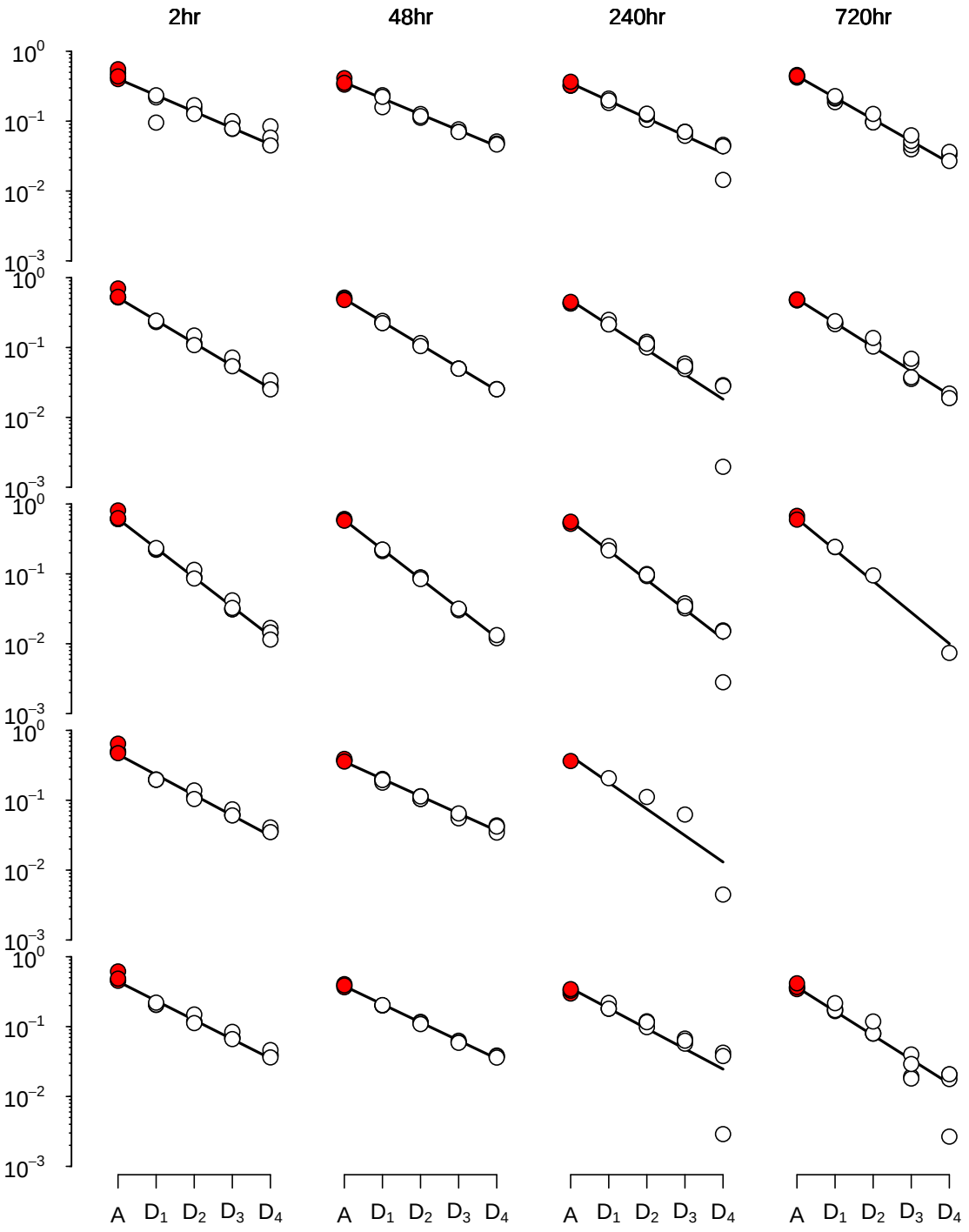


U

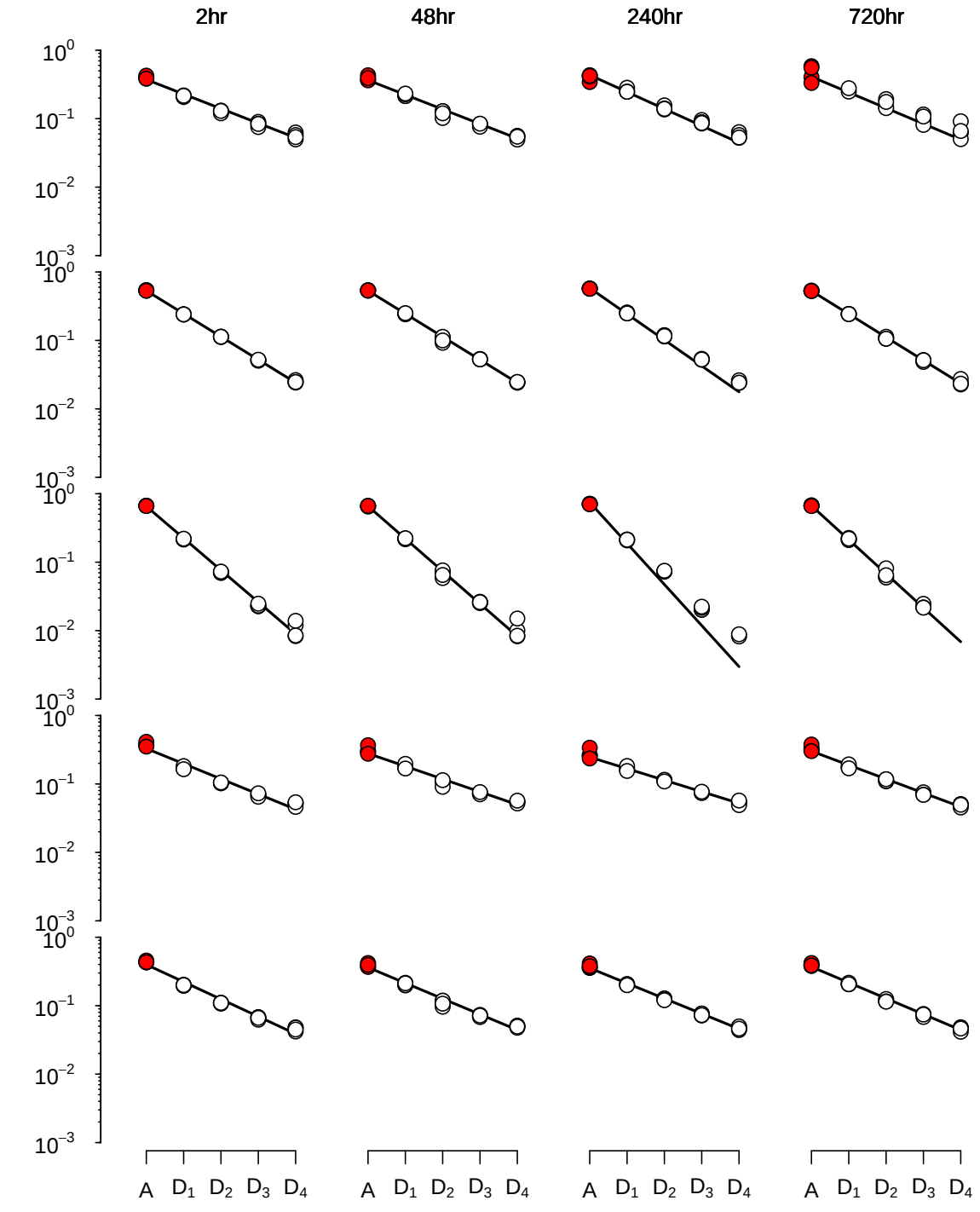


B

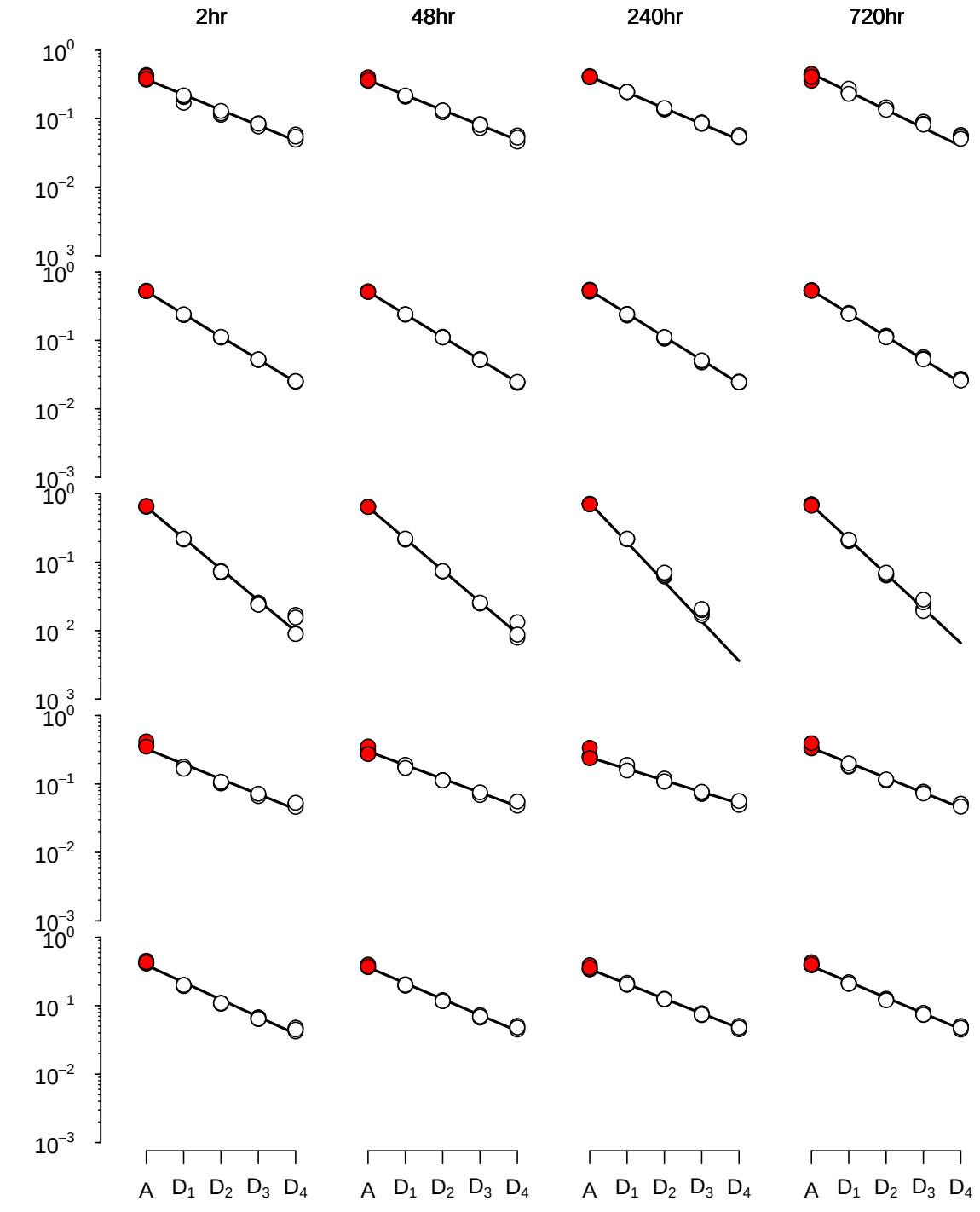

2hr
48hr
240hr
720hr
10^{0}
10^{-1}
10^{-2}
10^{-3}
A
D_1
D_2
D_3
D_4
FT



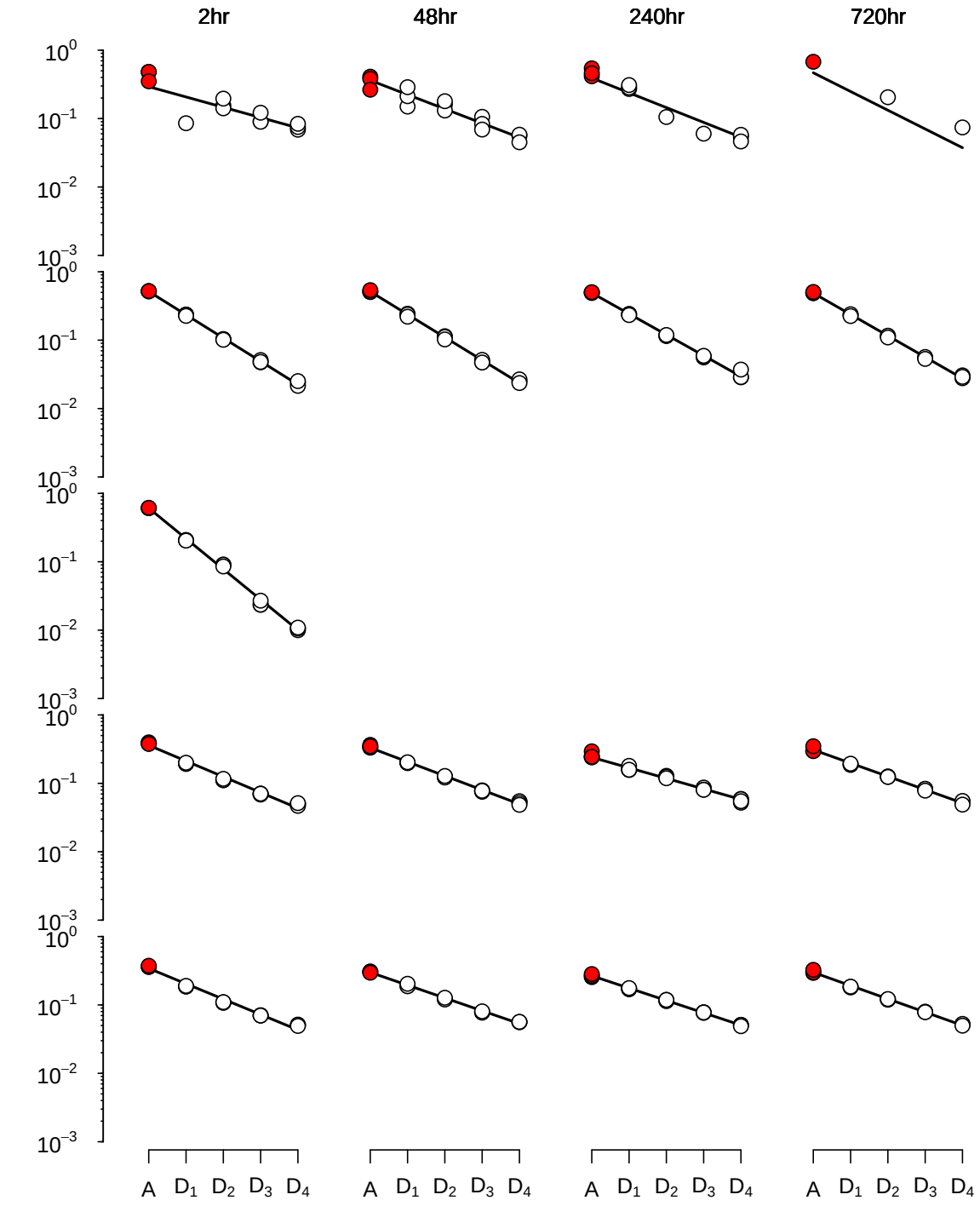
SOU



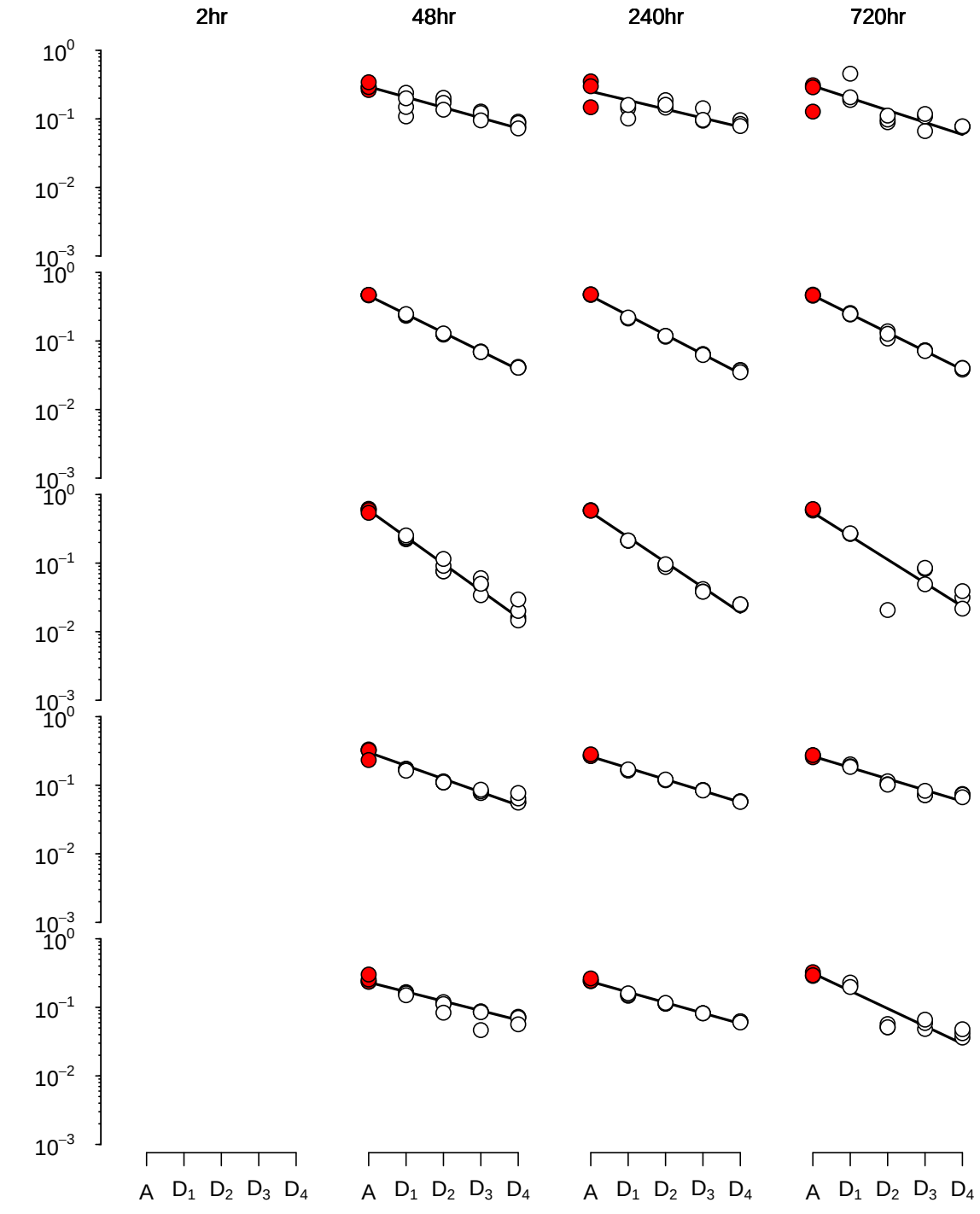
W1

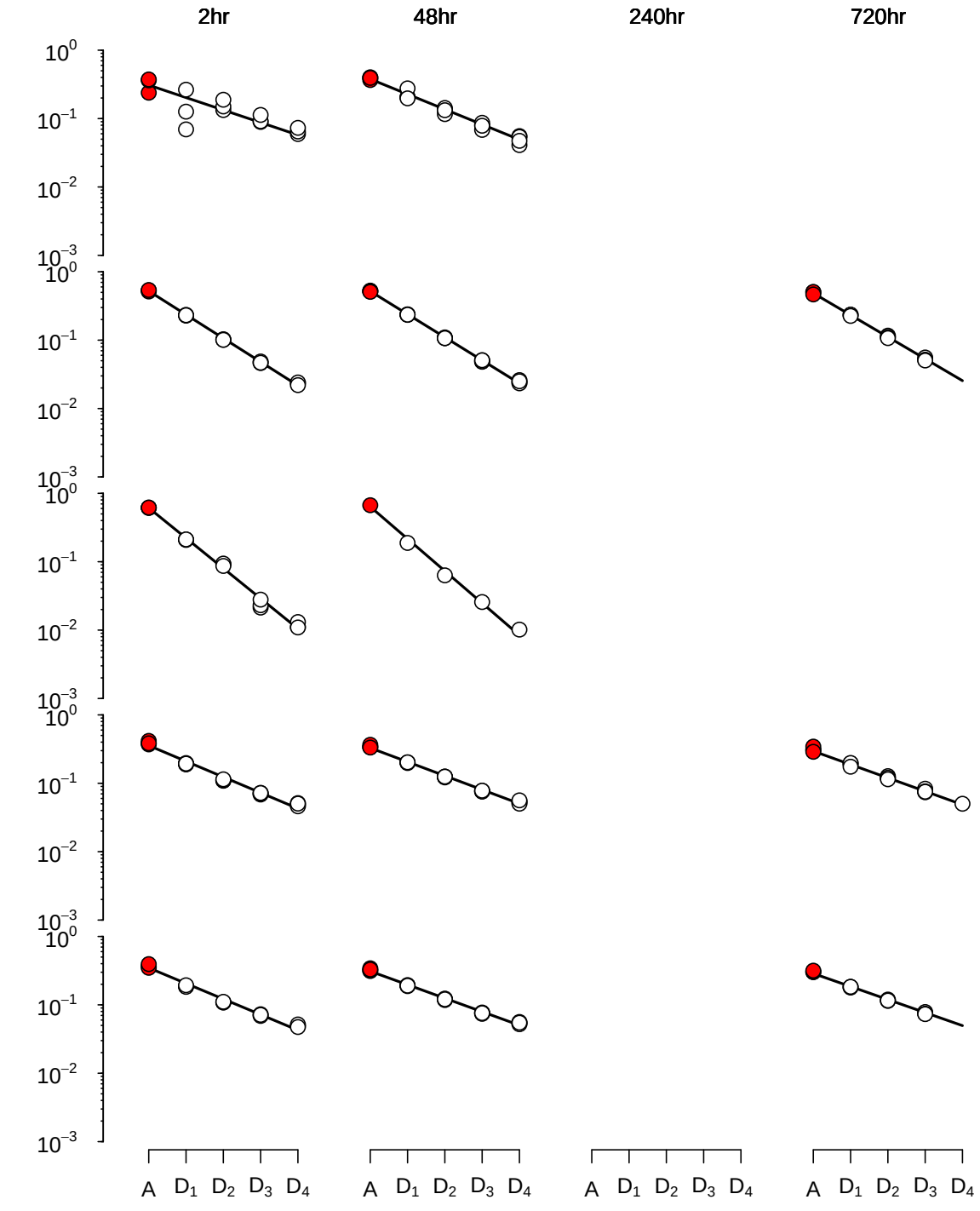


W2

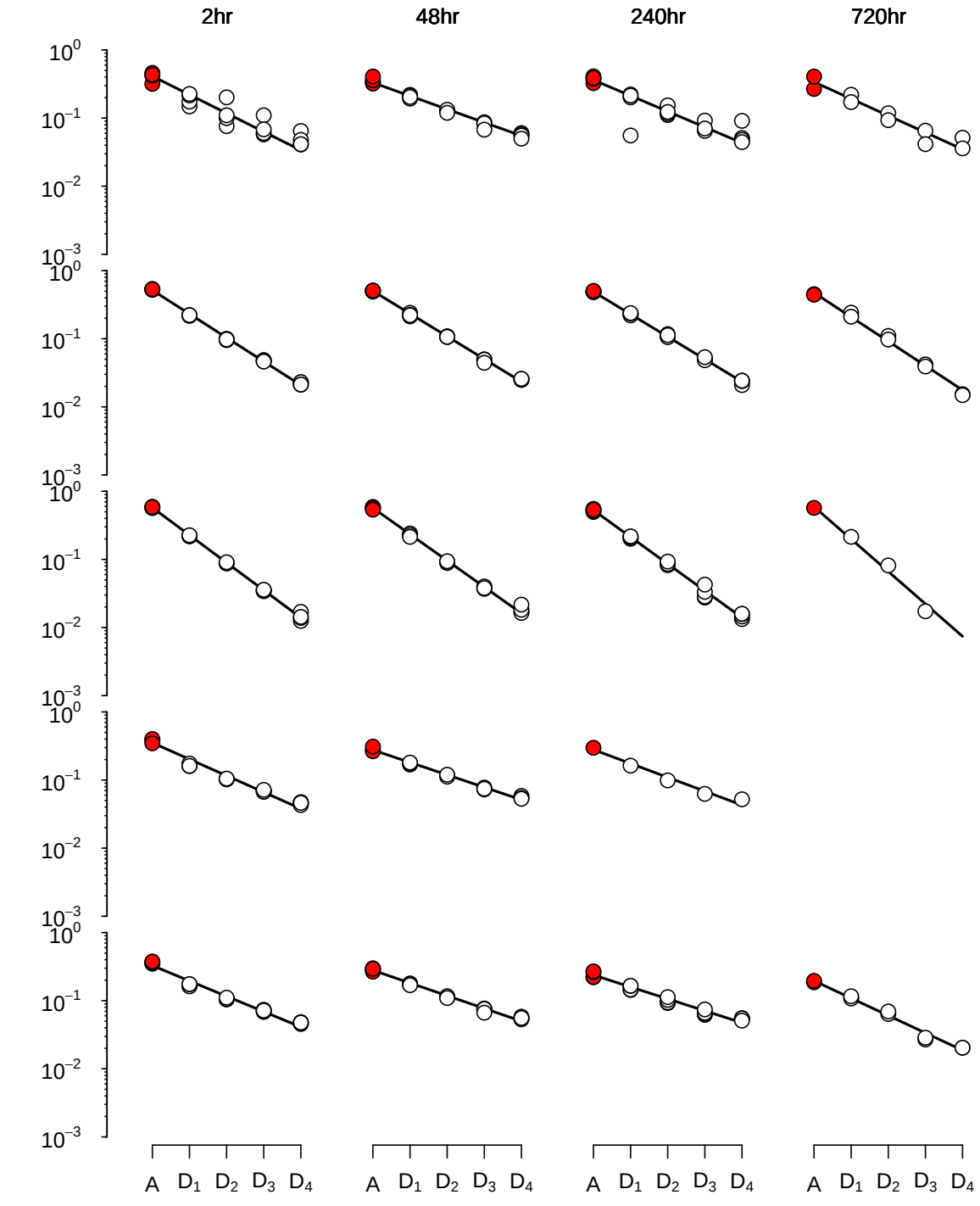


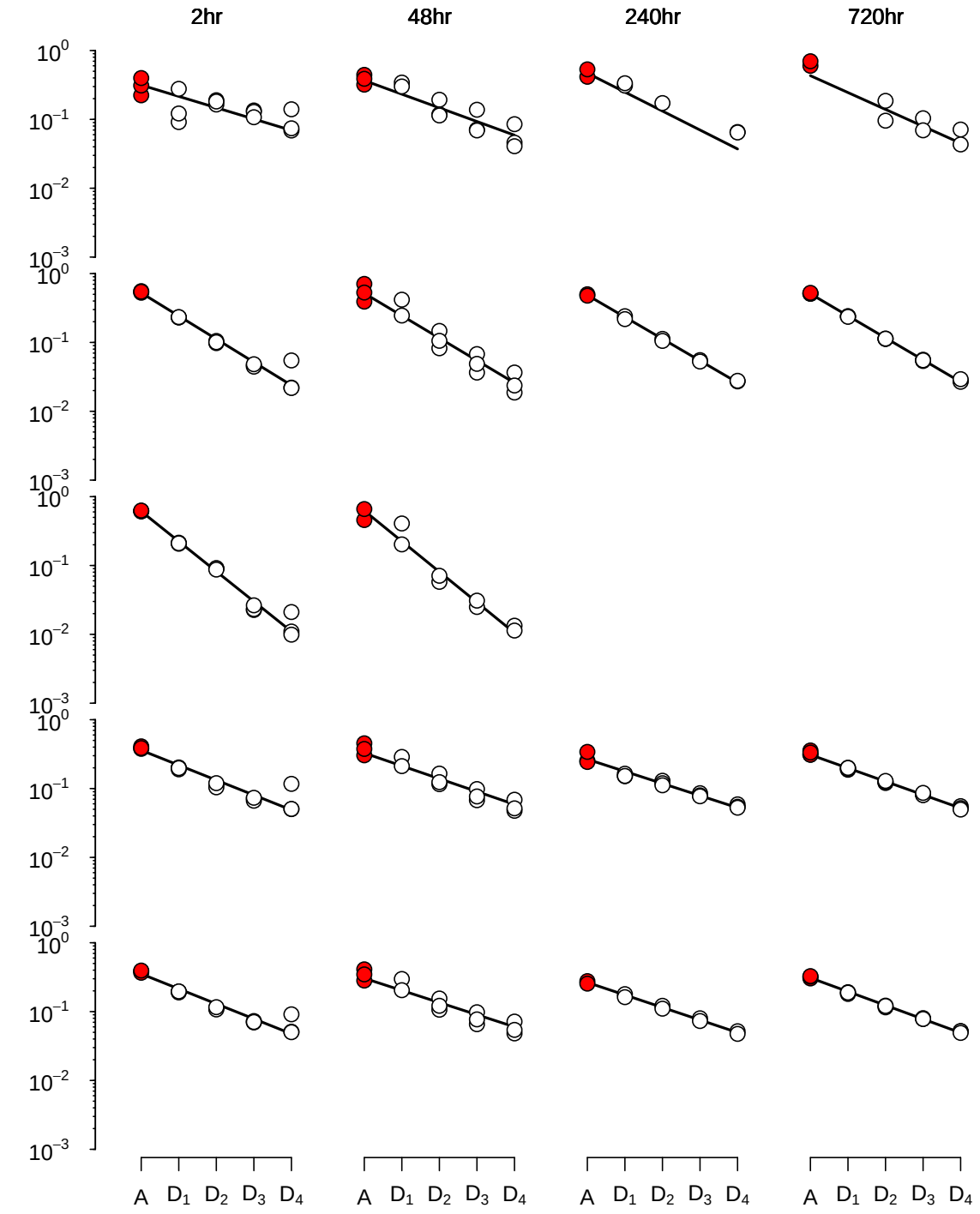
SAS


2hr
48hr
240hr
720hr
10^{0}
10^{-1}
10^{-2}
10^{-3}
A
D_1
D_2
D_3
D_4
CM

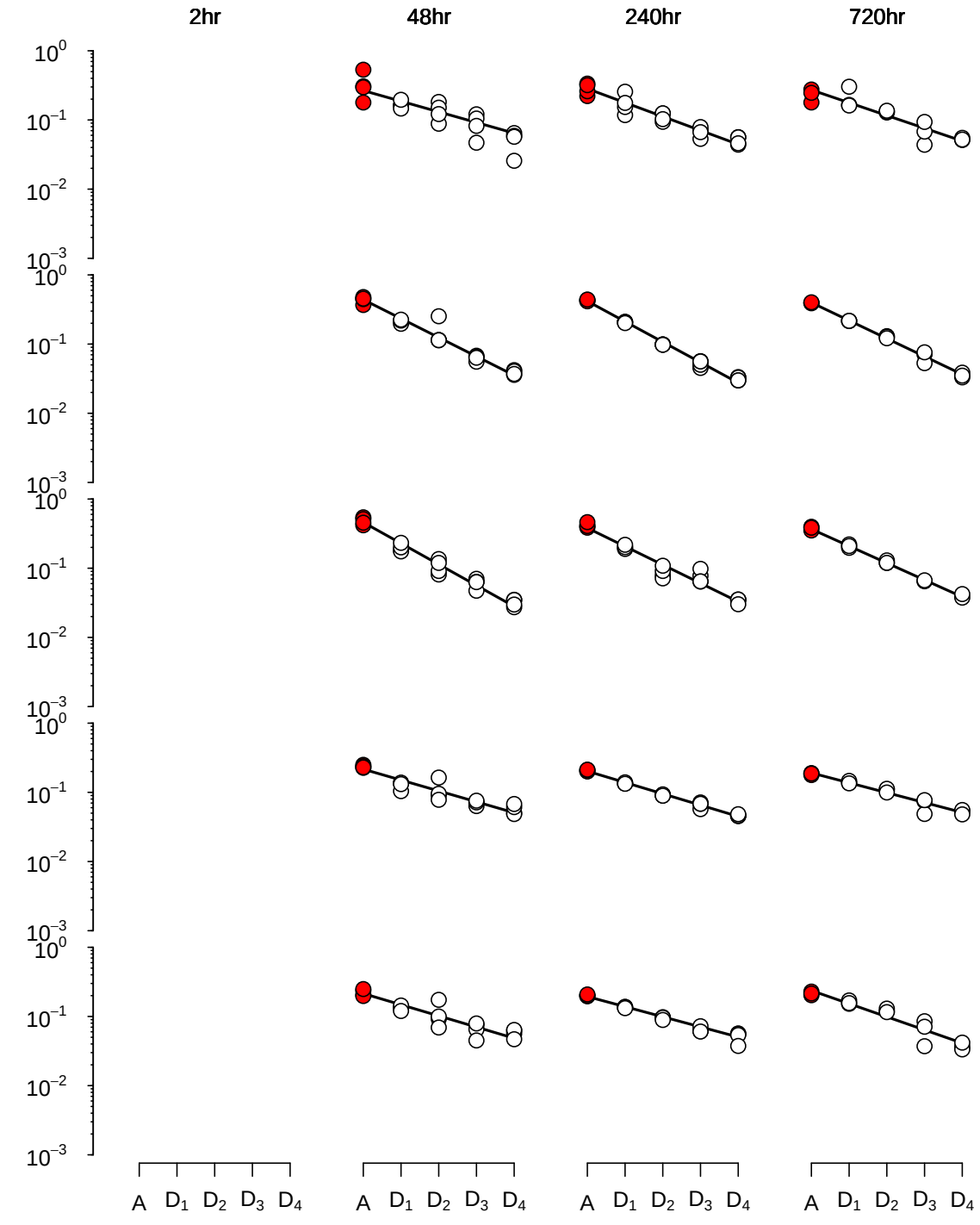


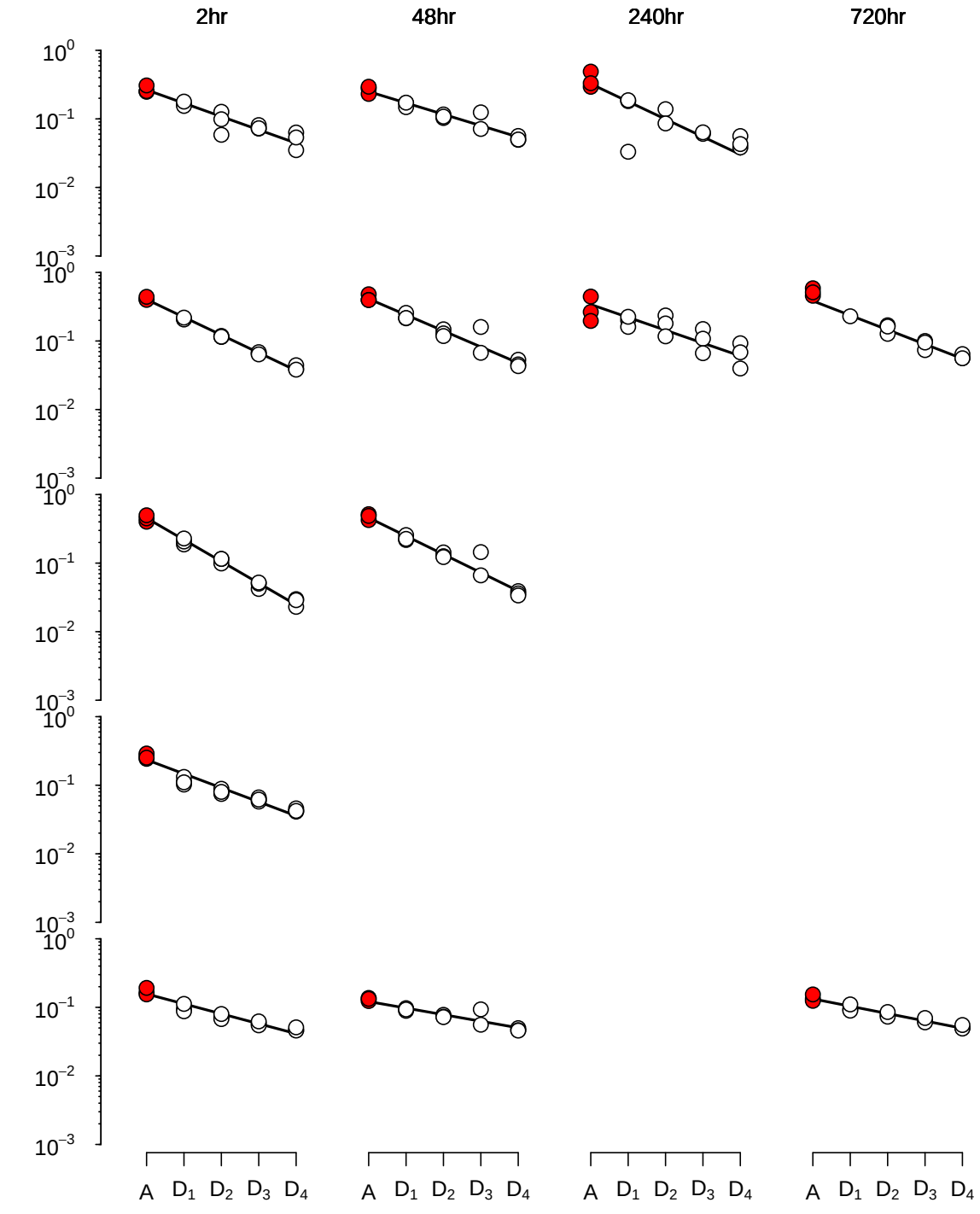
SSL


2hr
48hr
240hr
720hr
10^{0}
10^{-1}
10^{-2}
10^{-3}
A
D_1
D_2
D_3
D_4
MPK

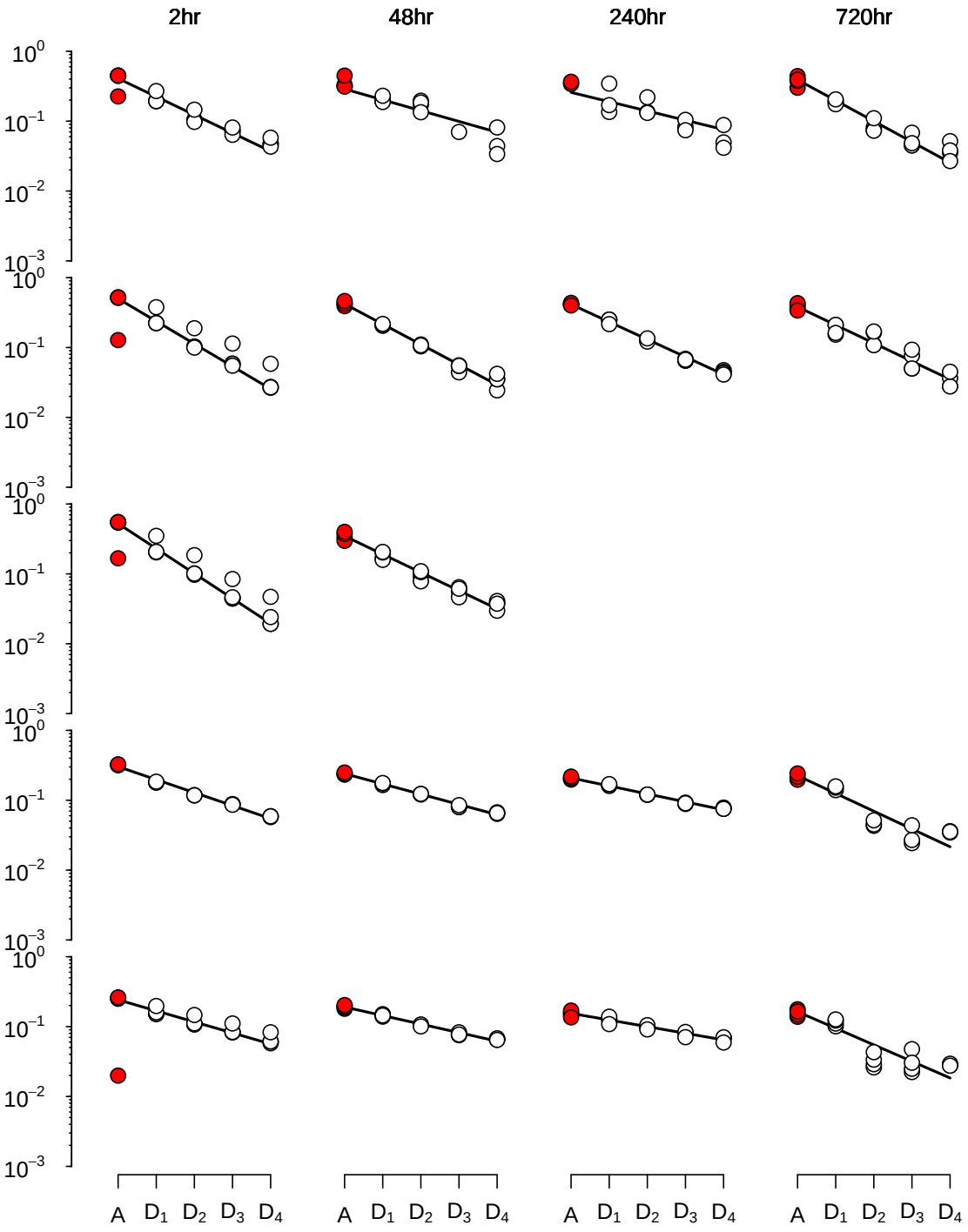


S2

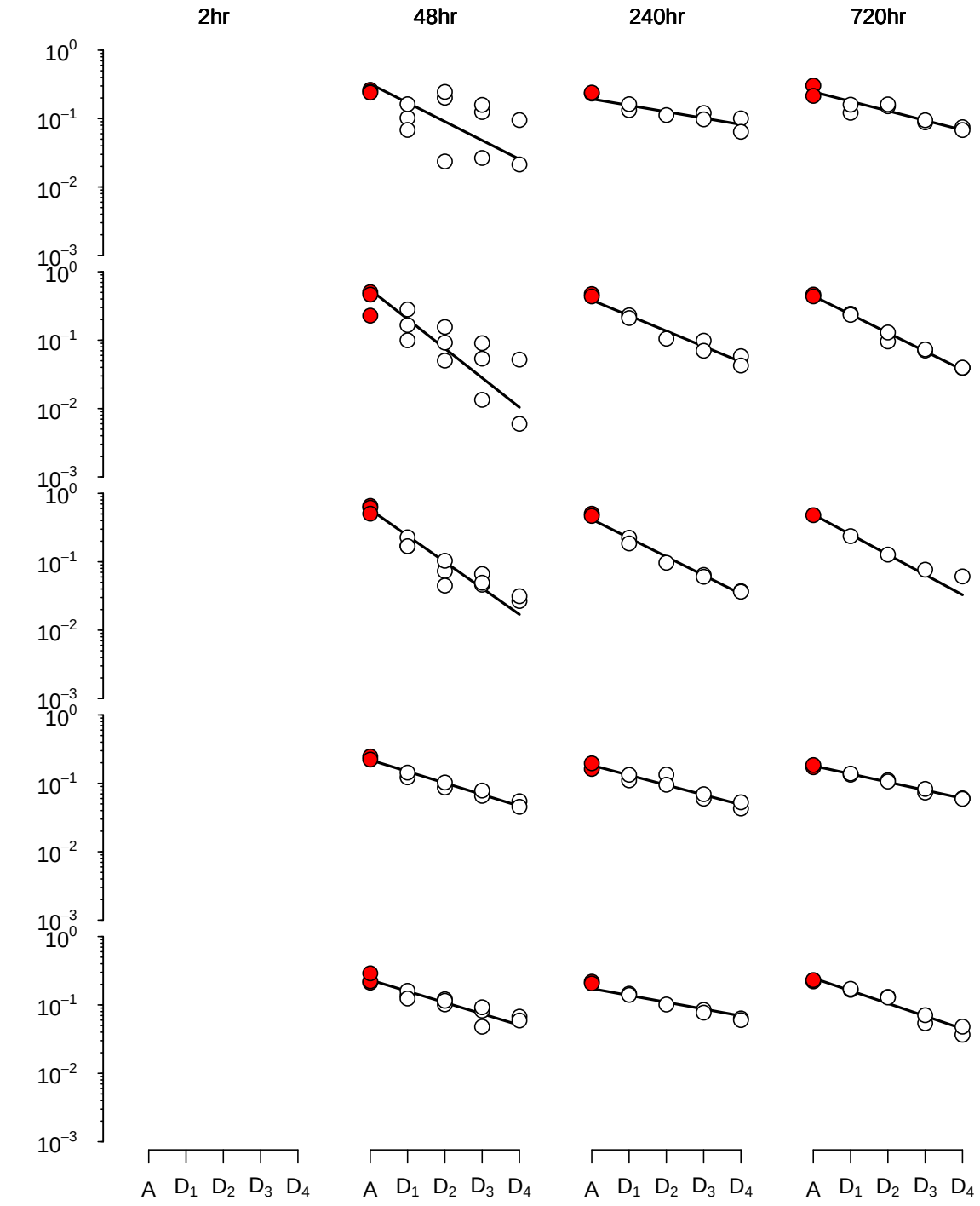

2hr
48hr
240hr
720hr
10^{0}
10^{-1}
10^{-2}
10^{-3}
A
D_1
D_2
D_3
D_4
W



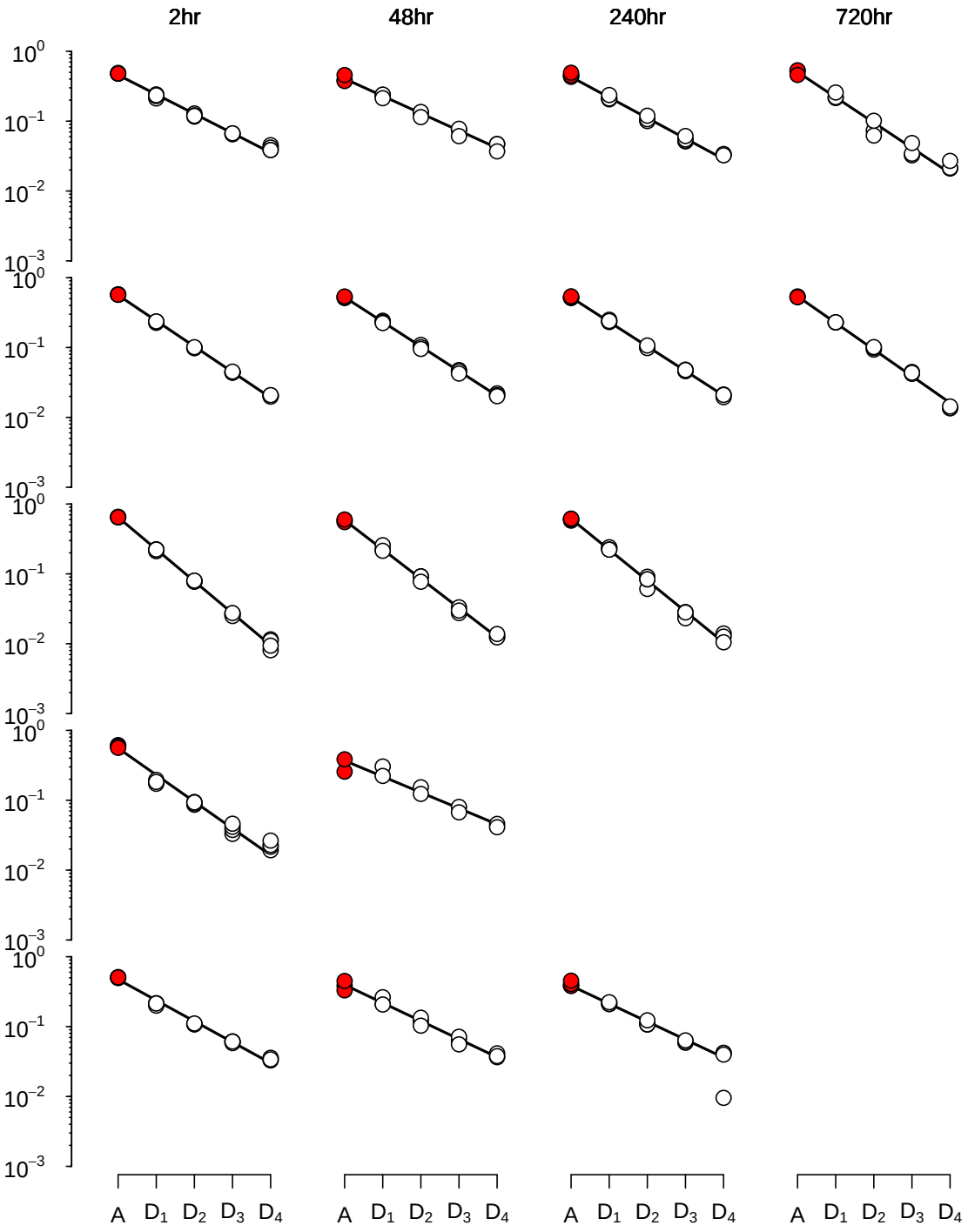
AM



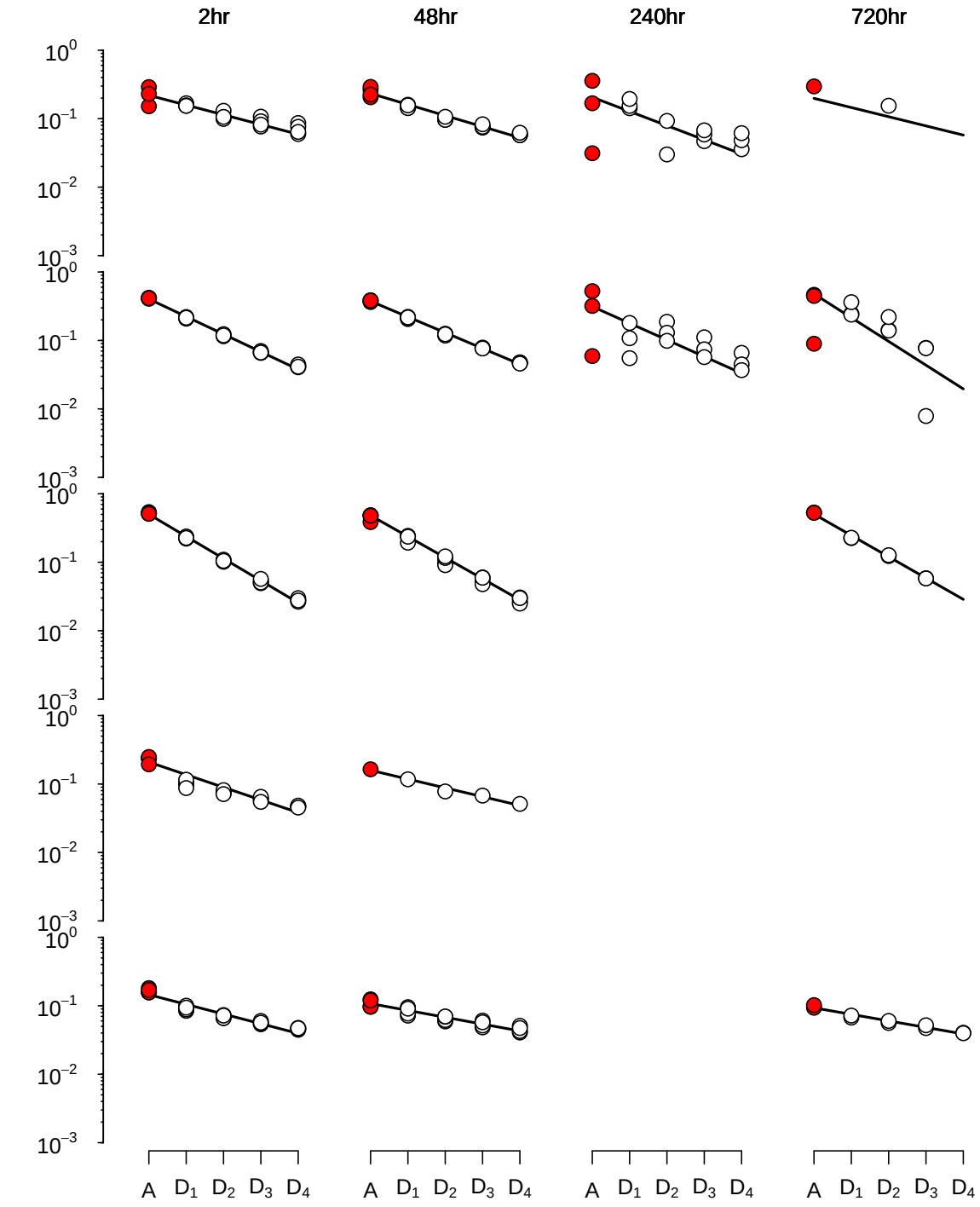
H



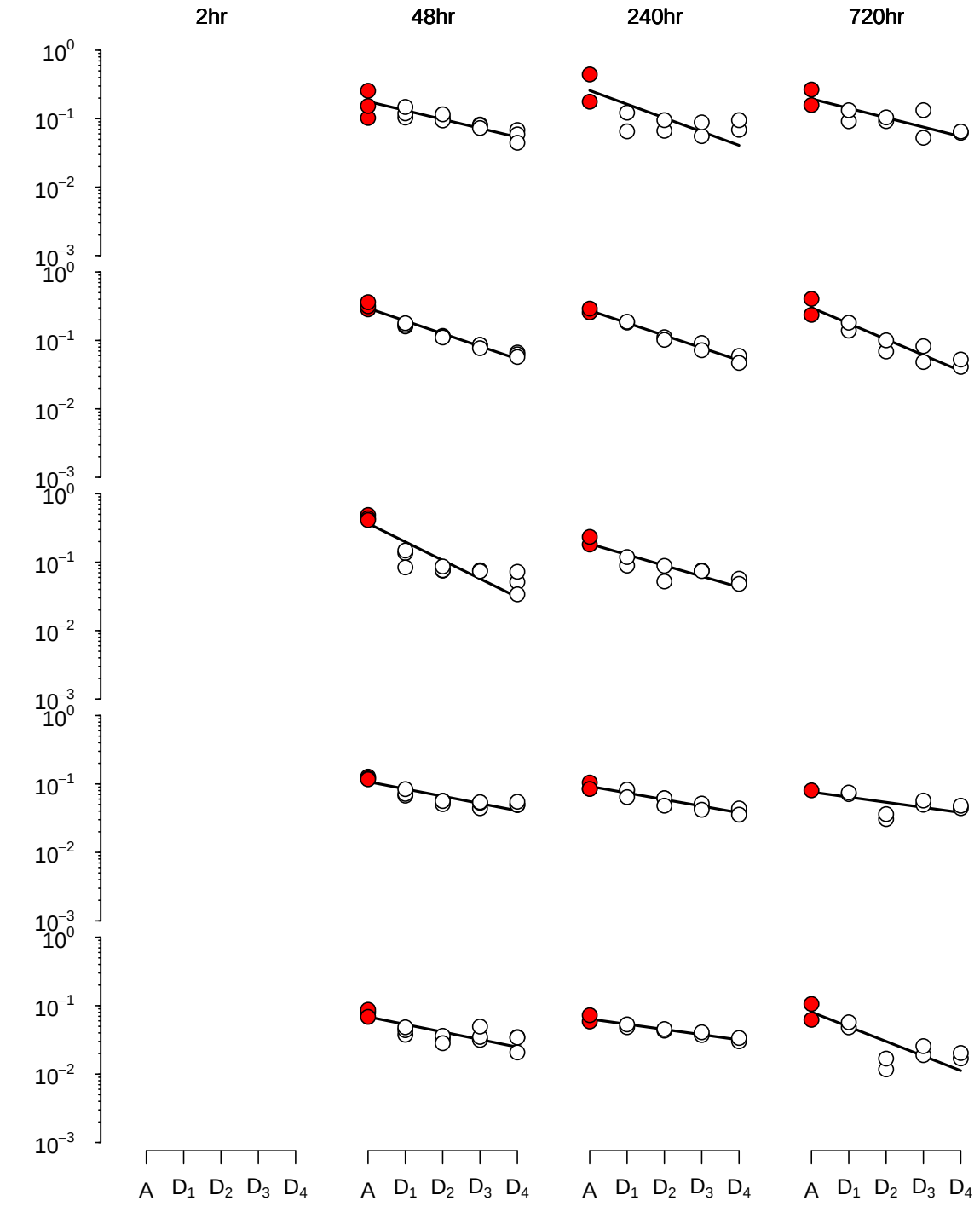
BOX



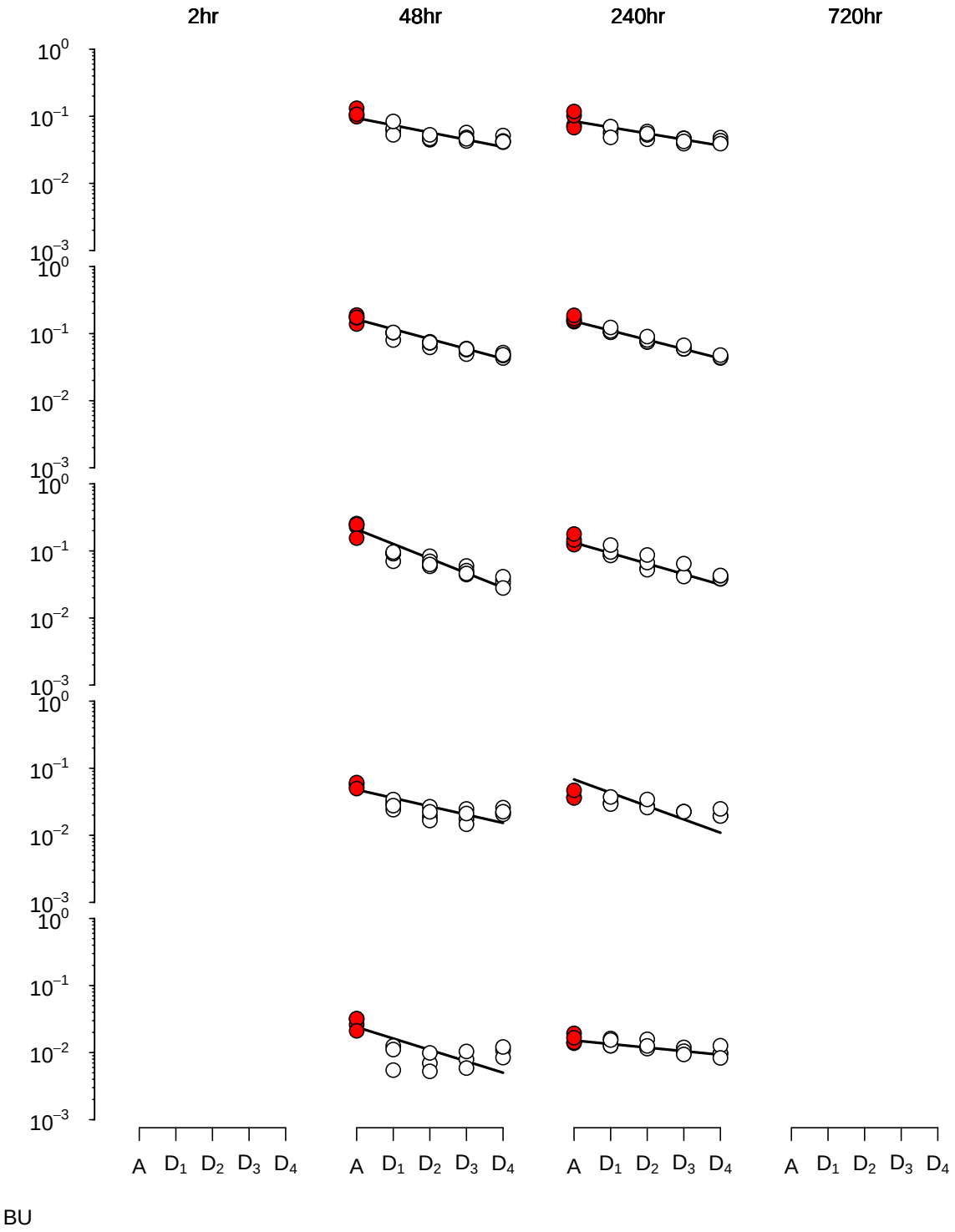
GUA

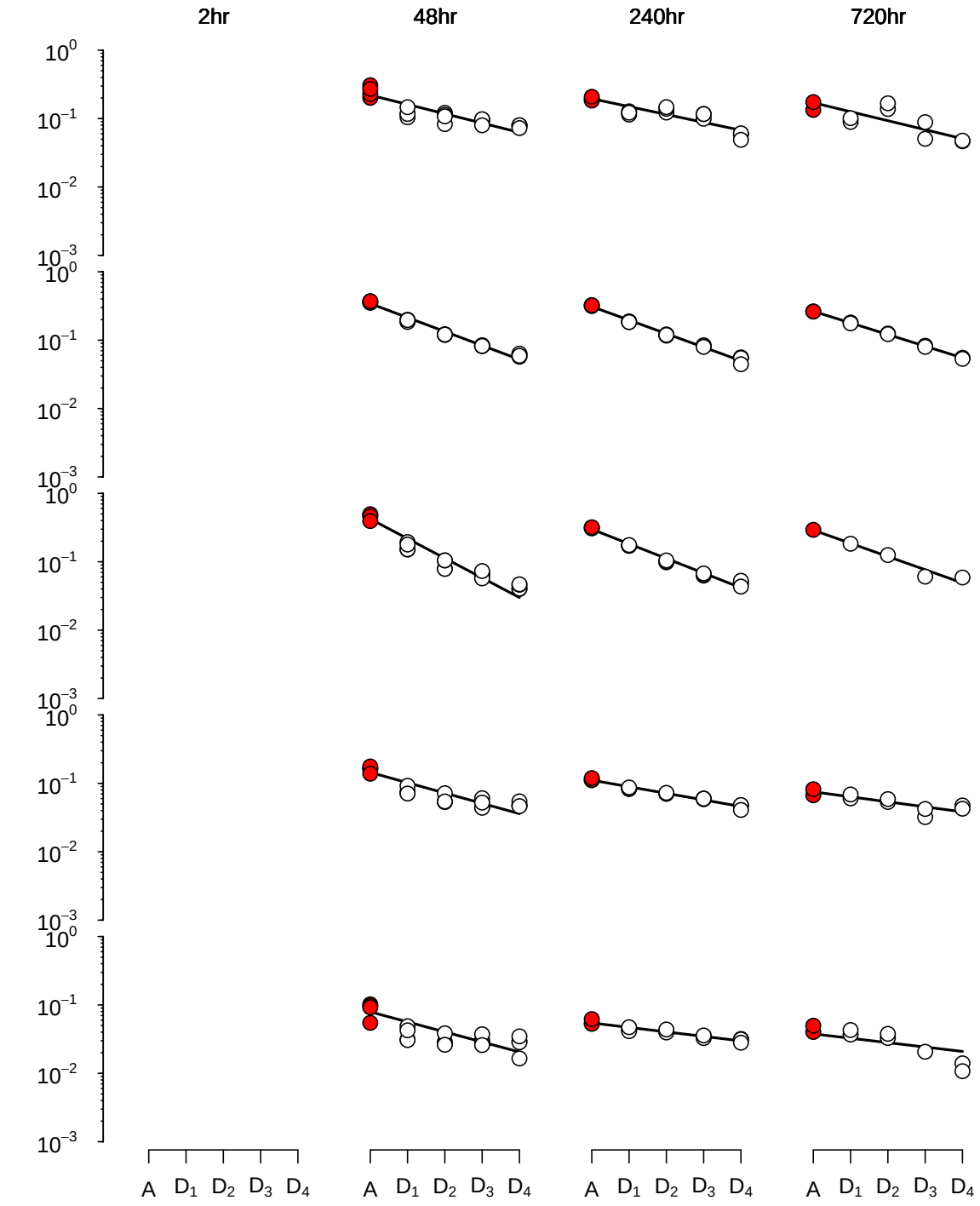


ELL

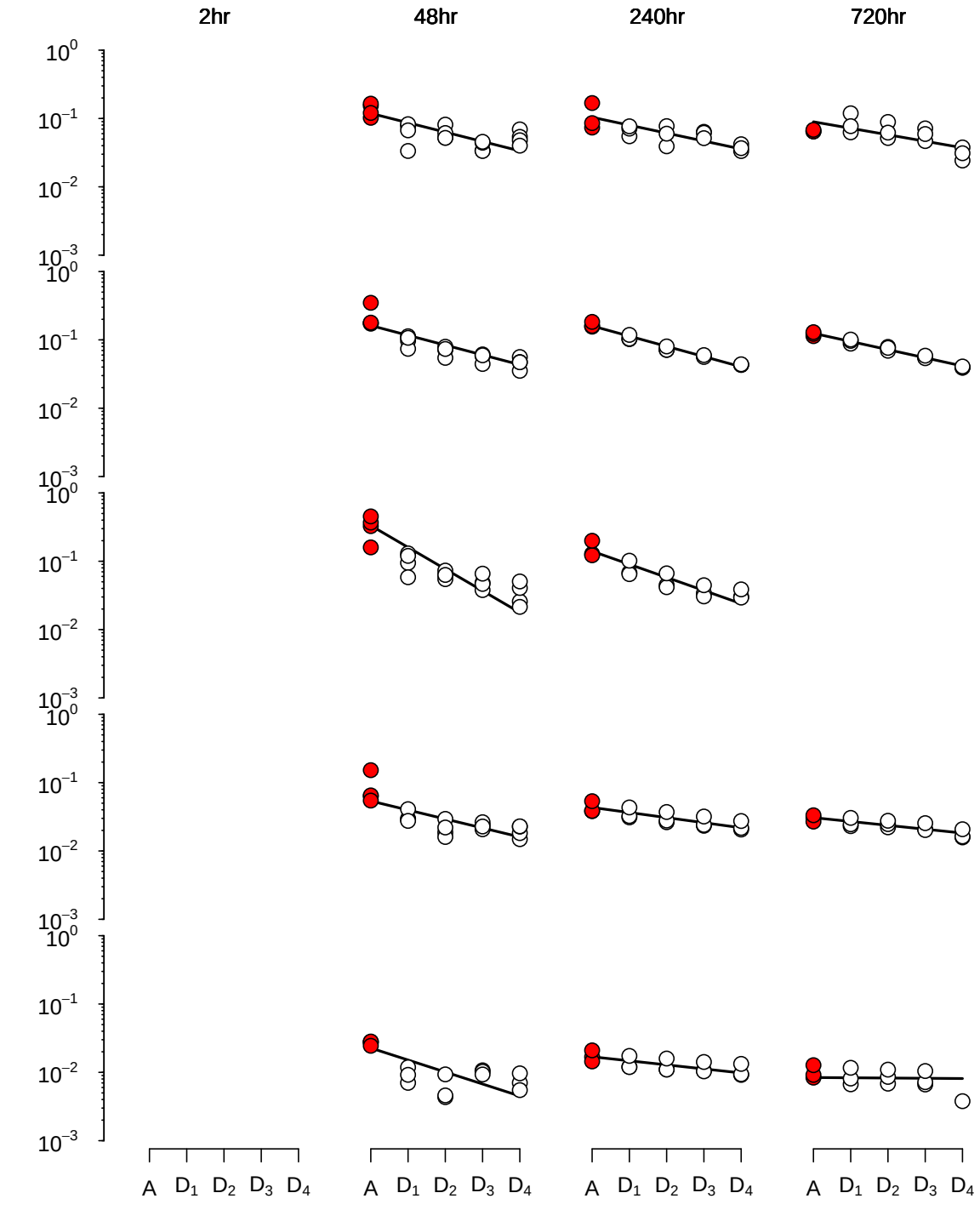


PO

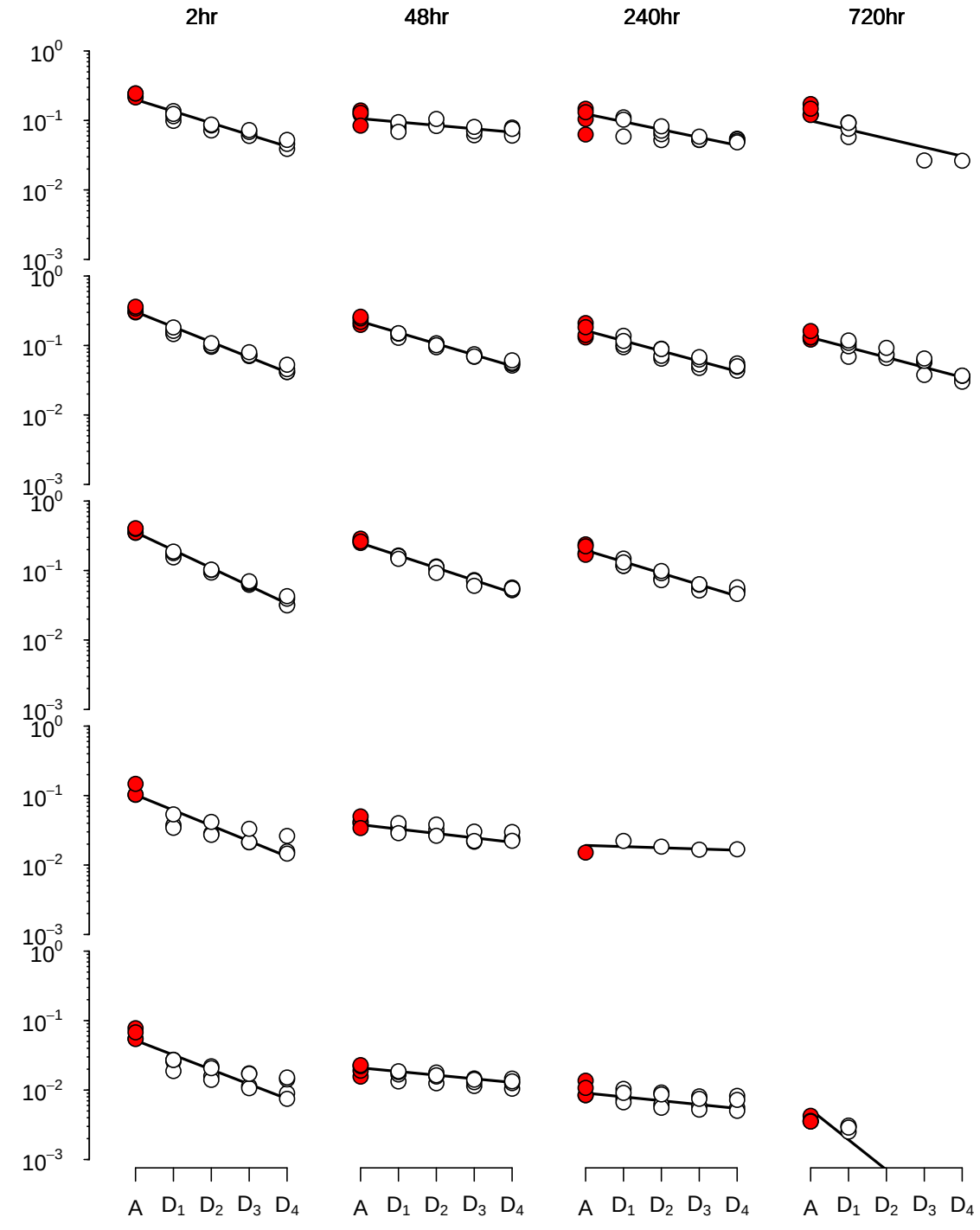

2hr
48hr
240hr
720hr
10^{0}
10^{-1}
10^{-2}
10^{-3}
A
D_1
D_2
D_3
D_4
BU



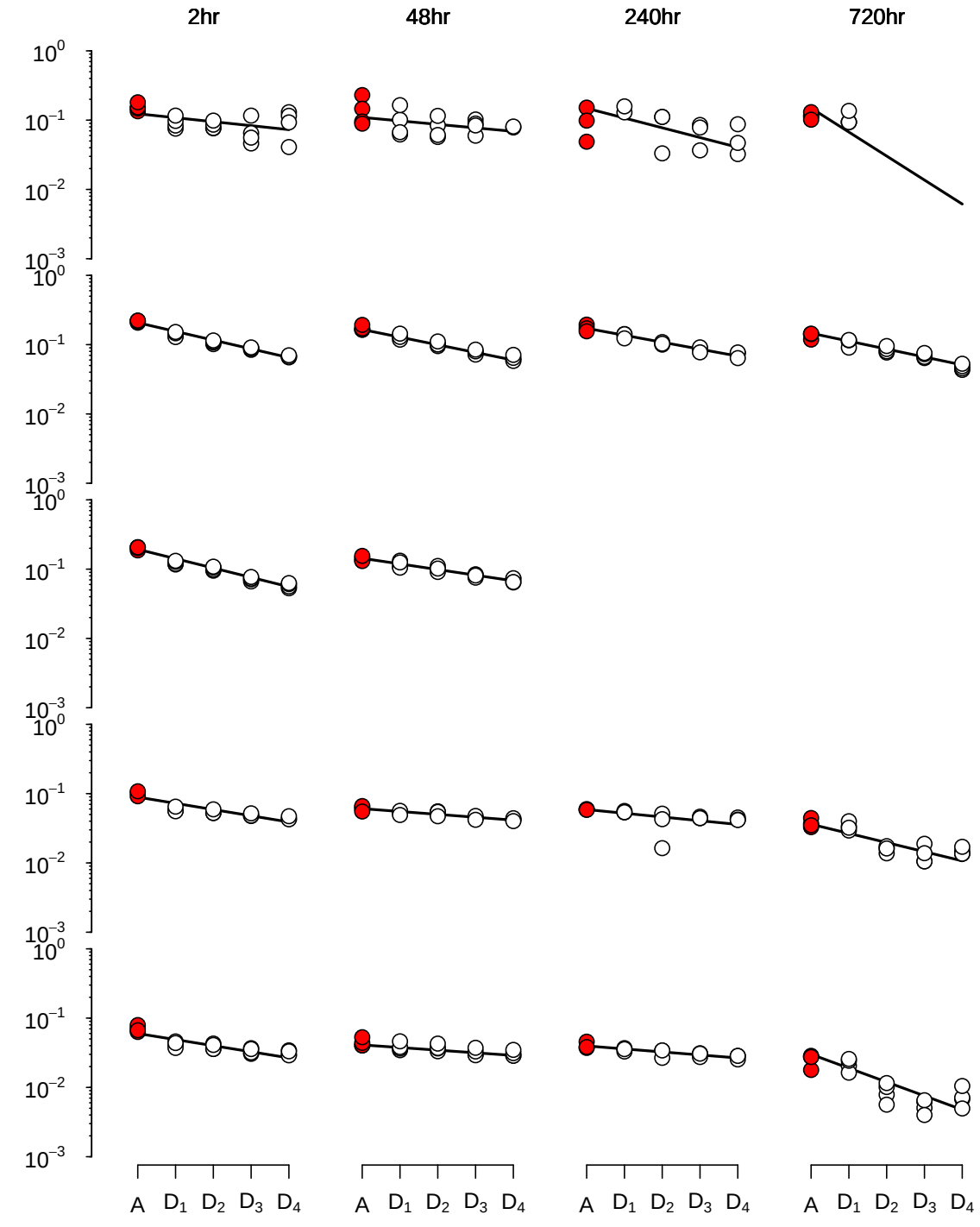
LCL

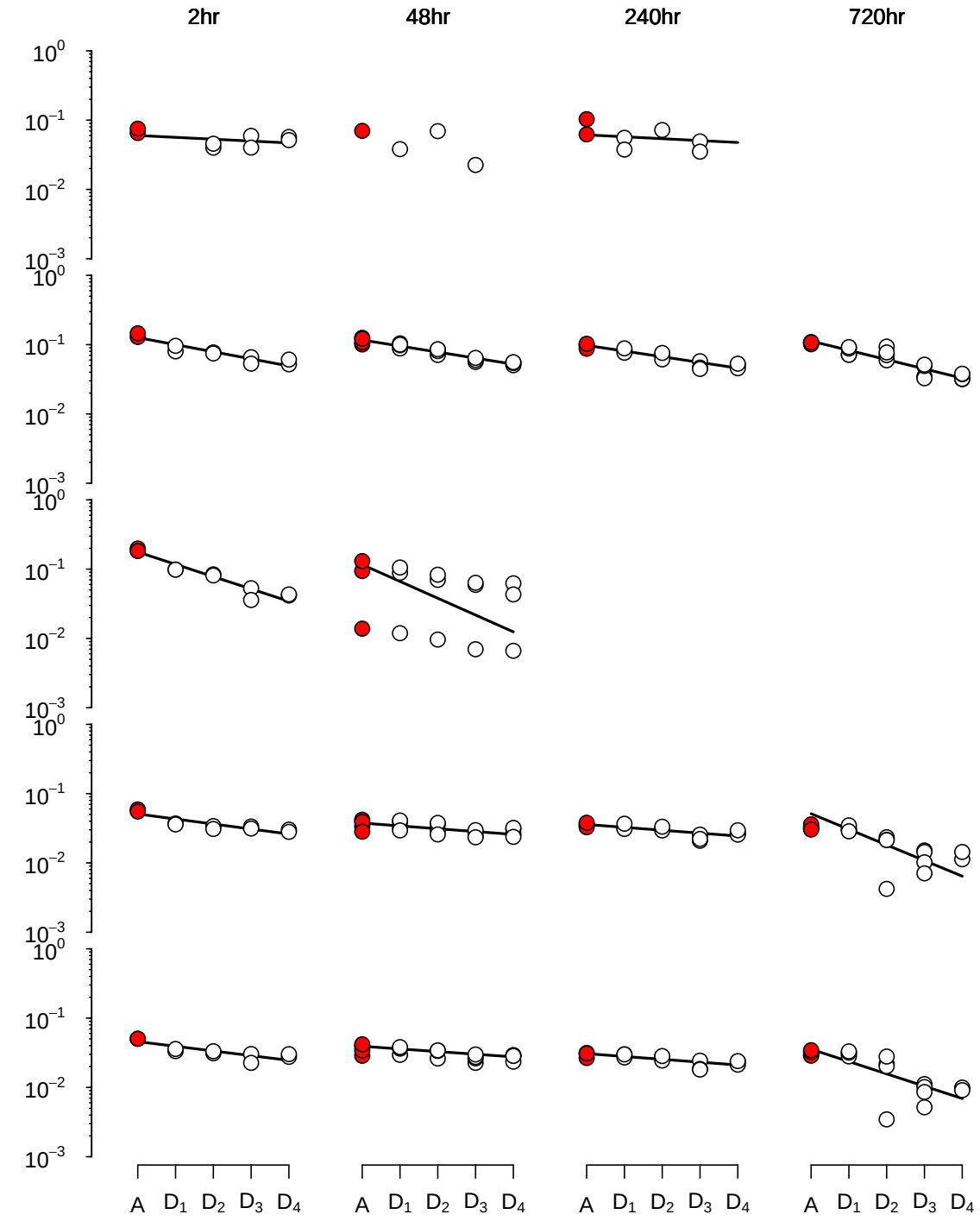


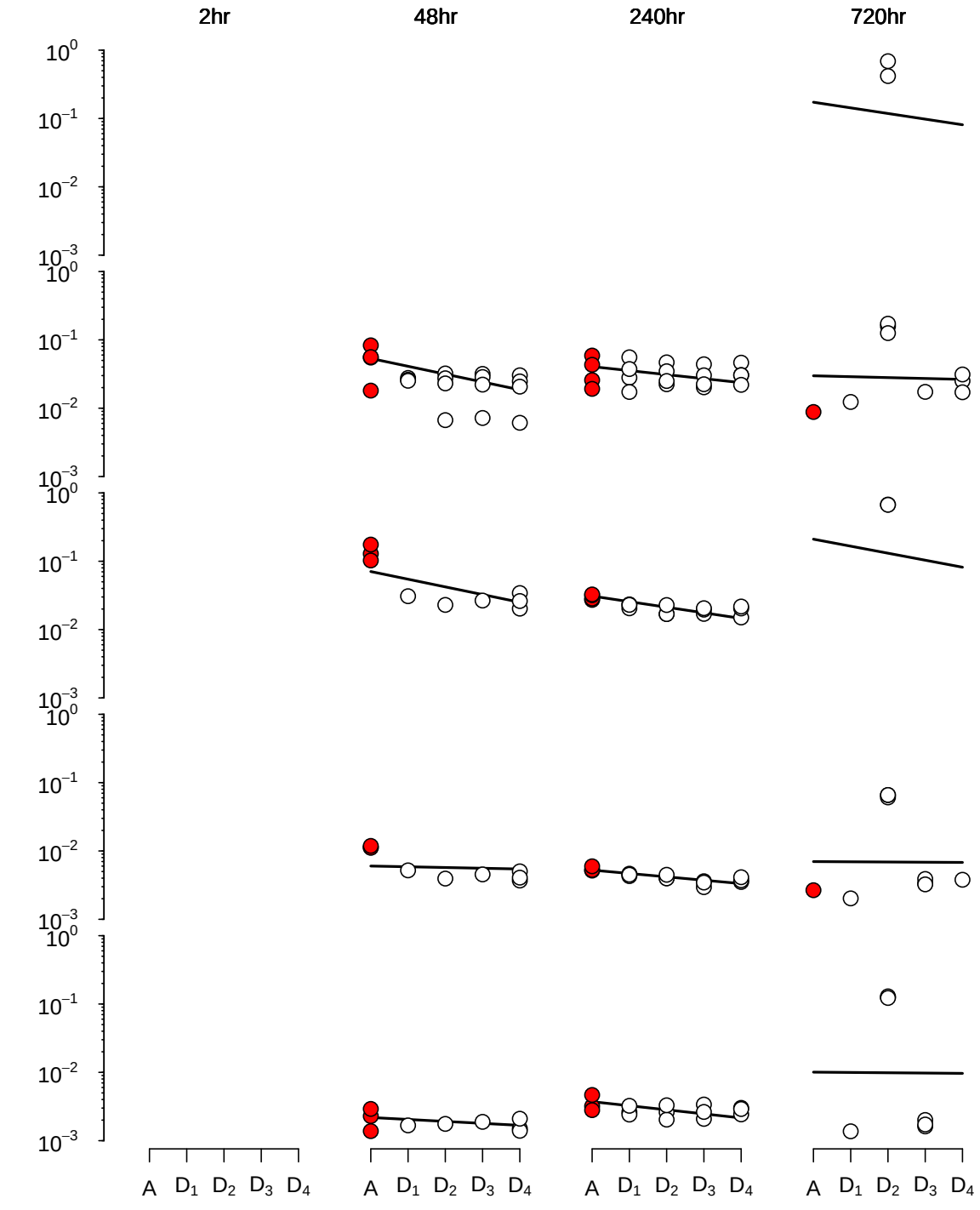
LCO

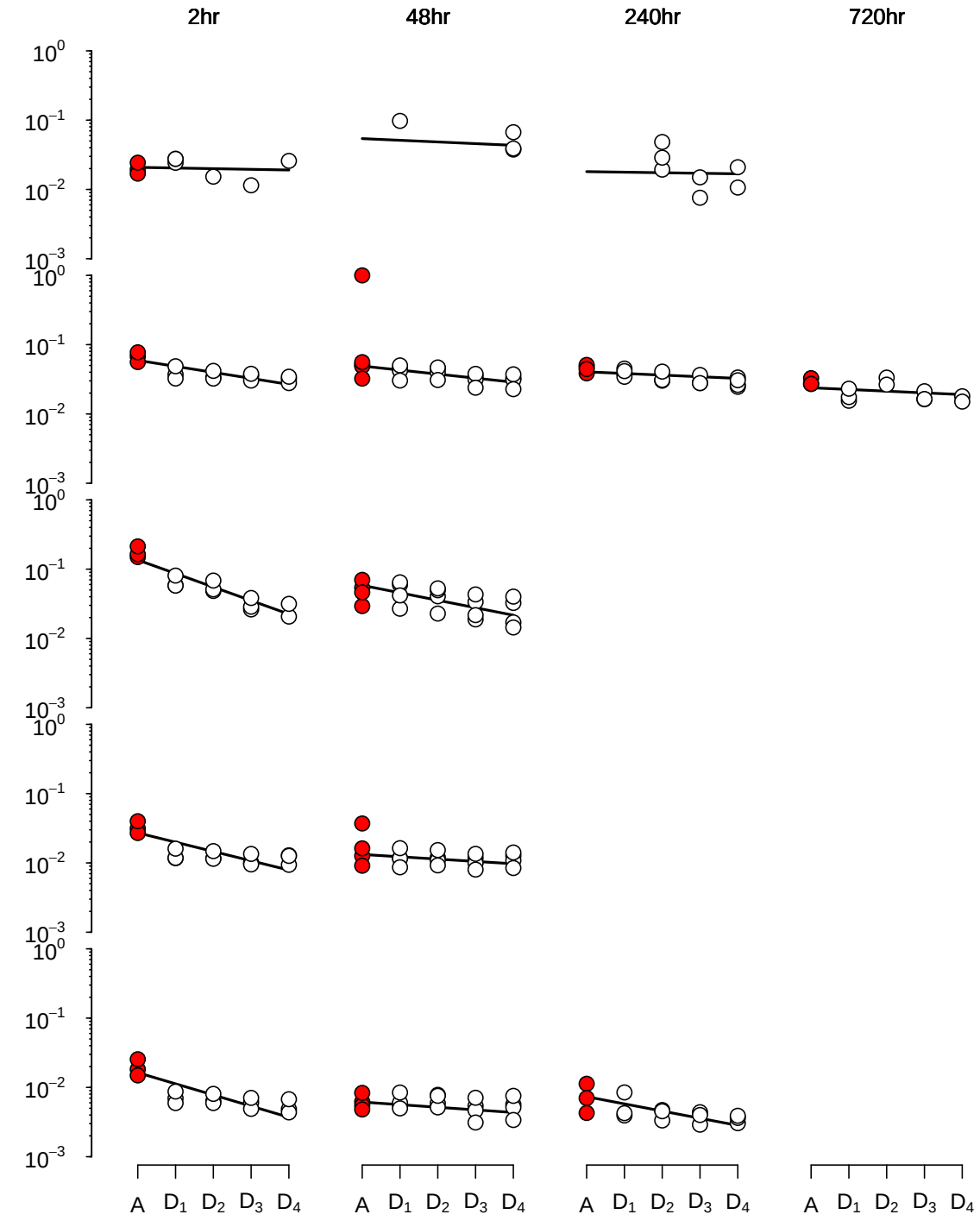


J


2hr
48hr
240hr
720hr
10^{0}
10^{-1}
10^{-2}
10^{-3}
A
D_1
D_2
D_3
D_4
R


2hr
48hr
240hr
720hr
10^{0}
10^{-1}
10^{-2}
10^{-3}
A
D_1
D_2
D_3
D_4
Z


2hr
48hr
240hr
720hr
10^{0}
10^{-1}
10^{-2}
10^{-3}
A
D_1
D_2
D_3
D_4
GAS


2hr
48hr
240hr
720hr
10^{0}
10^{-1}
10^{-2}
10^{-3}
A
D_1
D_2
D_3
D_4
P

Appendix B

SITE TRANSFORMATION MODEL SUPPLEMENTAL INFORMATION

B.1 Isotherms

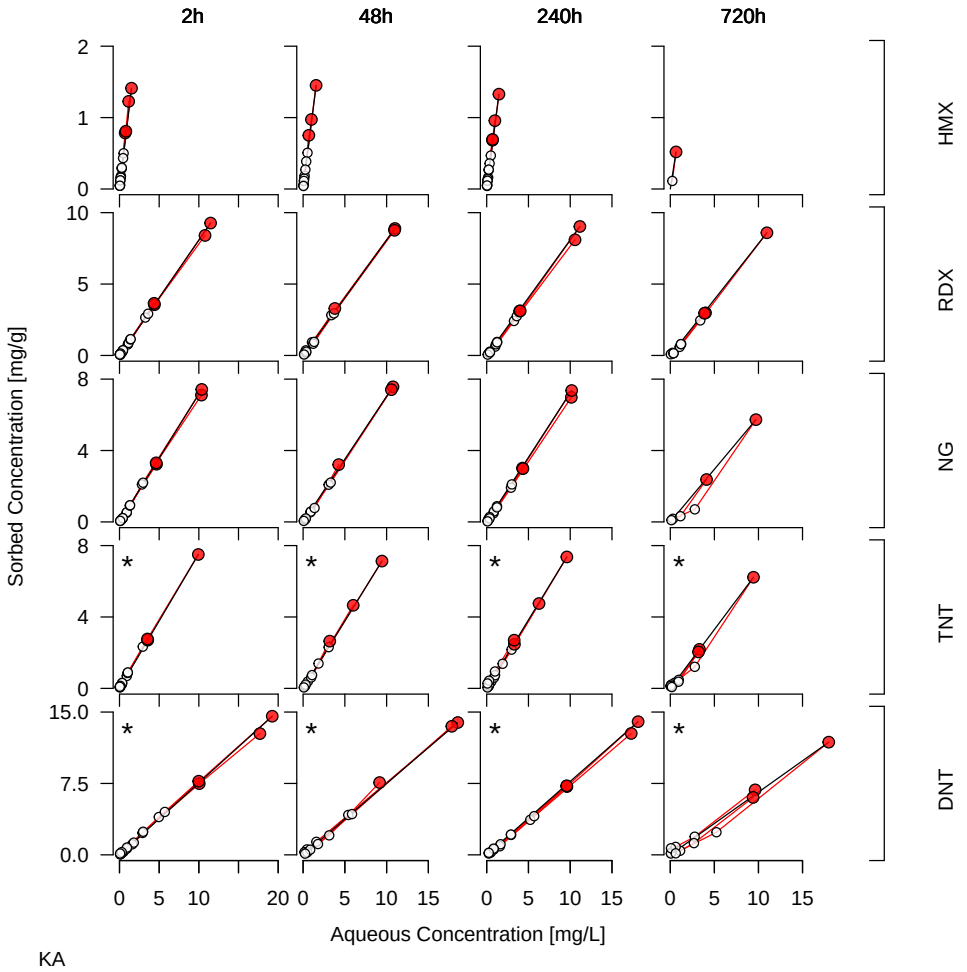
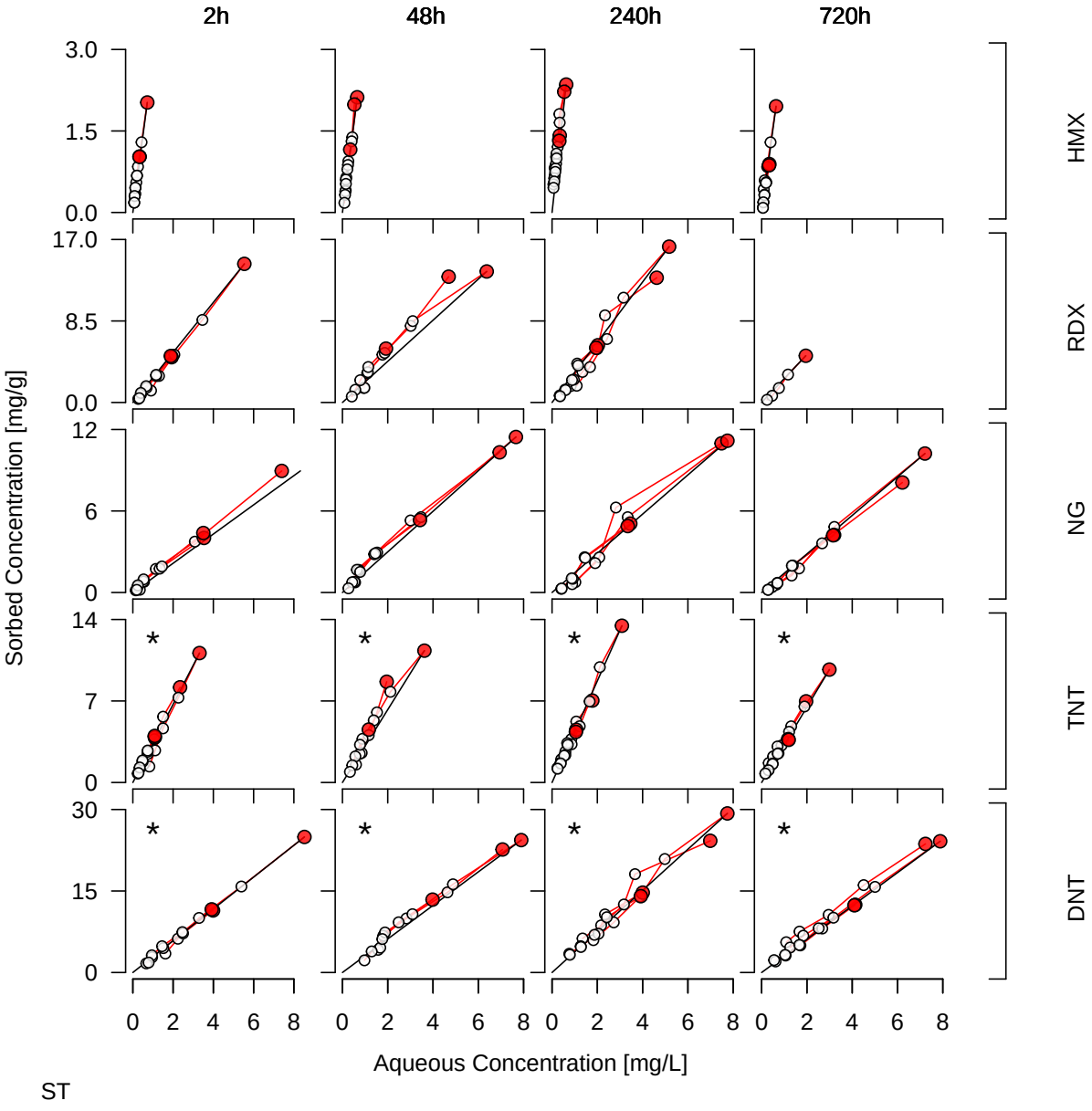
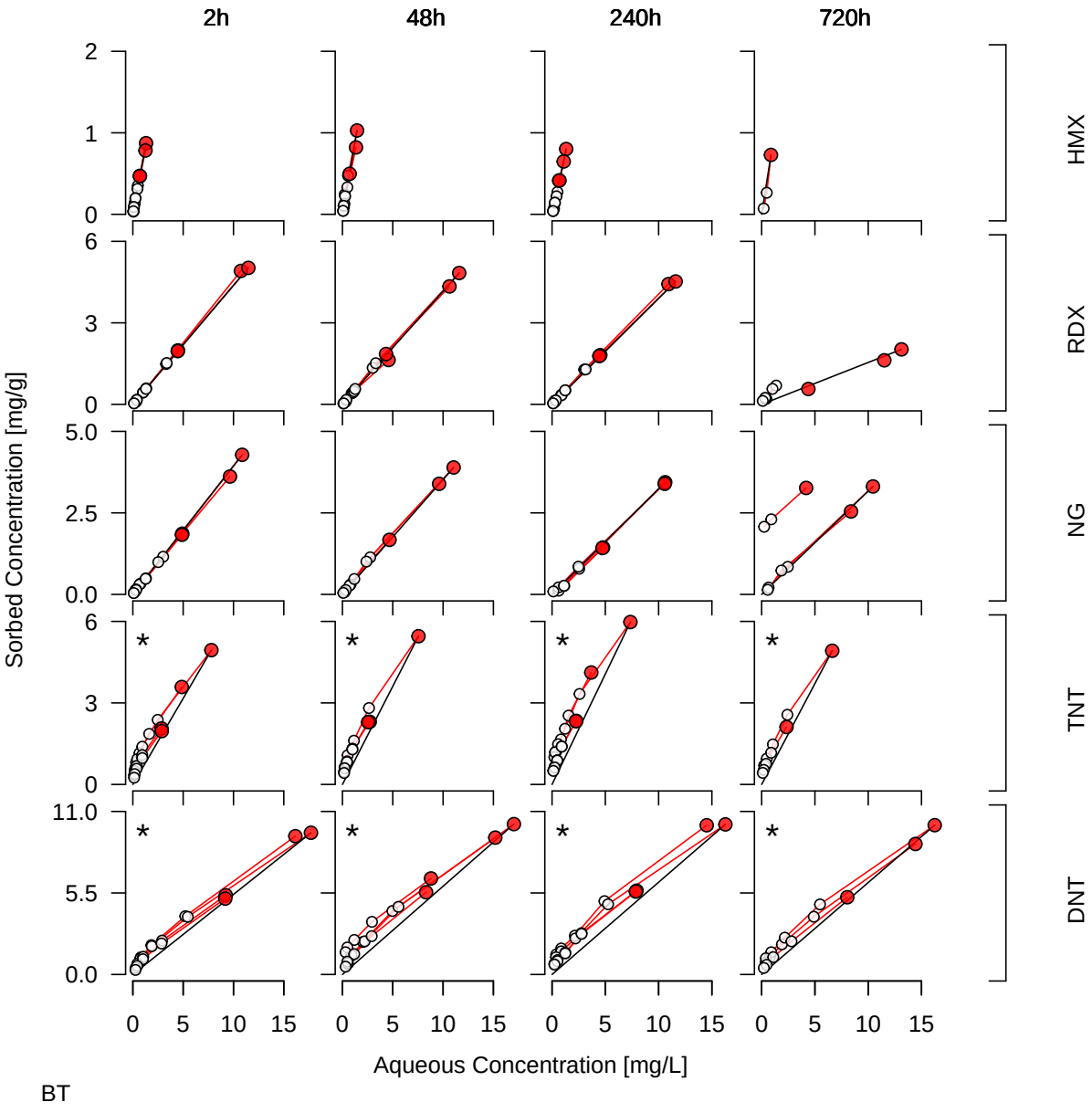
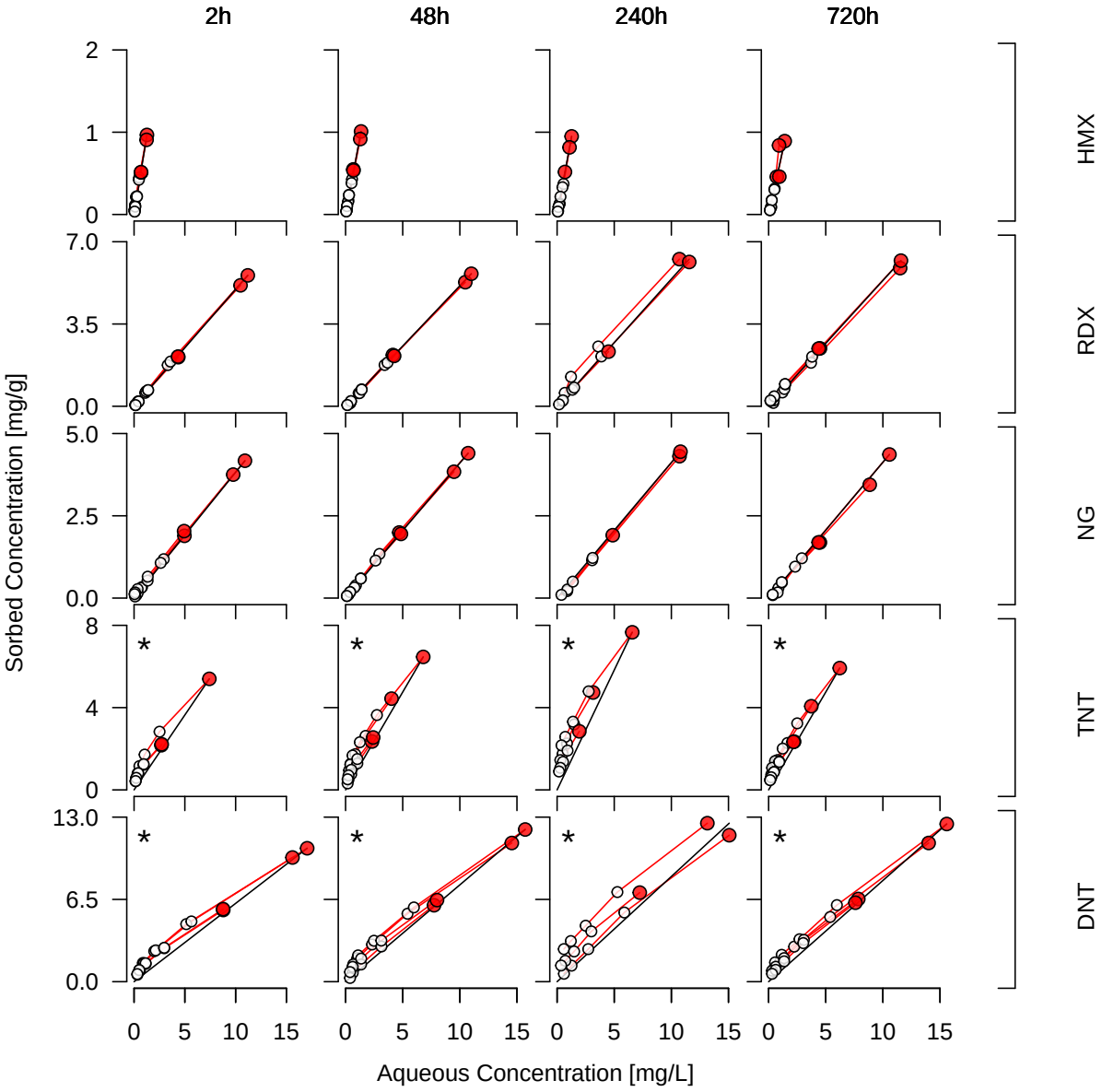
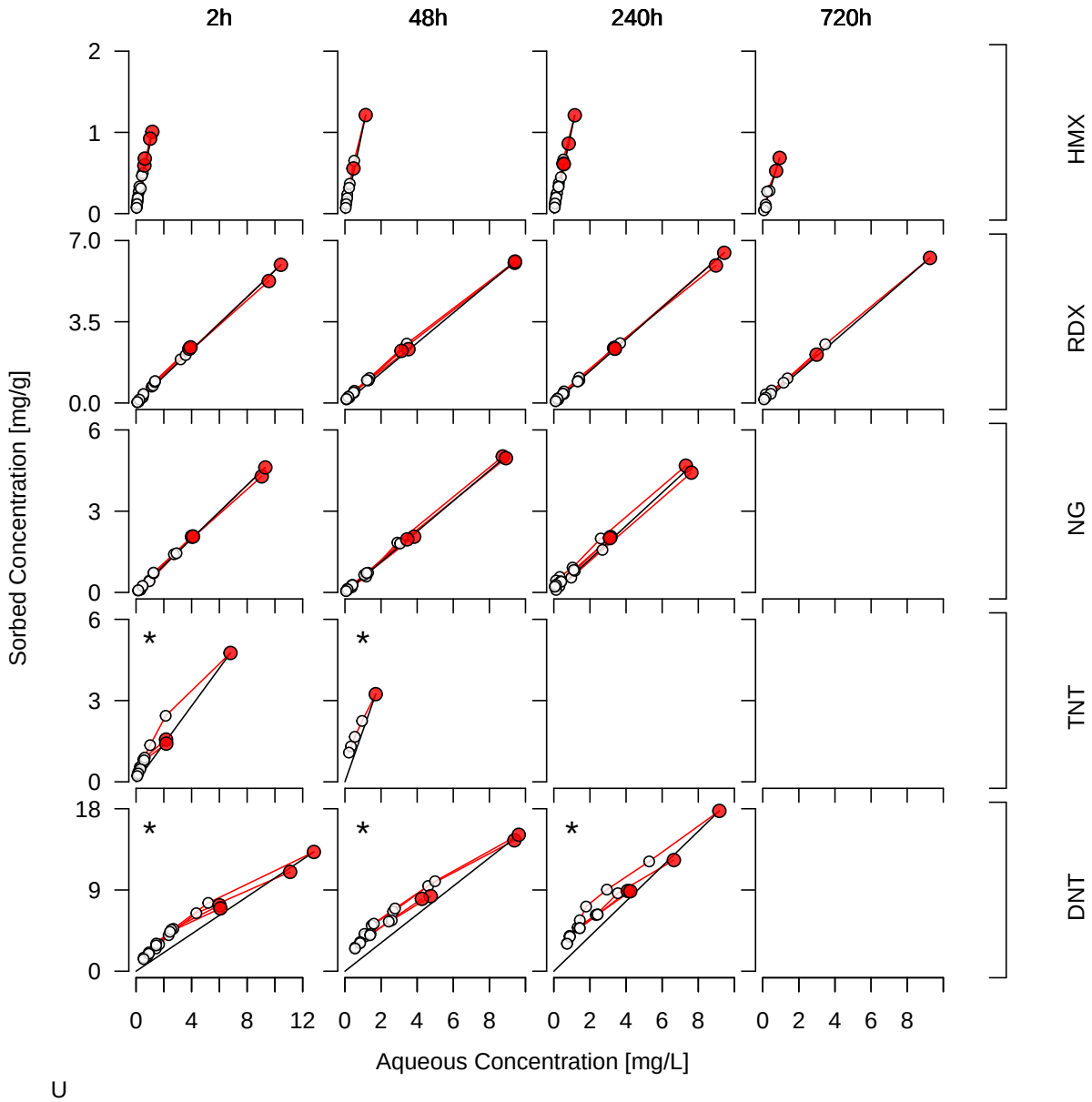


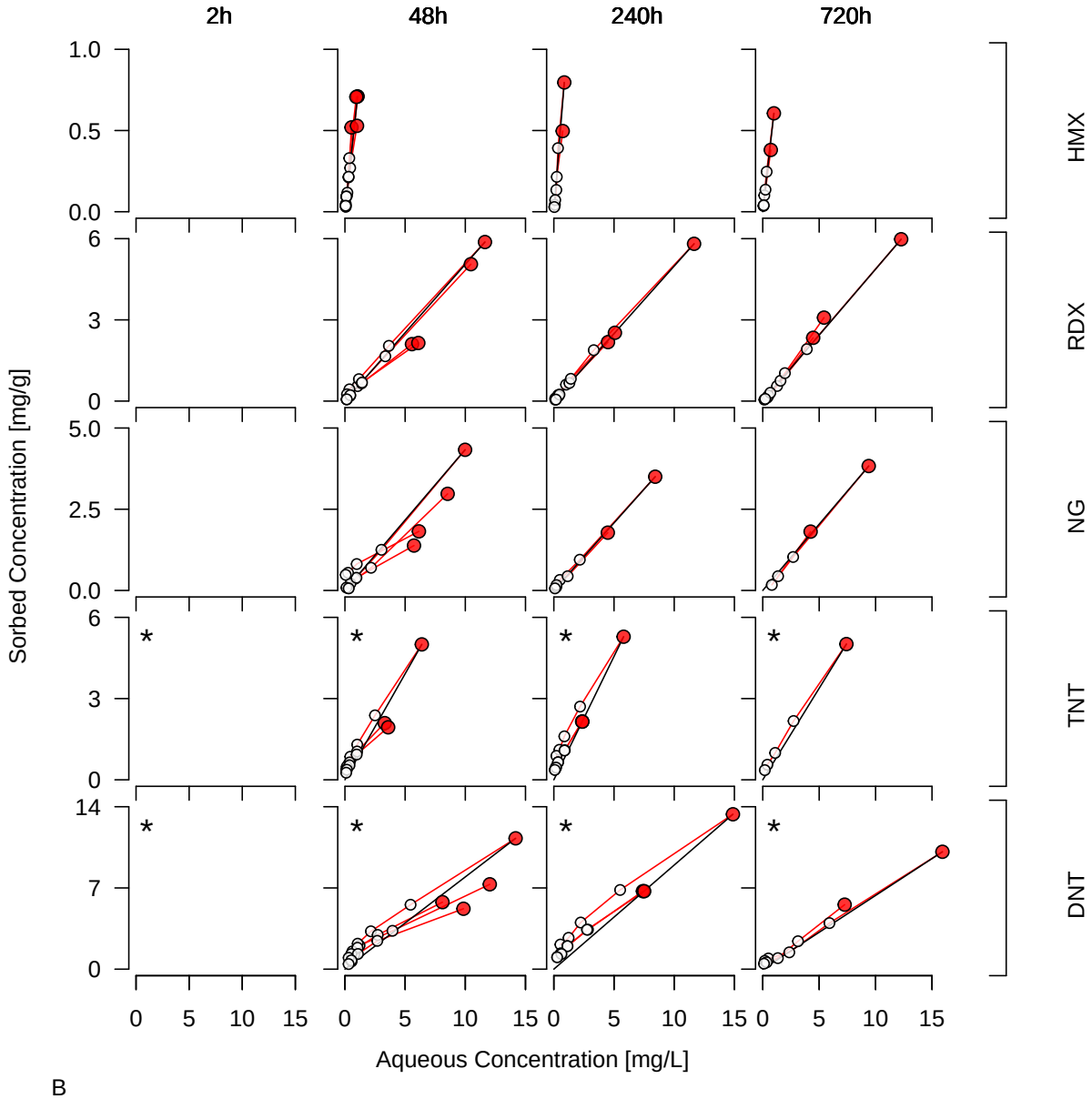
Figure B.1: Isotherms for all MC and sorbents with connective lines. Filled points are adsorption point, hollow points are desorption points.


2h
48h
240h
720h
HMX
RDX
NG
TNT
DNT
Sorbed Concentration [mg/g]
Aqueous Concentration [mg/L]
ST
3.0
1.5
0.0
17.0
8.5
0.0
12
6
0
14
7
0
30
15
0
0 2 4 6 8
*

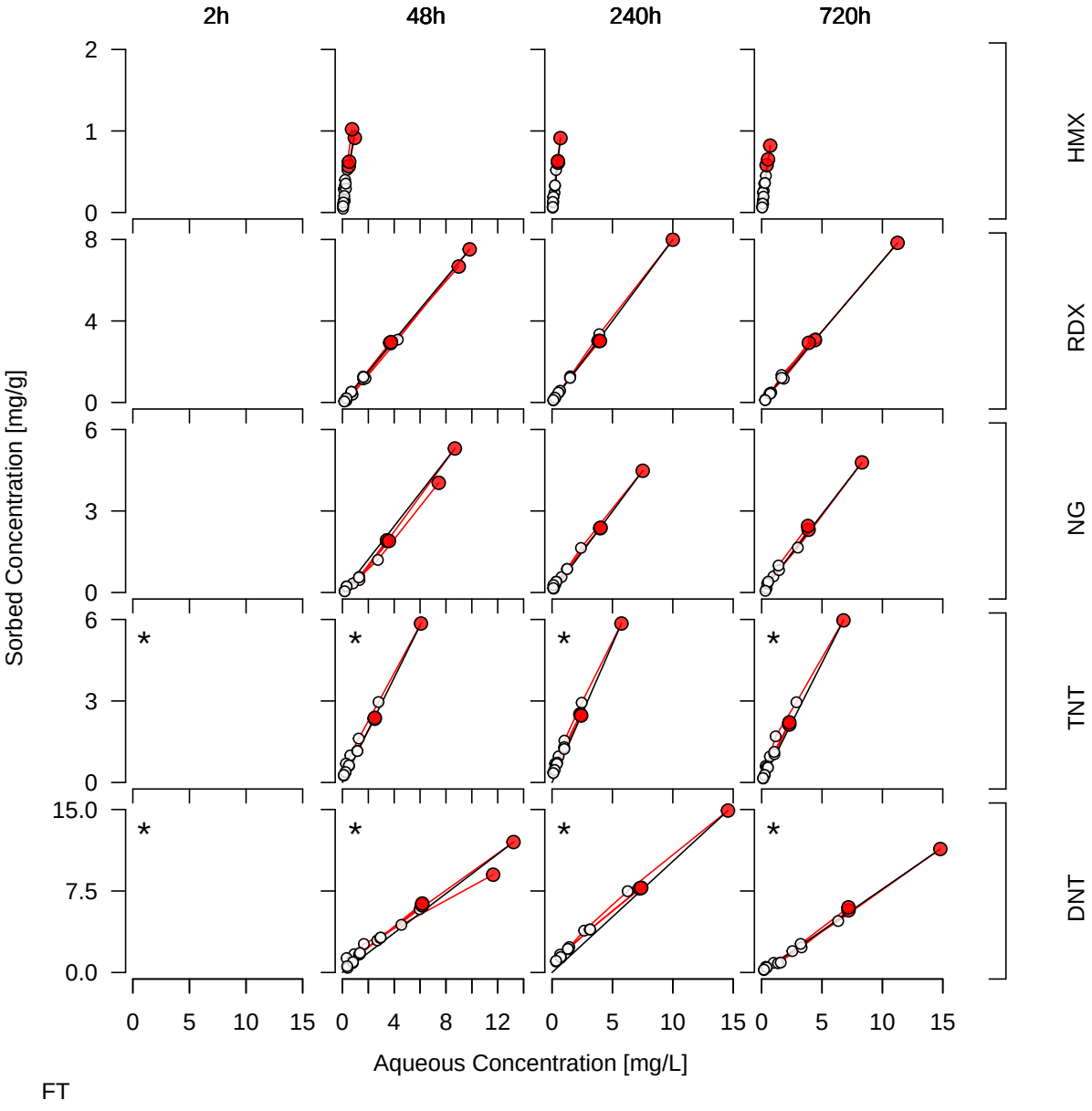

2h
48h
240h
720h
HMX
RDX
NG
TNT
DNT
Sorbed Concentration [mg/g]
Aqueous Concentration [mg/L]
BT

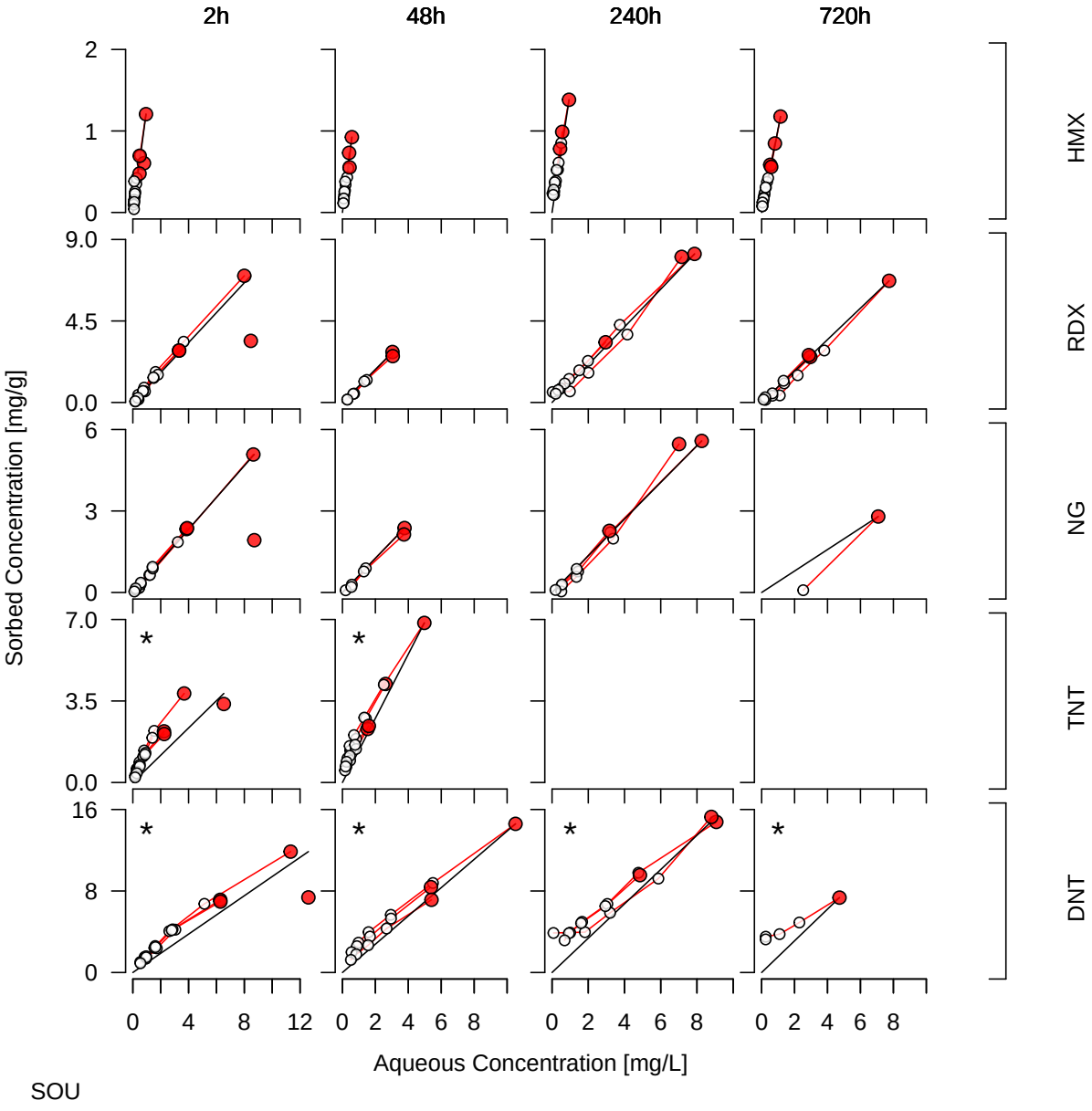

2h
48h
240h
720h
HMX
RDX
NG
TNT
DNT
Sorbed Concentration [mg/g]
Aqueous Concentration [mg/L]
BA

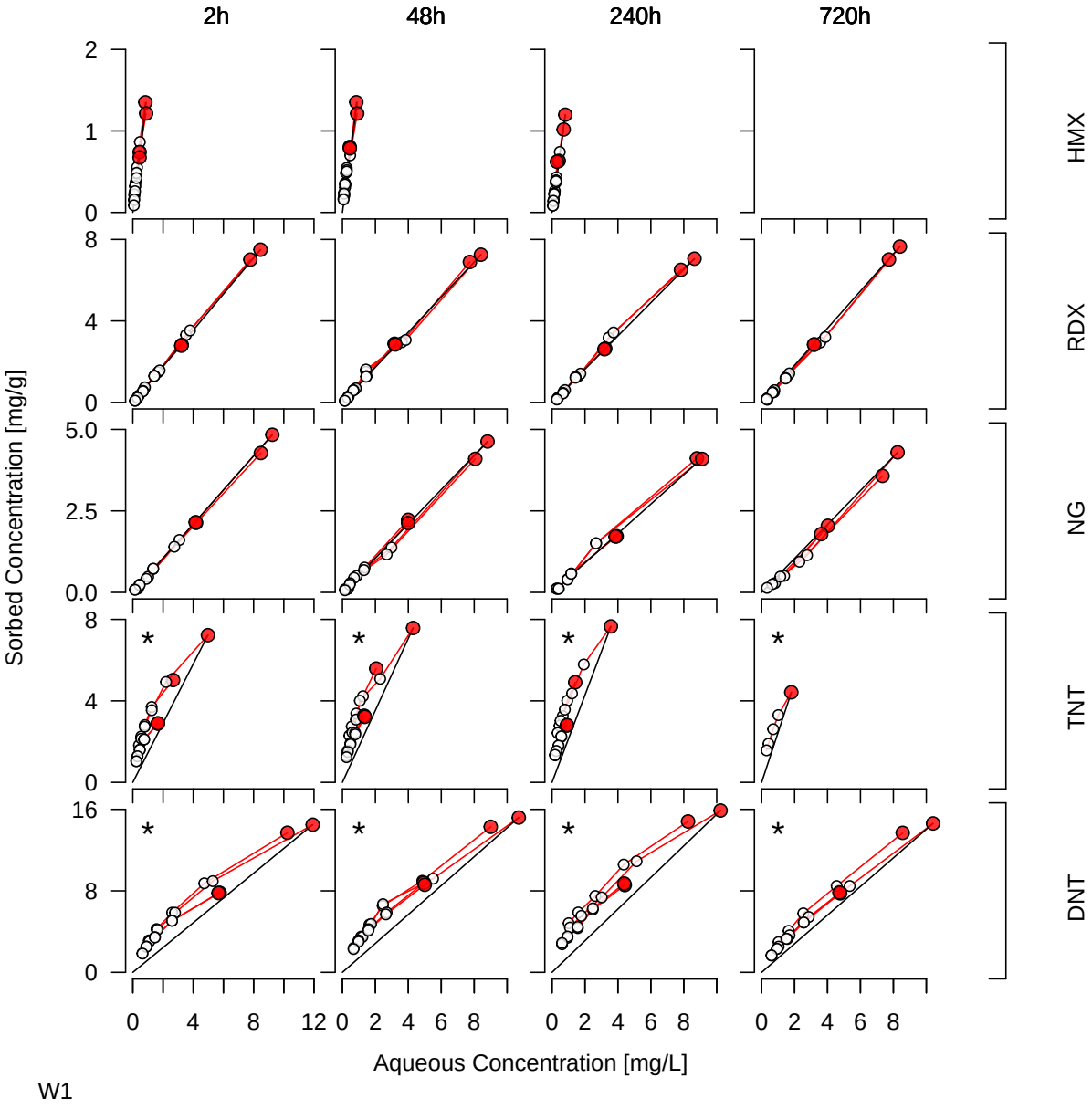

2h
48h
240h
720h
HMX
RDX
NG
TNT
DNT
Sorbed Concentration [mg/g]
Aqueous Concentration [mg/L]
U

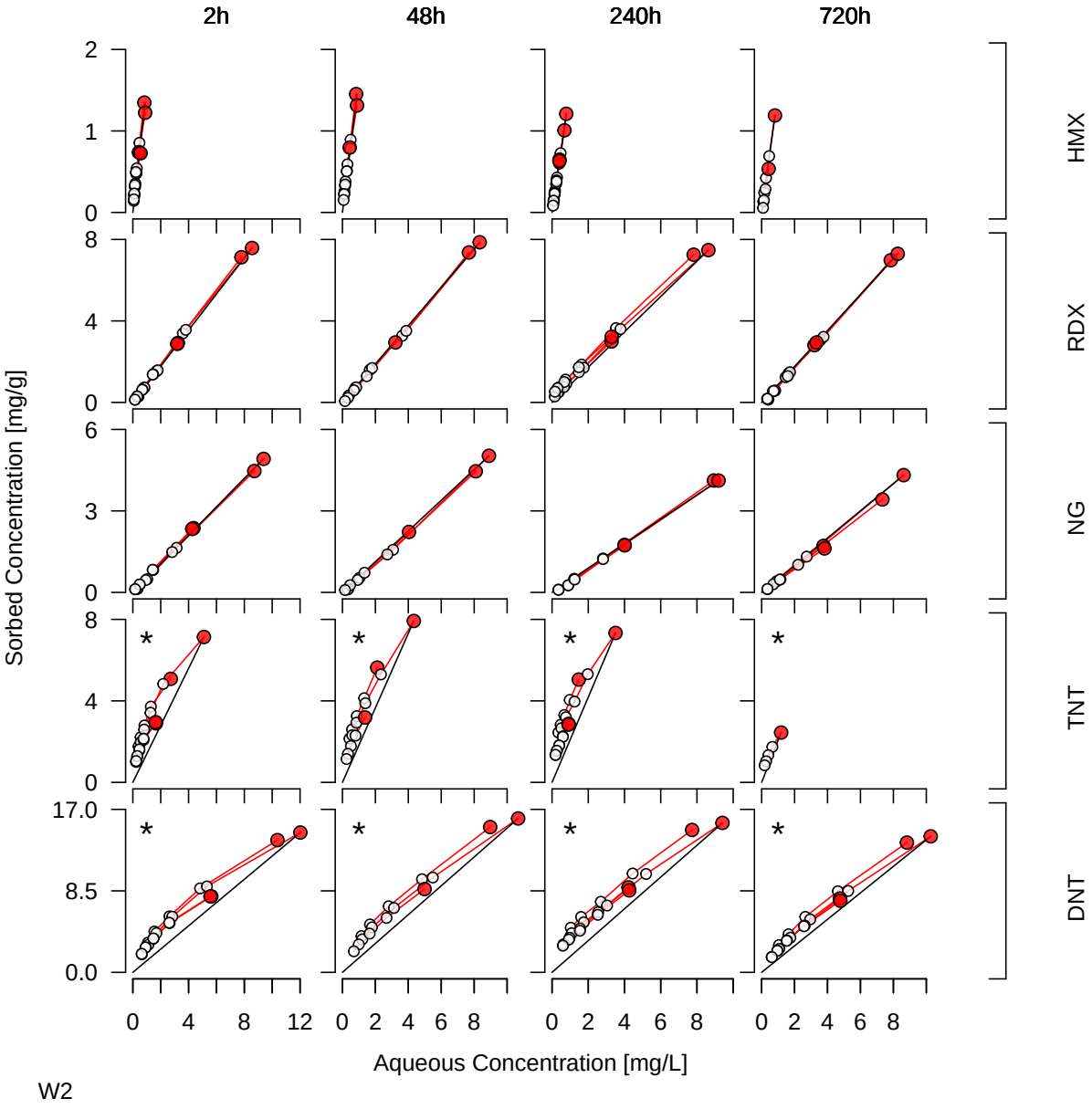

2h
48h
240h
720h
HMX
RDX
NG
TNT
DNT
Sorbed Concentration [mg/g]
Aqueous Concentration [mg/L]
1.0
0.5
0.0
6
3
0
5.0
2.5
0.0
6
3
0
14
7
0
*
0
5
10
15

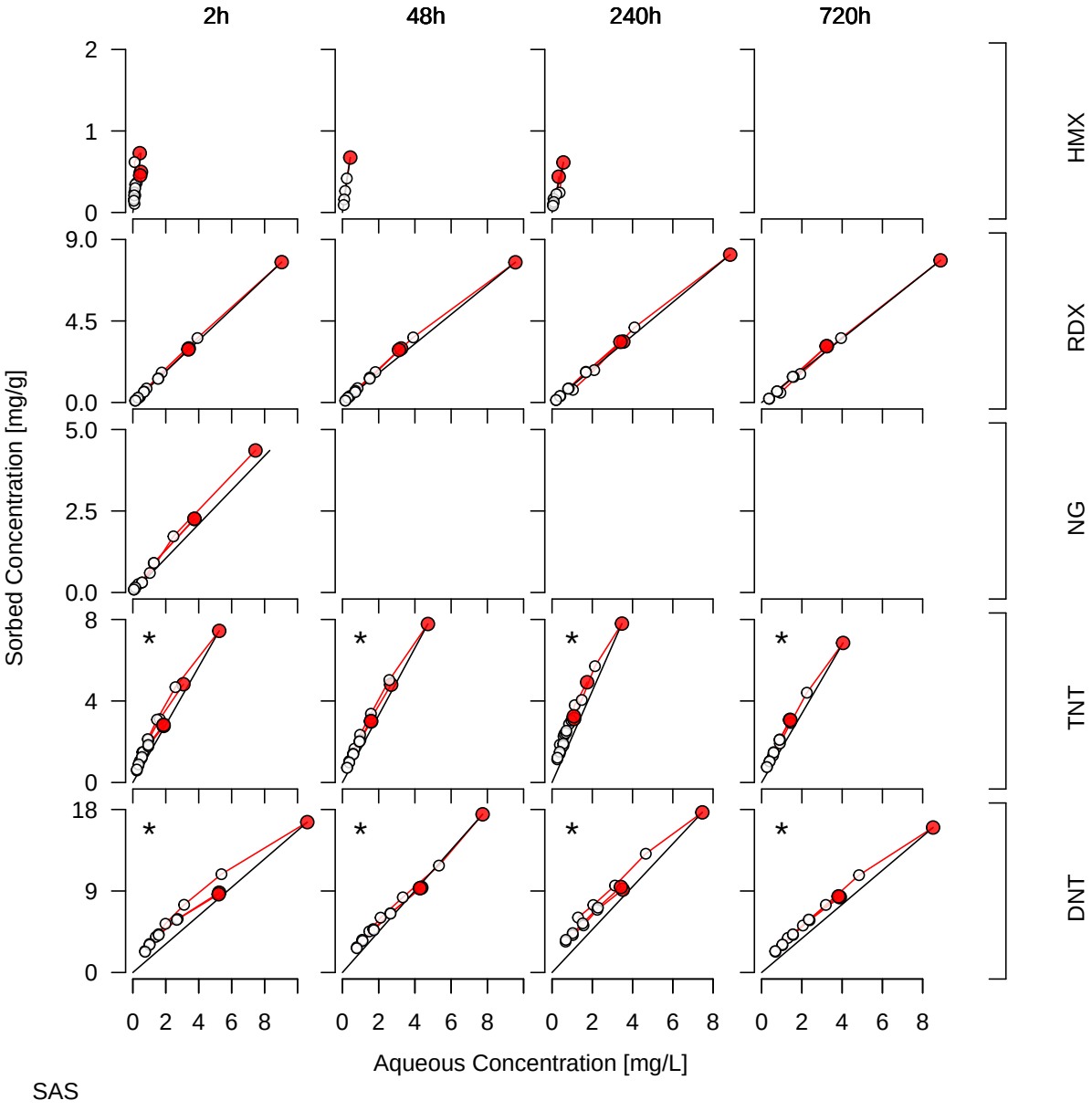
B

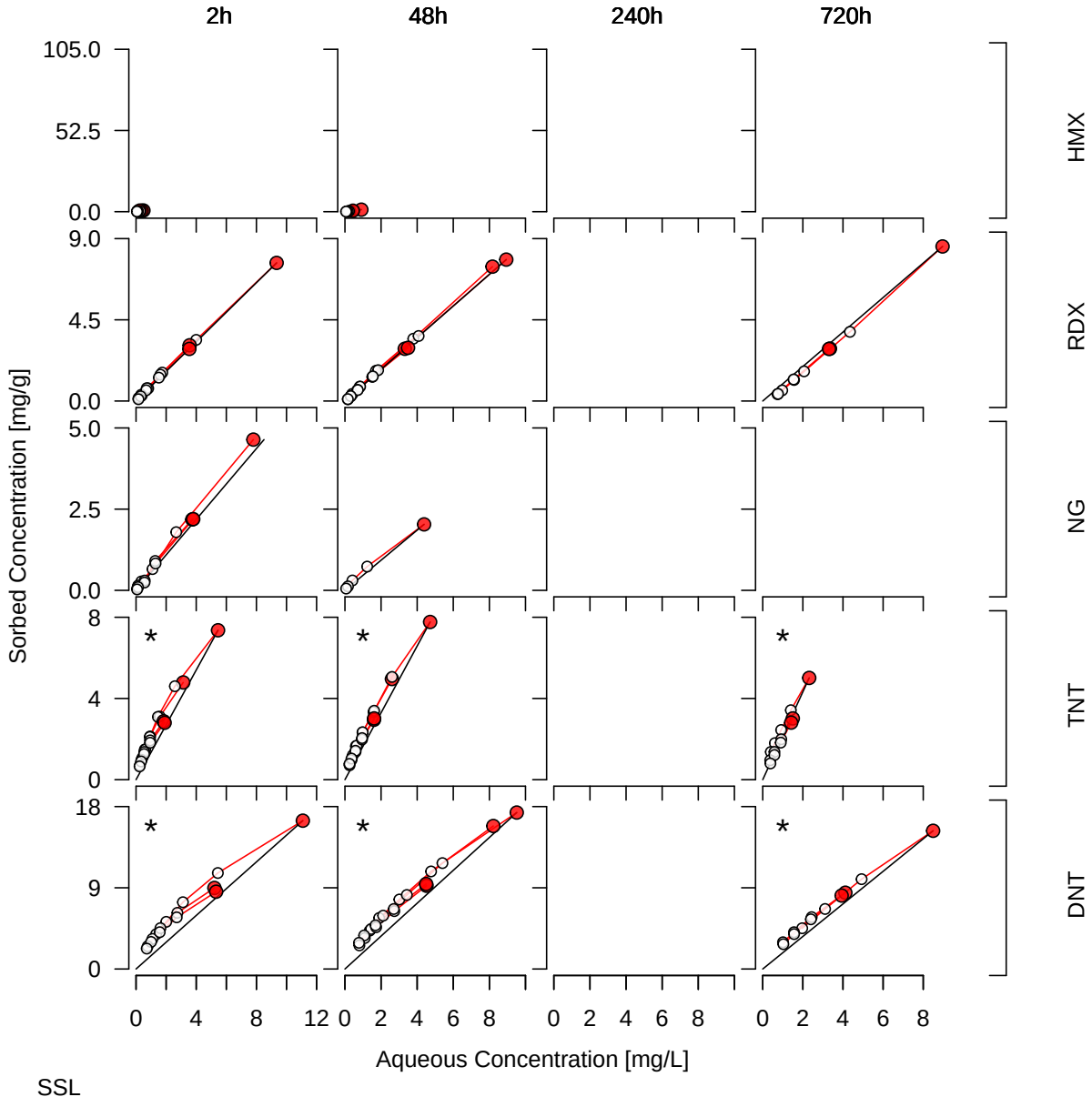

2h
48h
240h
720h
HMX
RDX
NG
TNT
DNT
Sorbed Concentration [mg/g]
Aqueous Concentration [mg/L]
FT


2h
48h
240h
720h
HMX
RDX
NG
TNT
DNT
Sorbed Concentration [mg/g]
Aqueous Concentration [mg/L]
SOU

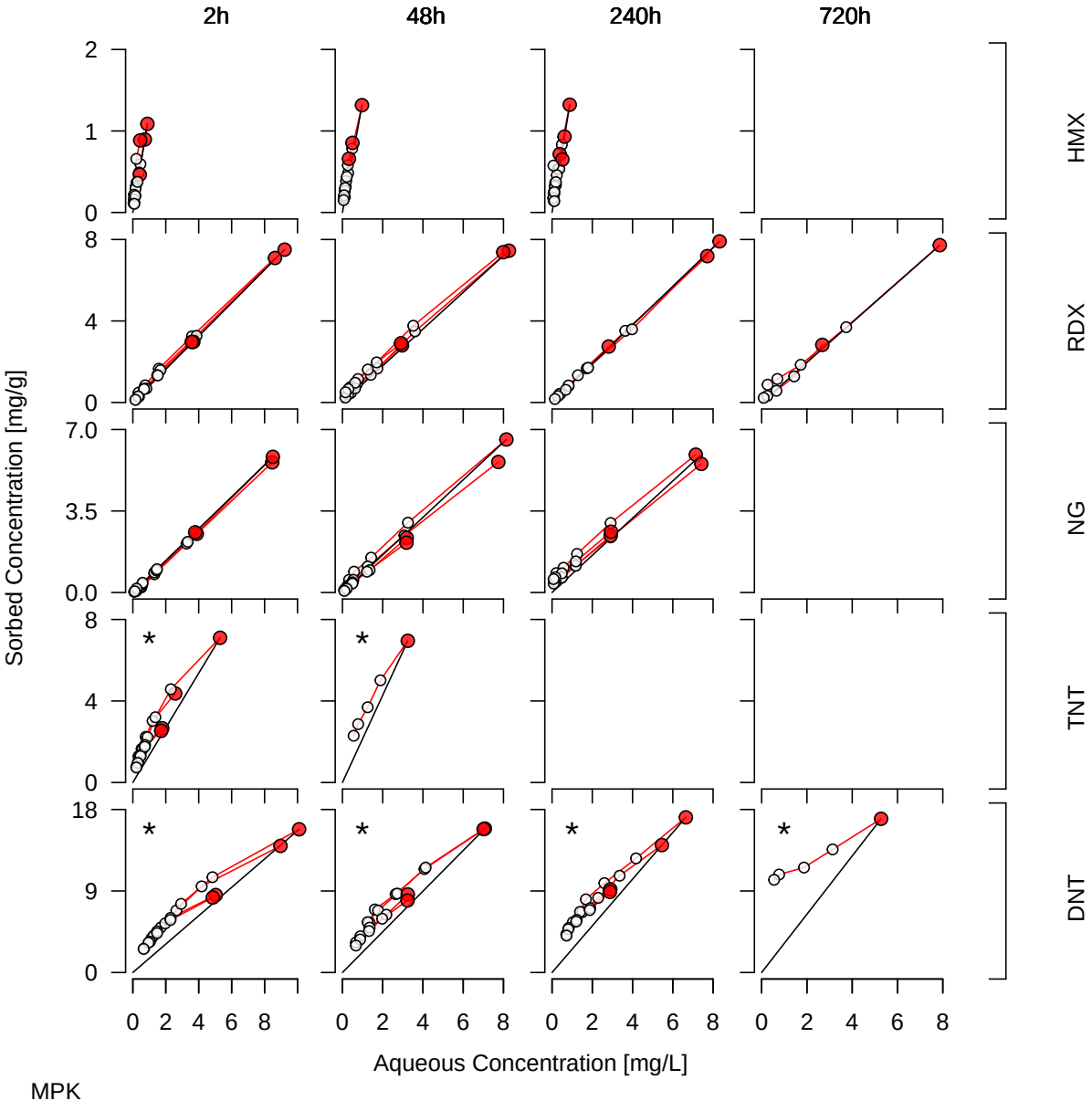

2h
48h
240h
720h
HMX
RDX
NG
TNT
DNT
Sorbed Concentration [mg/g]
Aqueous Concentration [mg/L]
W1

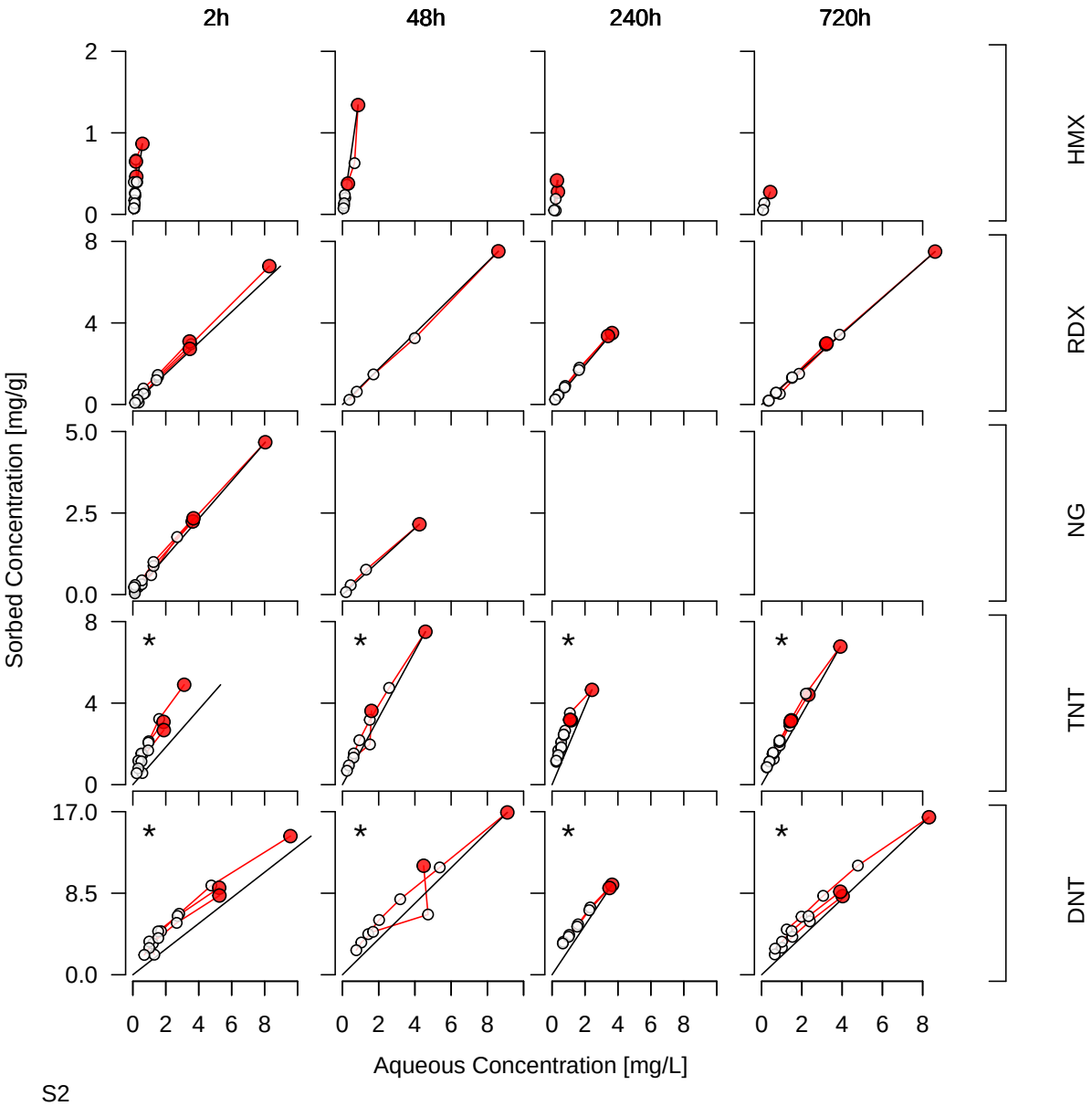

2h
48h
240h
720h
HMX
RDX
NG
TNT
DNT
Sorbed Concentration [mg/g]
Aqueous Concentration [mg/L]
W2


2h
48h
240h
720h
HMX
RDX
NG
TNT
DNT
Sorbed Concentration [mg/g]
Aqueous Concentration [mg/L]
SAS

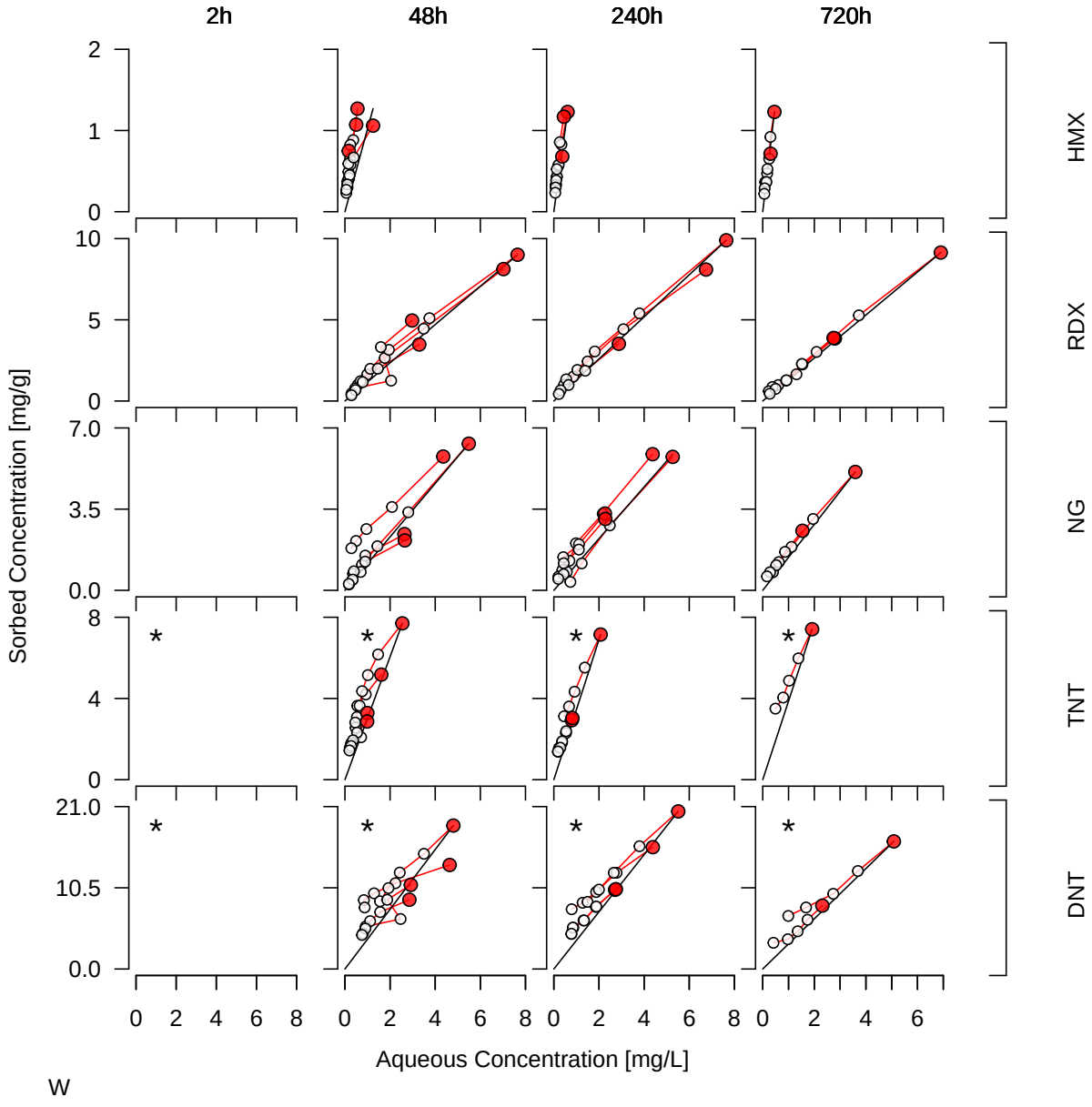

2h
48h
240h
720h
HMX
RDX
NG
TNT
DNT
Sorbed Concentration [mg/g]
Aqueous Concentration [mg/L]
105.0
52.5
0.0
9.0
4.5
0.0
5.0
2.5
0.0
8
4
0
18
9
0
0 4 8 12
0 2 4 6 8
0 2 4 6 8
0 2 4 6 8
*

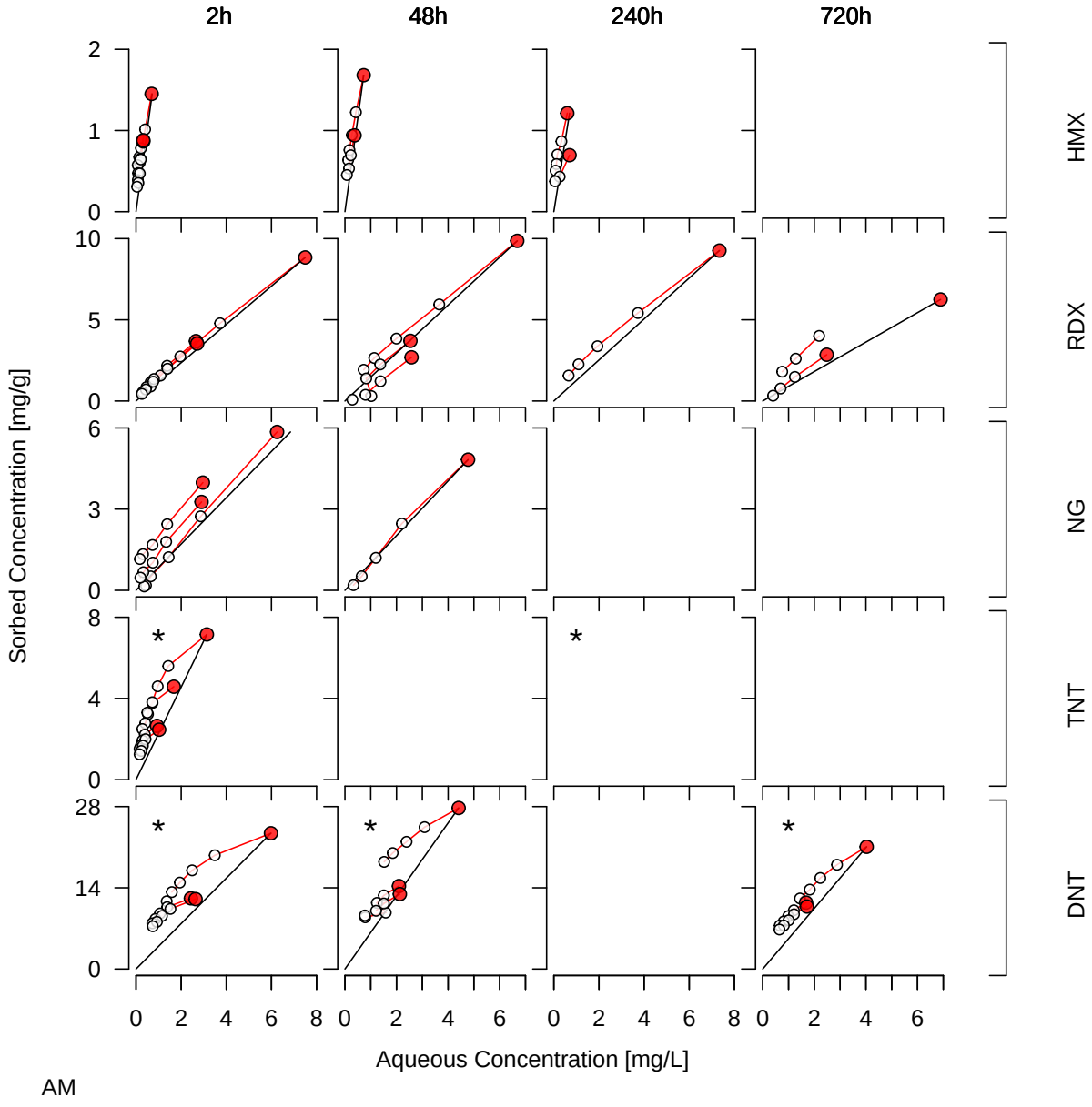
SSL

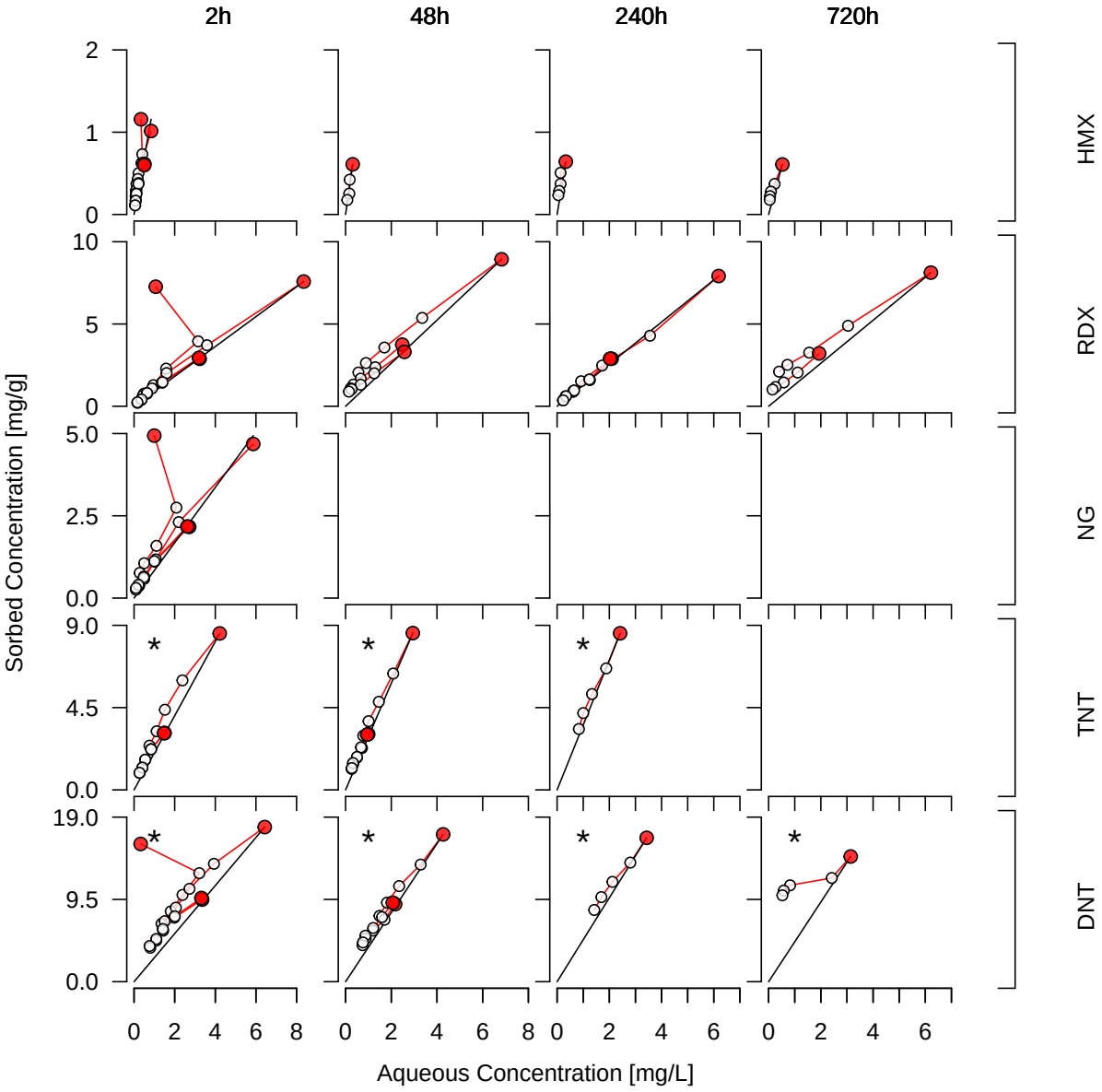

2h
48h
240h
720h
HMX
RDX
NG
TNT
DNT
Sorbed Concentration [mg/g]
Aqueous Concentration [mg/L]
MPK


2h
48h
240h
720h
HMX
RDX
NG
TNT
DNT
Sorbed Concentration [mg/g]
Aqueous Concentration [mg/L]
0
1
2
4
8
2.5
5.0
8.5
17.0
*

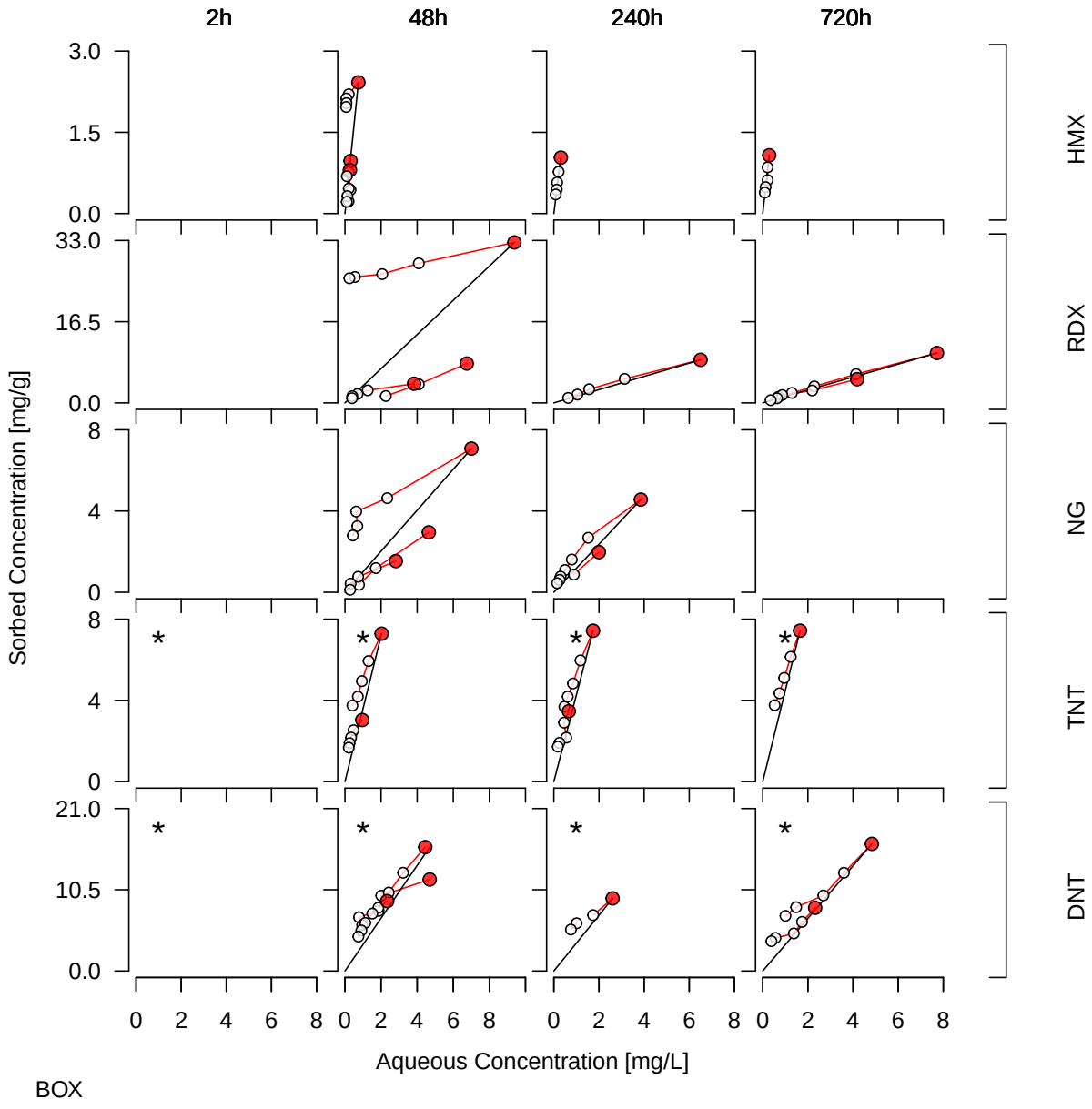
S2

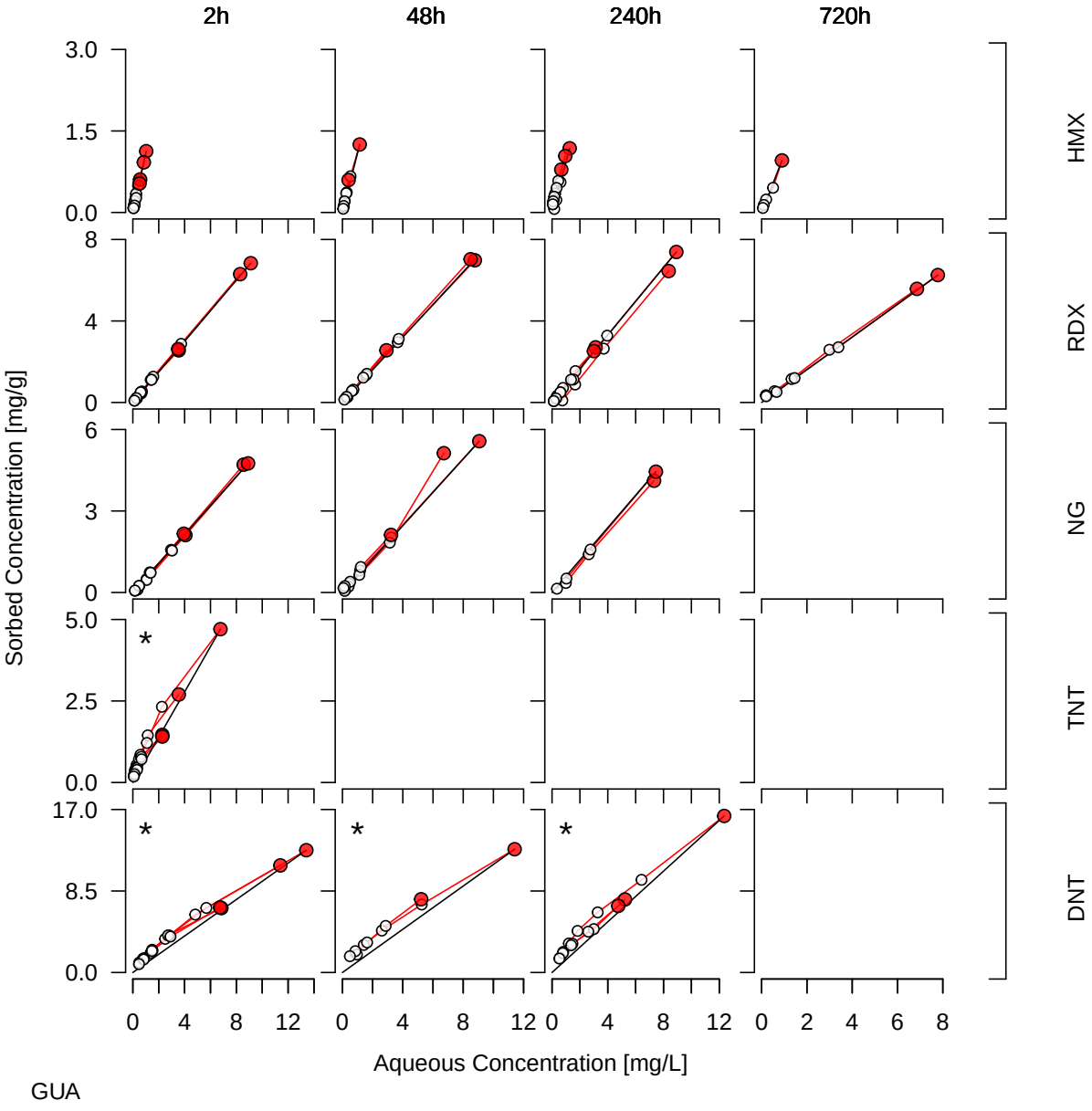

2h
48h
240h
720h
HMX
RDX
NG
TNT
DNT
Sorbed Concentration [mg/g]
Aqueous Concentration [mg/L]
W

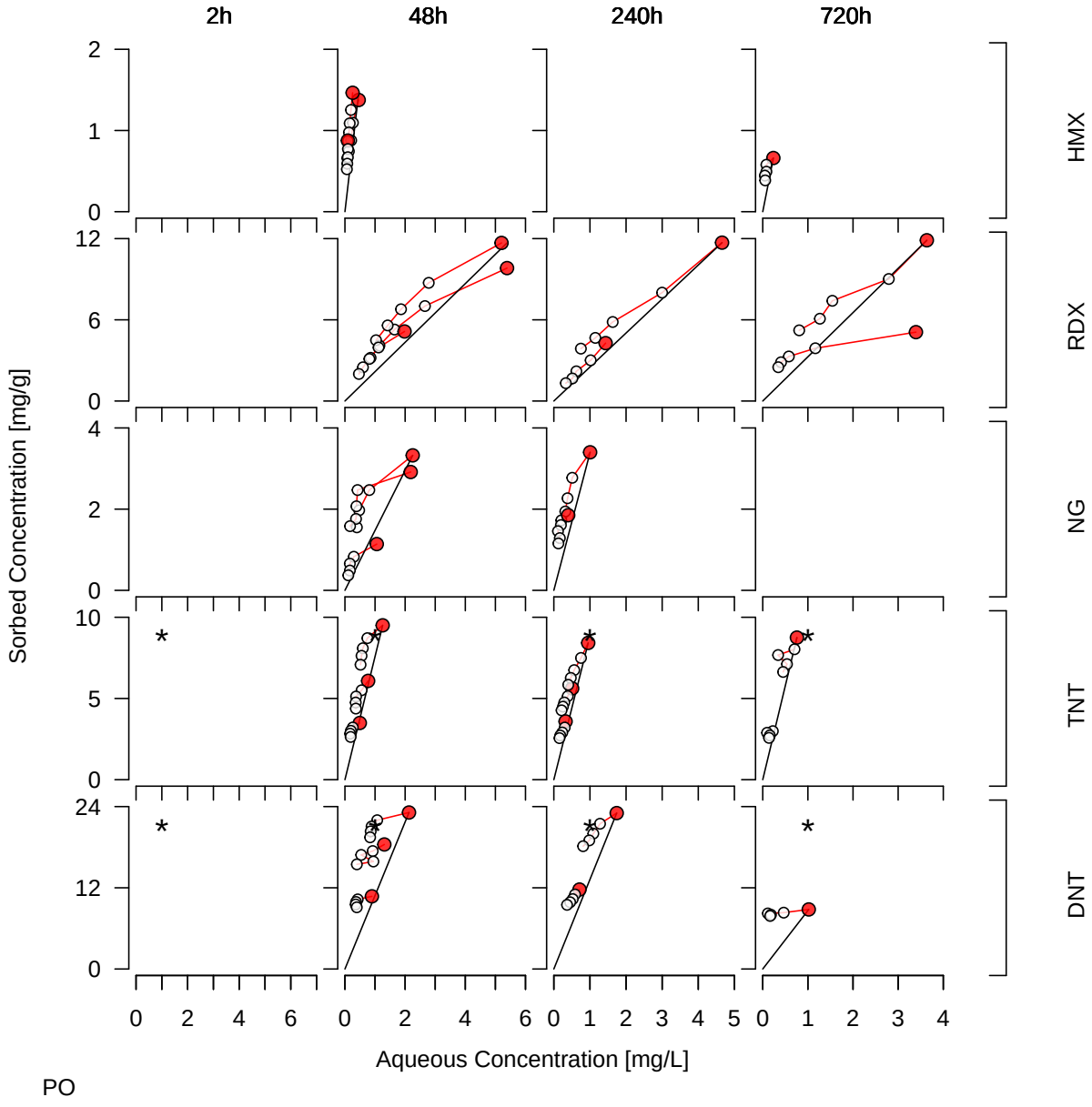

2h
48h
240h
720h
HMX
RDX
NG
TNT
DNT
Sorbed Concentration [mg/g]
Aqueous Concentration [mg/L]
AM

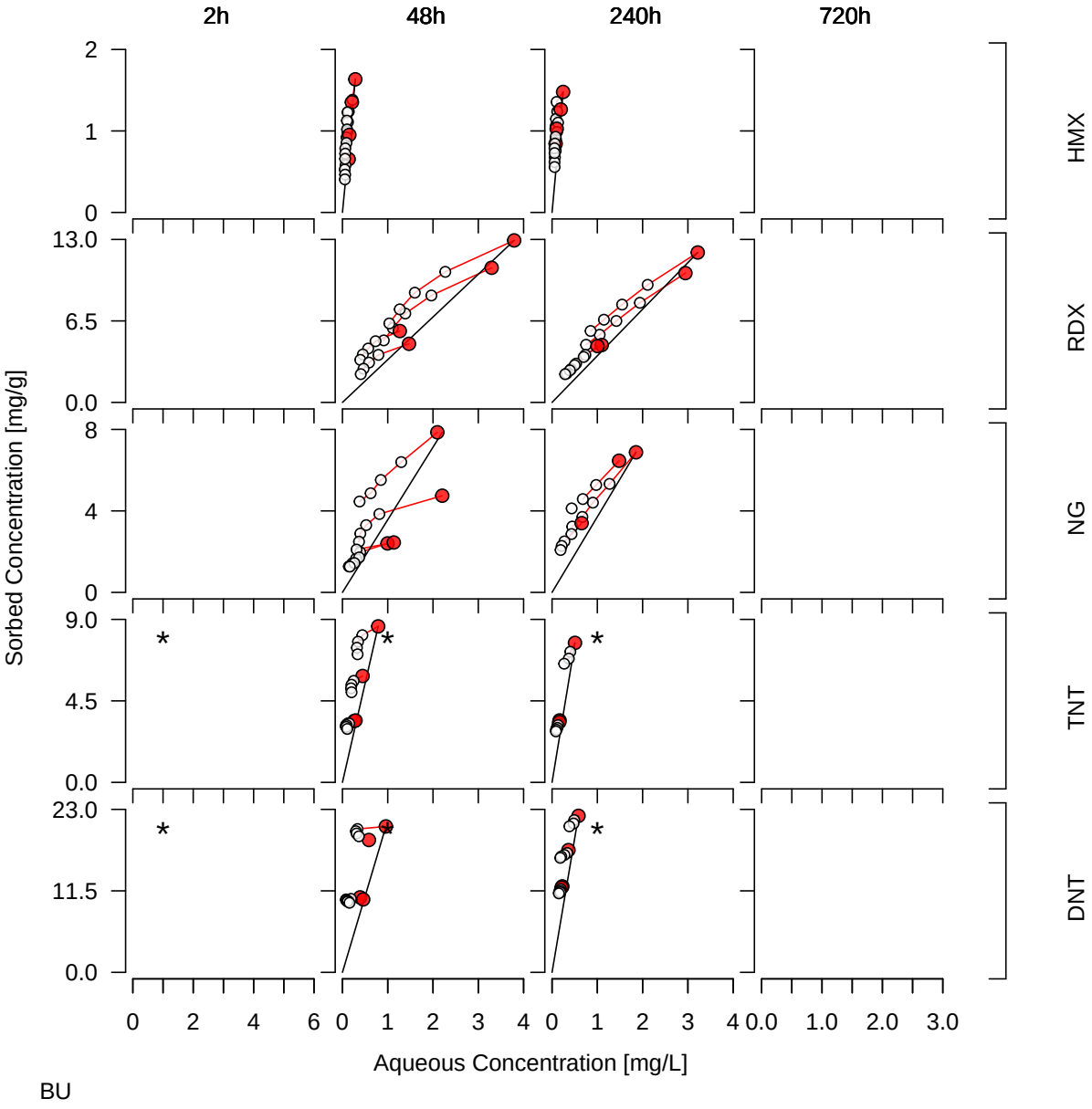

2h
48h
240h
720h
HMX
RDX
NG
TNT
DNT
Sorbed Concentration [mg/g]
Aqueous Concentration [mg/L]

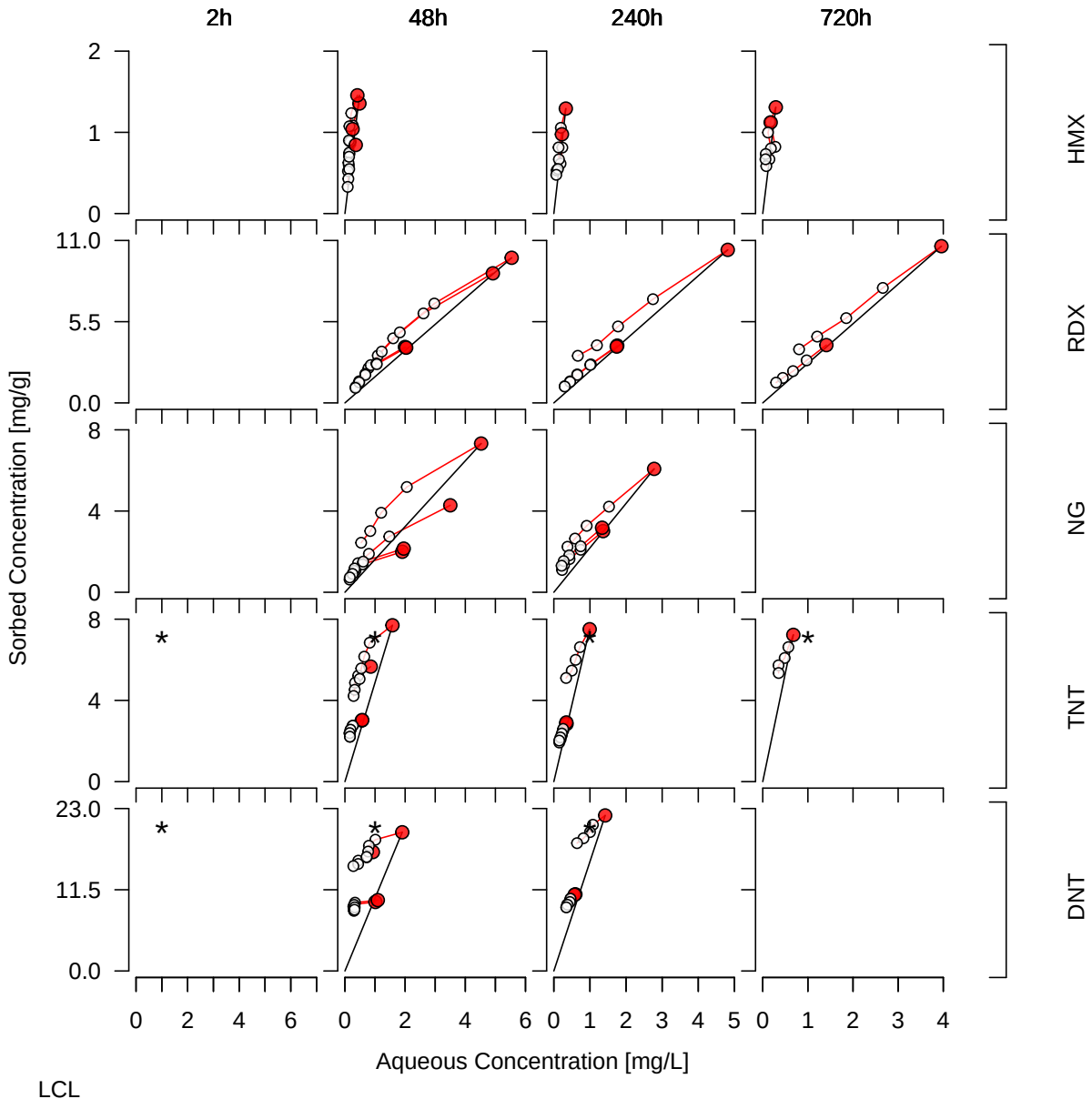
H

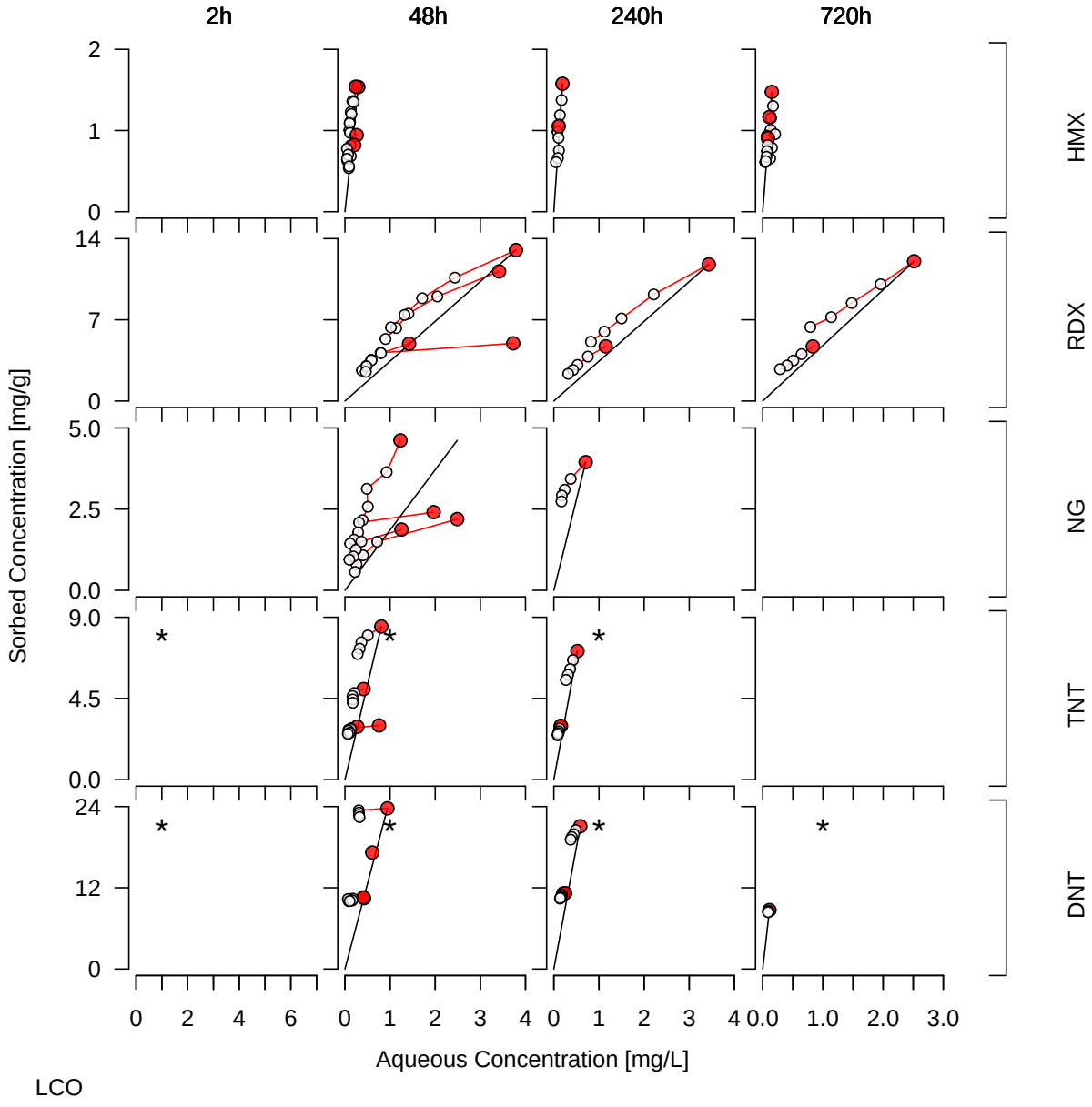

2h
48h
240h
720h
HMX
RDX
NG
TNT
DNT
Sorbed Concentration [mg/g]
Aqueous Concentration [mg/L]
BOX

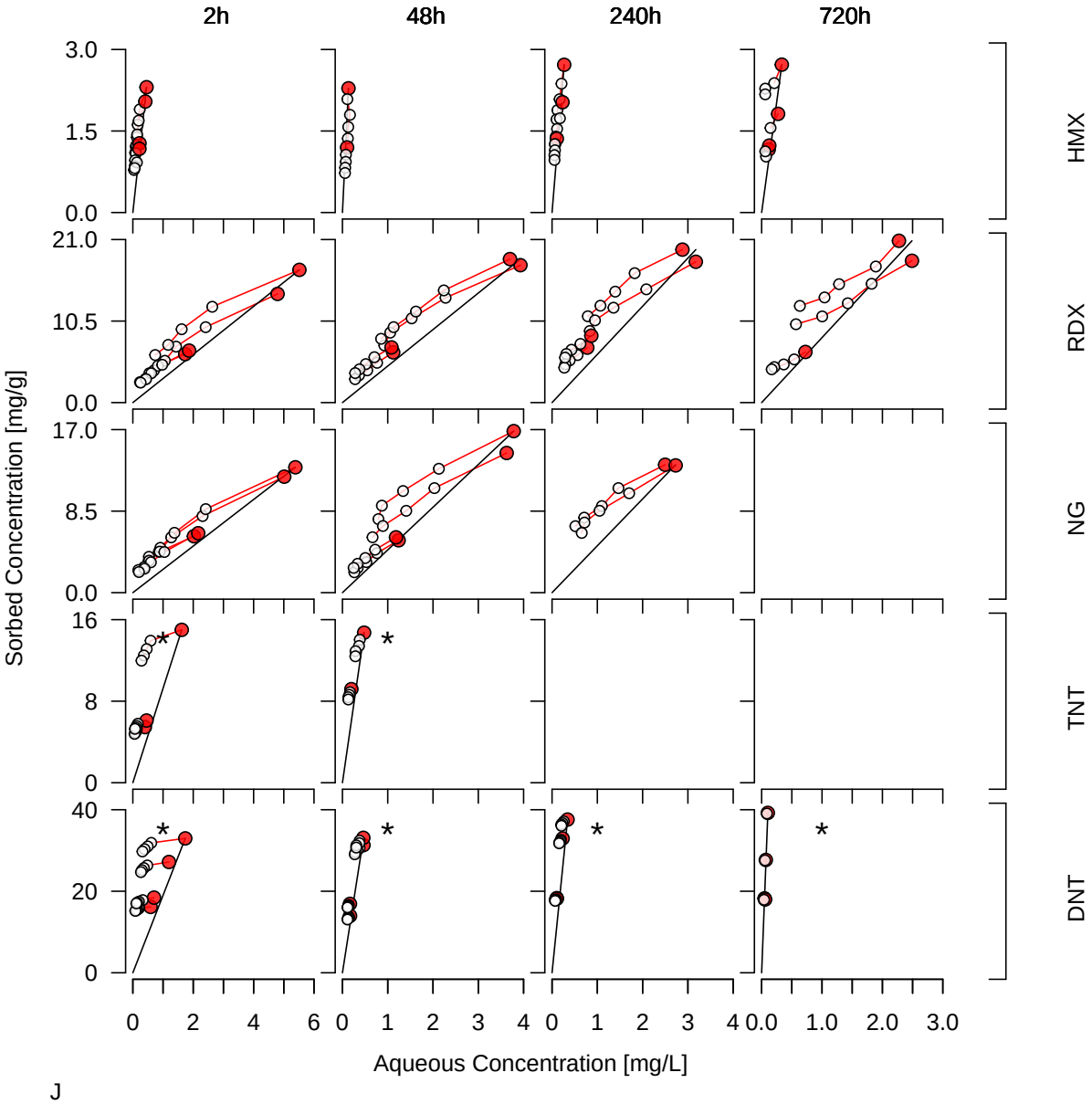

2h
48h
240h
720h
HMX
RDX
NG
TNT
DNT
Sorbed Concentration [mg/g]
Aqueous Concentration [mg/L]
GUA


2h
48h
240h
720h
HMX
RDX
NG
TNT
DNT
Sorbed Concentration [mg/g]
Aqueous Concentration [mg/L]
PO

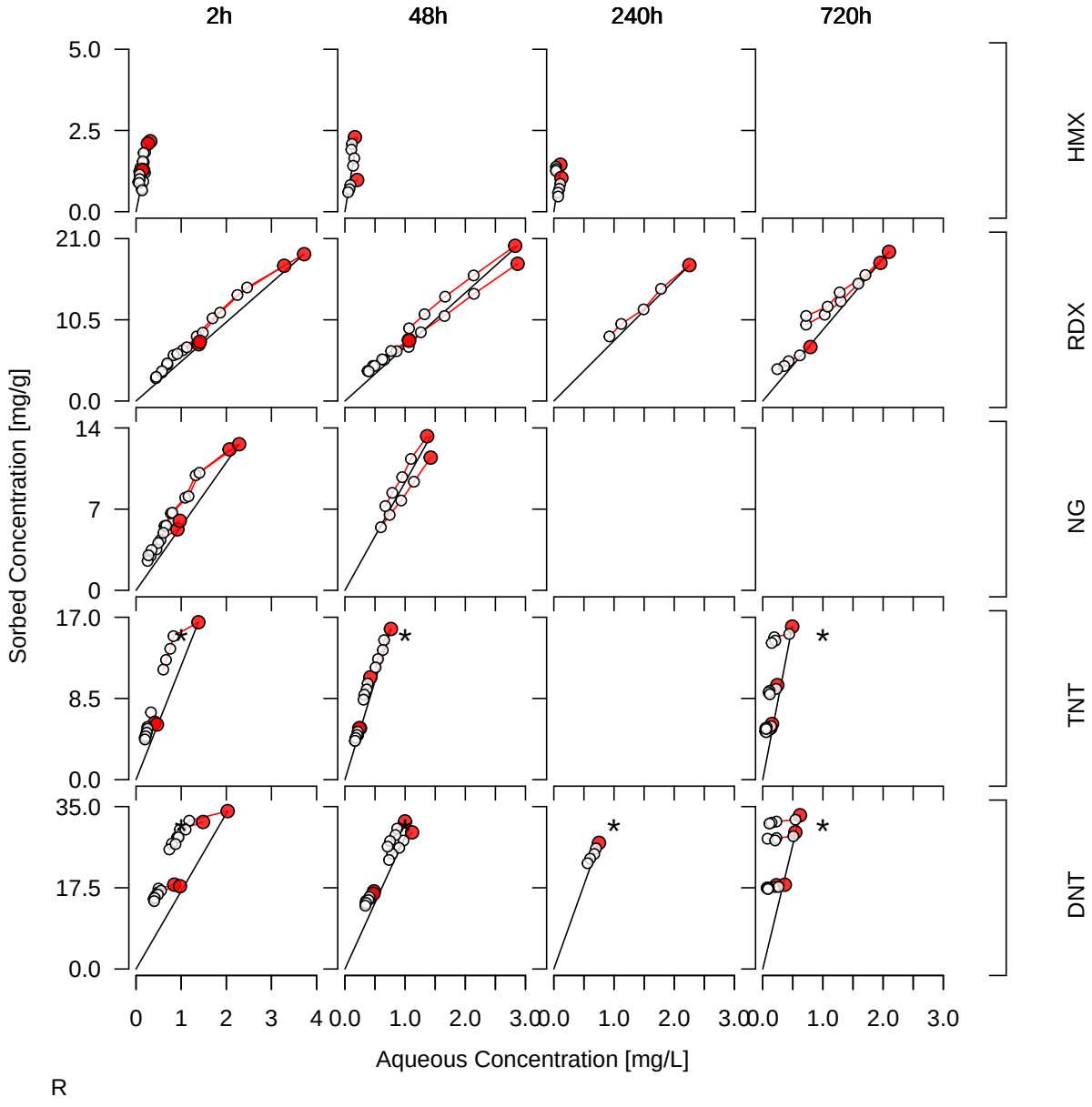

2h
48h
240h
720h
HMX
RDX
NG
TNT
DNT
Sorbed Concentration [mg/g]
Aqueous Concentration [mg/L]
BU

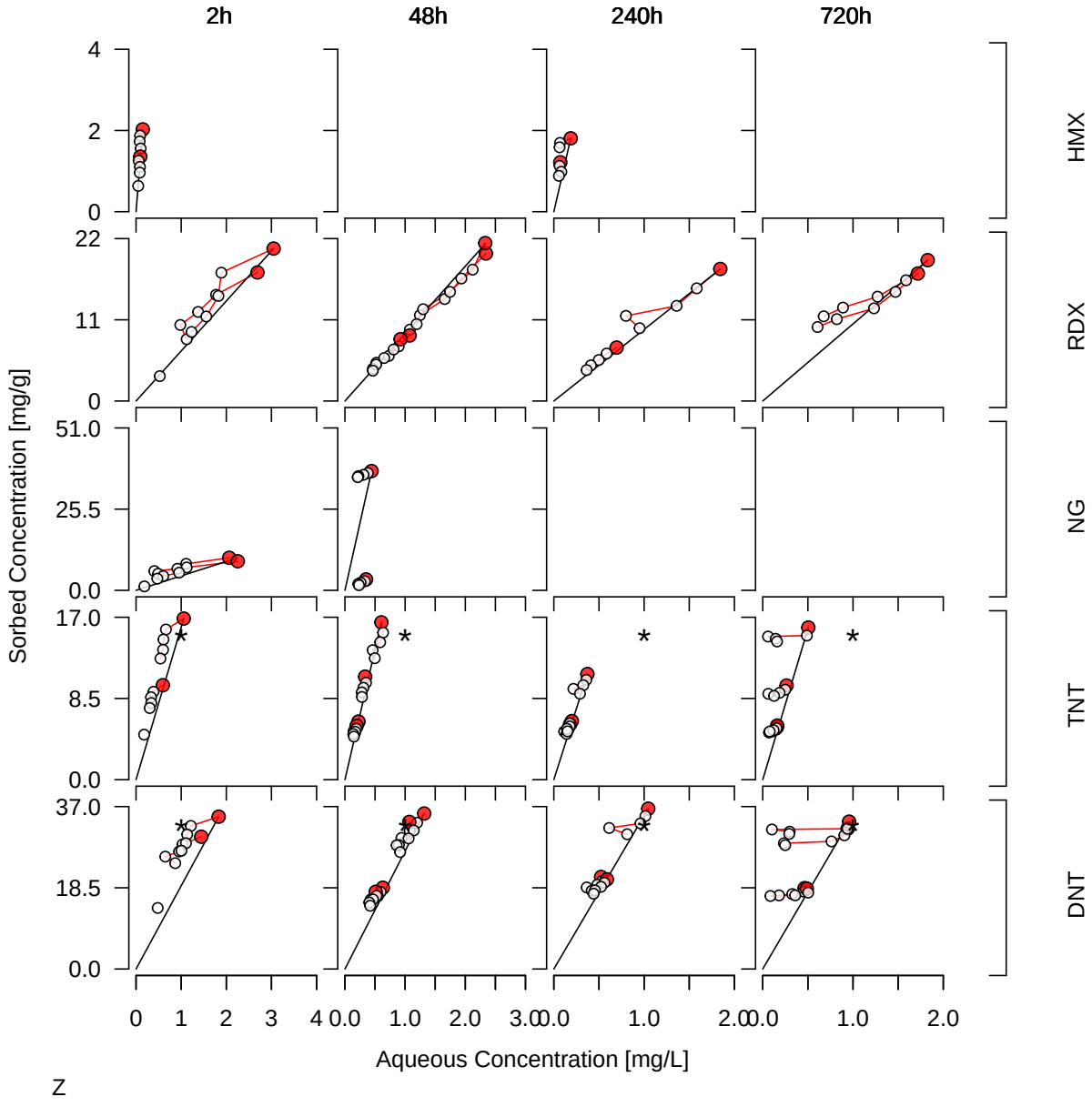

2h
48h
240h
720h
HMX
RDX
NG
TNT
DNT
Sorbed Concentration [mg/g]
Aqueous Concentration [mg/L]
LCL

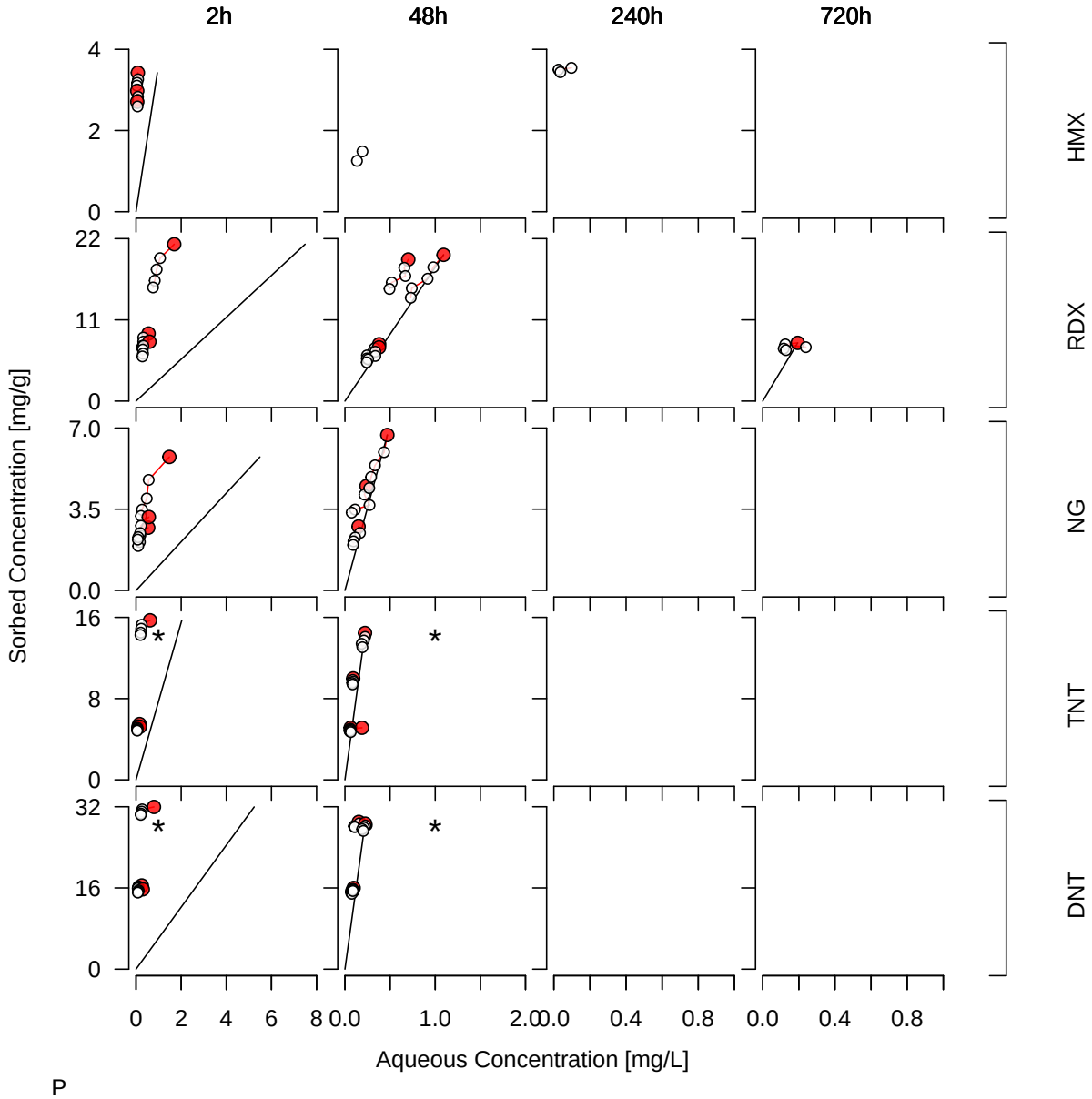

2h
48h
240h
720h
HMX
RDX
NG
TNT
DNT
Sorbed Concentration [mg/g]
Aqueous Concentration [mg/L]
LCO


2h
48h
240h
720h
HMX
RDX
NG
TNT
DNT
Sorbed Concentration [mg/g]
Aqueous Concentration [mg/L]
3.0
1.5
0.0
21.0
10.5
0.0
17.0
8.5
0.0
16
8
0
40
20
0
0 2 4 6
0 1 2 3 4
0 1 2 3 4
0.0 1.0 2.0 3.0
*

J


2h
48h
240h
720h
HMX
RDX
NG
TNT
DNT
Sorbed Concentration [mg/g]
Aqueous Concentration [mg/L]
R


2h
48h
240h
720h
HMX
RDX
NG
TNT
DNT
Sorbed Concentration [mg/g]
Aqueous Concentration [mg/L]
Z


2h
48h
240h
720h
HMX
RDX
NG
TNT
DNT
Sorbed Concentration [mg/g]
Aqueous Concentration [mg/L]
4
2
0
22
11
0
7.0
3.5
0.0
16
8
0
32
16
0
0 2 4 6 8
0.0 1.0 2.0
0.0 0.4 0.8
0.0 0.4 0.8

P

B.2 Derivation of Langmuir STM

The Langmuir isotherm is:

$$q = \frac{q_T K_L C}{1 + K_L C} \tag{B.1}$$

where q, q_T, K_L, and C are the sorbed concentration, total site density, Langmuir constant, and aqueous concentration, respectively.

If we allow for two binding strengths, weak (w) and strong (s), then the total sorbed concentration is:

$$q = \frac{q_{T,w} K_{L,w} C}{1 + K_{L,w} C} + \frac{q_{T,s} K_{L,s} C}{1 + K_{L,s} C} \tag{B.2}$$

If the strong sites are proportional to the weakly sorbed concentration at adsorption then their relationship is governed by:

$$q_{T,s} = f_{ST} \frac{q_T K_{L,w} C_A}{1 + K_{L,w} C_A} \tag{B.3}$$

where f_{ST} is the proportionality between weak and strong sites and C_A is the adsorption aqueous concentration. This allows for a differentiation between adsorption and desorption, where the adsorption isotherm is:

$$q_A = q_{T,w} \frac{K_{L,w} C_A}{1 + K_{L,w} C_A} + q_{T,s} \frac{K_s C_A}{1 + K_s C_A} \tag{B.4}$$

and the desorption isotherm is:

$$q_D = q_{T,w} \frac{K_{L,w} C_D}{1 + K_{L,w} C_D} + q_{T,s} \frac{K_s C_D}{1 + K_s C_D} \tag{B.5}$$

If there are only two site strengths, then the weak sites are the difference between the total and the strong sites:

$$q_{T,w} = q_T - q_{T,s} \tag{B.6}$$

and the isotherms are

$$q_A = (q_T - q_{T,s}) \frac{K_{L,w} C_A}{1 + K_{L,w} C_A} + q_{T,s} \frac{K_s C_A}{1 + K_s C_A} \tag{B.7}$$

$$q_D = (q_T - q_{T,s}) \frac{K_{L,w} C_D}{1 + K_{L,w} C_D} + q_{T,s} \frac{K_s C_D}{1 + K_s C_D} \tag{B.8}$$

Then, substituting eqn. B.3 into B.7 and B.8 yields

$$q_A = \left(q_T - f_s q_T \frac{K_{L,w} C_A}{1 + K_{L,w} C_A} \right) \frac{K_{L,w} C_A}{1 + K_{L,w} C_A} + f_s q_T \frac{K_{L,w} C_A}{1 + K_{L,w} C_A} \frac{K_s C_A}{1 + K_s C_A} \tag{B.9}$$

$$q_D = \left(q_T - f_s q_T \frac{K_{L,w} C_A}{1 + K_{L,w} C_A} \right) \frac{K_{L,w} C_D}{1 + K_{L,w} C_D} + f_s q_T \frac{K_{L,w} C_A}{1 + K_{L,w} C_A} \frac{K_s C_D}{1 + K_s C_D} \tag{B.10}$$

If the strong sites are saturated at all C and $K_s C >> 1$ then

$$\frac{K_s C}{1 + K_s C} \approx 1 \tag{B.11}$$

So, eqns. B.9 and B.10 become

$$\begin{aligned} q_A &= \left(q_T - f_s q_T \frac{K_{L,w} C_A}{1 + K_{L,w} C_A} \right) \frac{K_{L,w} C_A}{1 + K_{L,w} C_A} + f_s q_T \frac{K_{L,w} C_A}{1 + K_{L,w} C_A} \\ &= (q_T - q_{T,s}) \frac{K_{L,w} C_A}{1 + K_{L,w} C_A} + q_{T,s} \end{aligned} \tag{B.12}$$

$$\begin{aligned} q_D &= \left(q_T - f_s q_T \frac{K_{L,w} C_A}{1 + K_{L,w} C_A} \right) \frac{K_{L,w} C_D}{1 + K_{L,w} C_D} + f_s q_T \frac{K_{L,w} C_A}{1 + K_{L,w} C_A} \\ &= (q_T - q_{T,s}) \frac{K_{L,w} C_D}{1 + K_{L,w} C_D} + q_{T,s} \end{aligned} \tag{B.13}$$

If the concentration of strong sites is << than the total number of sites, then $q_T - q_{T,s} \approx q_T$ so the Langmuir STM is

$$q_A = q_T \frac{K_{L,w} C_A}{1 + K_{L,w} C_A} + f_s q_T \frac{K_{L,w} C_A}{1 + K_{L,w} C_A} \tag{B.14}$$

$$q_D = q_T \frac{K_{L,w} C_D}{1 + K_{L,w} C_D} + f_s q_T \frac{K_{L,w} C_A}{1 + K_{L,w} C_A} \tag{B.15}$$

In the linear case where $K_{L,w}C \ll 1$, the model reduces to

$$q_A = q_T K_{L,w} C_A + f_s q_T K_{L,w} C_A \tag{B.16}$$
$$q_D = q_T K_{L,w} C_D + f_s q_T K_{L,w} C_A \tag{B.17}$$

which is similar to the Reversible Resistant model:

$$q_A = K_x C_A + K_0 C_A \tag{B.18}$$
$$q_D = K_x C_D + K_0 C_A \tag{B.19}$$

By comparison, it can be seen that

$$K_x = q_T K_{L,w} \tag{B.20}$$
$$K_0 = f_{ST} q_T K_{L,w} \tag{B.21}$$

which yields the relationship

$$f_{ST} = \frac{K_0}{K_x} \tag{B.22}$$

B.3 Model code

B.3.1 Determination of dependencies

```
graphics.off()
rm(list=ls(all=TRUE))

### Read data files
##  HPLC
hplc.raw     <-  read.table(file='../data/hplc_data.csv',header=TRUE,
    stringsAsFactor=FALSE,sep=',',as.is=TRUE)
     #   Add Mass Total Column
     hplc.raw$MTOT   <-  hplc.raw$A.C*hplc.raw$V.A+
                         hplc.raw$D1.C*hplc.raw$V.D1+
                         hplc.raw$D2.C*hplc.raw$V.D2+
                         hplc.raw$D3.C*hplc.raw$V.D3+
                         hplc.raw$D4.C*hplc.raw$V.D4+
                         hplc.raw$E1.C*hplc.raw$V.E1+
                         hplc.raw$E2.C*hplc.raw$V.E2+
                         hplc.raw$E3.C*hplc.raw$V.E3
##  Properties
prop.raw     <-  read.table(file='../data/soil_properties.csv',header=
    TRUE,stringsAsFactors=FALSE,sep=',',as.is=TRUE)
##  Mass Balance Check
mbal.yesno   <-  read.table(file='../data/MB_yesno_v3.csv',header=TRUE,
    sep=',',as.is=TRUE,stringsAsFactors=FALSE)
##  reversible Fit Data
irp.fit      <-  read.table(file='../data/IRP_wErr_v2.csv',header=TRUE,
    sep=',',as.is=TRUE,stringsAsFactors=FALSE)
##  RR Fit Data
nrr.fit      <-  read.table(file='../data/RR_Norm_nls_v5.csv',header=TRUE
    ,sep=',',as.is=TRUE,stringsAsFactors=FALSE)
##  STM Fit
stm.fit      <-  read.table(file='../data/fit_st_v4.csv',header=TRUE,sep=
    ',',as.is=TRUE,stringsAsFactors=FALSE)
stm.err      <-  read.table(file='../data/err_st_v4.csv',header=TRUE,sep=
    ',',as.is=TRUE,stringsAsFactors=FALSE)
stm.lin      <-  read.table(file='../data/lin_covv2.csv',header=TRUE,sep=
    ',',as.is=TRUE,stringsAsFactors=FALSE)
##  STM Residuals
stm.res      <-  read.table(file='../data/ssqtotoptim_KQ_v3.csv',header=
    TRUE,sep=',',as.is=TRUE,stringsAsFactors=FALSE)

### Known Variables
mc_list      <-  c('HMX','RDX','NG','TNT','DNT')

soil_list    <-  c('KA','ST','BT','BA','U','B','FT','SOU','W1','W2','SAS'
    ,'SSL','MPK','S2','W','AM','H','BOX','GUA','PO','BU','LCL','LCO','J'
    ,'R','Z','P')

soil_order   <-  prop.raw[prop.raw[,1] %in% soil_list,]
soil_order   <-  soil_order[order(soil_order$TOC),]
```

```
38 nSoil        <- length(soil_list)
39 nMC          <- length(mc_list)
40
41 # Test models
42 # kmst_fmst ==> each MC/sorbent/adsorption pair is independent i.e. k(MC
       ,Sorbent,Ads), f(MC,Sorbent,Ads)
43 kmst_fmst_model_opt   <- function(pars,Obs,Lin) {
44     Kq       <- 10^pars[1:4]
45     K        <- 10^pars[5:8]
46     fS       <- 10^pars[9:12]
47
48     fS[fS<1e-5] <- 1e-5
49
50     KQfit    <- Kq[Obs[,2]]
51     Kfit     <- K[Obs[,2]]
52     fFit     <- fS[Obs[,2]]
53     linear   <- Lin
54
55     c.obs    <- Obs[,3:7]
56     q.obs    <- Obs[,8:12]
57
58     q.lan    <- matrix(NA,nc=5,nr=length(Kfit))
59     q.lin    <- matrix(NA,nc=5,nr=length(Kfit))
60     q.mod    <- matrix(NA,nc=5,nr=length(Kfit))
61     for (ii in 1:dim(Obs)[1]) {
62         for (jj in 1:5){
63             q.lan[ii,jj]   <- KQfit[ii]*c.obs[ii,jj]/(1+Kfit[ii]*c.obs[
                   ii,jj]) +
64                               fFit[ii]*KQfit[ii]*c.obs[ii,1]/(1+Kfit[ii
                                   ]*c.obs[ii,1])
65
66             q.lin[ii,jj]   <- KQfit[ii]*c.obs[ii,jj] +
67                               fFit[ii]*KQfit[ii]*c.obs[ii,1]
68
69             q.mod[ii,jj]    <- linear*q.lin[ii,jj]+(1-linear)*q.lan[ii,
                   jj]
70         }
71     }
72     qres     <- (log10(q.obs)-log10(q.mod))^2
73     is.na(qres) <- !is.finite(qres)
74     ssq      <- sum(qres,na.rm=T)
75     return(ssq)
76 }
77 # kms_fmst  ==> kp is dependent on MC, sorbent, fst is dependent on MC,
       sorbent,ads
78 kms_fmst_model_opt <- function(pars,Obs,Lin) {
79     Kq       <- 10^pars[1]
80     K        <- 10^pars[2]
81     fS       <- 10^pars[3:6]
82
83     #fS[fS<1e-5] <- 1e-5
```

```
84
85      KQfit   <-  rep(Kq,length(Obs[,2]))
86      Kfit    <-  rep(K,length(Obs[,2]))
87      fFit    <-  fS[Obs[,2]]
88      linear  <-  rep(Lin,length(Obs[,2]))
89
90      c.obs   <-  Obs[,3:7]
91      q.obs   <-  Obs[,8:12]
92
93      q.lan   <-  matrix(NA,nc=5,nr=length(Kfit))
94      q.lin   <-  matrix(NA,nc=5,nr=length(Kfit))
95      q.mod   <-  matrix(NA,nc=5,nr=length(Kfit))
96      for (ii in 1:length(fFit)) {
97          for (jj in 1:5){
98              q.lan[ii,jj]   <-  KQfit[ii]*c.obs[ii,jj]/(1+Kfit[ii]*c.obs[
                    ii,jj]) +
99                                 fFit[ii]*KQfit[ii]*c.obs[ii,1]/(1+Kfit[ii
                                    ]*c.obs[ii,1])
100
101             q.lin[ii,jj]   <-  KQfit[ii]*c.obs[ii,jj] +
102                                fFit[ii]*KQfit[ii]*c.obs[ii,1]
103
104             q.mod[ii,jj]    <-  linear[ii]*q.lin[ii,jj]+(1-linear[ii])*q
                    .lan[ii,jj]
105         }
106     }
107     #print(q.mod)
108     qres    <-  (log10(q.obs)-log10(q.mod))^2
109     is.na(qres) <-  !is.finite(qres)
110     ssq     <-  sum(qres,na.rm=T)
111     return(ssq)
112 }
113
114 # Output matrix
115 p.kMST_fMST <-  array(NA,c(nSoil,5,6))
116 p.kMS_fMST  <-  array(NA,c(nSoil,4,10))
117 err.fin <-  c()
118 pars.fin<-  c()
119
120 # parameters and error output matrix
121 pars.kMST_fMST  <-  array(NA,c(nSoil,5,8))
122 pars.kMS_fMST   <-  array(NA,c(nSoil,5,8))
123
124 for (ii in 1:nSoil) {
125     print(paste('Soil ',ii,sep=''))
126     flush.console()
127     # Select Soil Data
128     sub.soil    <-  hplc.raw[hplc.raw[,2]==soil_order$SoilCode[ii],]
129
130     # Check Mass Balance
131     for (jj in 1:dim(sub.soil)[1]) {
```

```
132         is.na(sub.soil[jj,4:32])    <- ifelse((sub.soil[jj,3]==4 | sub.
                soil[jj,3]==9 | sub.soil[jj,3]==14 | sub.soil[jj,3]==19) &
                sub.soil[jj,1]=='TNT',TRUE,ifelse((sub.soil[jj,3]==5 | sub.
                soil[jj,3]==10 | sub.soil[jj,3]==15 | sub.soil[jj,3]==20) &
                sub.soil[jj,1]!='TNT',TRUE,FALSE))
133         is.na(sub.soil[jj,4:32])    <- ifelse(mbal.yesno[mbal.yesno
                [,3]==sub.soil[jj,1] & mbal.yesno[,1]==soil_list[ii] & mbal.
                yesno[,2]==sub.soil[jj,3],4]==1,FALSE,TRUE)
134     }
135
136     # Indexing for MC, Adsorption time
137     mtmp          <- data.matrix(sub.soil[,1])
138     M.List        <- ifelse(mtmp=='HMX',1,
139                       ifelse(mtmp=='RDX',2,
140                       ifelse(mtmp=='NG',3,
141                       ifelse(mtmp=='TNT',4,5))))
142     V.List        <- data.matrix(sub.soil[,3])
143     T.List        <- ifelse(V.List<6,1,
144                       ifelse(V.List<11,2,
145                       ifelse(V.List<16,3,4)))
146
147     # set up observed matrix
148     obs                   <- matrix(c(M.List,T.List,data.matrix(sub.soil
            [,6:10]),data.matrix(sub.soil[,28:32])),nc=12)
149     is.na(obs[,1])        <- obs[,3]==0
150     # Remove incomplete cases
151     obs                   <- obs[complete.cases(obs),]
152     m.obs                 <- obs[,1]
153     t.obs                 <- obs[,2]
154     c.obs                 <- obs[,3:7]
155     q.obs                 <- obs[,8:12]
156
157     st.obs                <- obs
158     lin.obs               <- data.matrix(stm.lin[ii,])
159
160     st.theta                 <- c(rep(0,5),rep(0,5),rep(-3,4))
161
162     for (jj in 1:5) {
163         mst.theta         <- c(rep(0,4),rep(0,4),rep(-3,4))
164         mst.obs           <- st.obs[st.obs[,1]==jj,]
165         mst.linear        <- lin.obs[jj]
166         err.fin           <- c(NA,NA,NA,NA)
167
168         # Fit least restrictive model
169         kmst_fmst.fit           <- optim(par=mst.theta,fn=kmst_fmst_model
                _opt,Lin=mst.linear,Obs=mst.obs,method='L-BFGS-B',hessian=
                TRUE,control=list(maxit=300))
170
171         pars.kMST_fMST[ii,jj,1:4]     <- kmst_fmst.fit$par[1:4]
172
173         hess.fit      <- kmst_fmst.fit$hessian[1:4,1:4]
```

```
174         fit.v       <-  c(1,2,3,4)
175         c.del       <-  c()
176
177         # Eliminate row/column from hessian for variables we don't care
                about
178         for (kk in 1:4) {
179             if (hess.fit[kk,kk]==0){
180                 c.del   <-  c(c.del,kk)
181             }
182         }
183         if (!is.null(c.del)) {
184             hess.fit    <-  hess.fit[-c.del,-c.del]
185             fit.v       <-  fit.v[-c.del]
186         }
187         if (is.null(dim(hess.fit))) {
188             err.fin[fit.v]  <-  sqrt(hess.fit)
189         } else {
190             vc          <- solve(matrix(NA,nrow=nrow(hess.fit),ncol=ncol
                    (hess.fit)))
191             try(vc      <-  solve(hess.fit))
192             err.tmp     <-  sqrt(diag(vc))
193             err.fin[fit.v]  <-  err.tmp
194         }
195         pars.kMST_fMST[ii,jj,5:8]    <-    err.fin
196
197         for (kk in 1:6) {
198             # pairwise comparison, k2h - k48h, k2h - k240h, ...
199             i.dex                   <-  c(1,1,1,2,2,3)
200             j.dex                   <-  c(2,3,4,3,4,4)
201             # Grand standard deviation = sqrt(0.5*(s1^2+s2^2))
202             # Assumes equal variance and equal sample size
203             s.pool                  <-  sqrt(0.5*(err.fin[i.dex[kk]]^2+
                    err.fin[j.dex[kk]]^2))
204             # Difference in means
205             x.diff                  <-  pars.kMST_fMST[ii,jj,i.dex[kk]]-
                    pars.kMST_fMST[ii,jj,j.dex[kk]]
206             # Compute t-test value
207             ttest                   <-  x.diff/s.pool
208             # Compute p-value
209             p.kMST_fMST[ii,jj,kk]   <-  2*pt(-abs(ttest),df=10)
210         }
211     }
212     print('Kmst_Fmst_OK')
213
214     fit.out <-  matrix(NA,nc=4,nr=5)
215     err.out <-  fit.out
216
217     # Do the same for kms_fmst model
218     for (jj in 1:5) {
219         mst.theta       <-  c(0,0,rep(-3,4))
220         mst.obs         <-  st.obs[st.obs[,1]==jj,]
```

```
221         mst.linear      <-  lin.obs[jj]
222
223         kms_fmst.fit          <-  optim(par=mst.theta,fn=kms_fmst_model_
                opt,Lin=mst.linear,Obs=mst.obs,method='L-BFGS-B',hessian=
                TRUE,control=list(maxit=300))
224
225         pars.fit <-  kms_fmst.fit$par[3:6]
226         hess.fit <-  kms_fmst.fit$hessian[3:6,3:6]
227
228         fit.v       <-  c(1,2,3,4)
229         c.del       <-  c()
230         # Eliminate row/column from hessian for variables we don't care
              about
231         for (kk in 1:4) {
232             if (hess.fit[kk,kk]==0){
233                 c.del   <-  c(c.del,kk)
234             }
235         }
236         if (!is.null(c.del)) {
237             hess.fit    <-  hess.fit[-c.del,-c.del]
238             fit.v       <-  fit.v[-c.del]
239         }
240         if (is.null(dim(hess.fit))) {
241             err.fin[fit.v]  <-  sqrt(hess.fit)
242         } else {
243             vc          <- solve(matrix(NA,nrow=nrow(hess.fit),ncol=ncol
                    (hess.fit)))
244             try(vc      <-  solve(hess.fit))
245             err.tmp     <-  sqrt(diag(vc))
246             err.fin[fit.v]  <-  err.tmp
247         }
248
249         fit.out[jj,]<-  pars.fit
250         err.out[jj,]<-  err.fin
251         pars.kMS_fMST[ii,jj,1:4]    <-  pars.fit
252         pars.kMS_fMST[ii,jj,5:8]    <-  err.fin
253     }
254
255     for (jj in 1:4)  {
256     for (kk in 1:10) {
257         i.dex                   <-  c(1,1,1,1,2,2,2,3,3,4)
258         j.dex                   <-  c(2,3,4,5,3,4,5,4,5,5)
259         s.pool                  <-  sqrt(0.5*(err.out[i.dex[kk],jj]^2+
                err.out[j.dex[kk],jj]^2))
260         x.diff                  <-  fit.out[i.dex[kk]]-fit.out[j.dex[kk
                ]]
261         # Generate t-test statistic
262         ttest                   <-  x.diff/s.pool
263         # Calculate p-value
264         p.kMS_fMST[ii,jj,kk]    <-  2*pt(-abs(ttest),df=10)
265     }
```

```
266         }
267         print('Kms_Fmst_OK')
268         flush.console()
269     }
270
271     # Perform Holm-Bonferroni stepdown test
272     # Null is kt(1)-kt(2)=0
273
274     # First K-MST
275     nConv   <-  sum(!is.na(p.kMST_fMST))/(dim(p.kMST_fMST)[1]*dim(p.kMST_
            fMST)[2]*dim(p.kMST_fMST)[3])
276     P   <-  c(p.kMST_fMST)
277     P   <-  P[!is.na(P)]
278     P   <-  P[order(P)]
279     m   <-  length(P)
280
281     alpha = 0.05
282     crit    <-  alpha/(m+1-seq(1:m))
283     # k is first observation > criteria
284     k   <-  match(FALSE,P<crit)
285     # Reject null for all H < k
286
287     # Next K-MS, F-MST
288     nConv   <-  sum(!is.na(p.kMS_fMST))/(dim(p.kMS_fMST)[1]*dim(p.kMS_fMST)
            [2]*dim(p.kMS_fMST)[3])
289     P   <-  c(p.kMS_fMST)
290     P   <-  P[!is.na(P)]
291     P   <-  P[order(P)]
292     m   <-  length(P)
293
294     alpha = 0.05
295     crit    <-  alpha/(m+1-seq(1:m))
296     # k is first observation > criteria
297     k   <-  match(FALSE,P<crit)
298     # Reject null for all H < k
299
300
301     ### Plots?
302     x11(8,8)
303     xFigs   <-  seq(0.1,0.95,length=2)
304     yFigs   <-  seq(0.95,0.1,length=6)
305     for (ii in 1:5) {
306         par(fig=c(xFigs[1],xFigs[2],yFigs[ii+1],yFigs[ii]),new=ifelse(ii==1,
                FALSE,TRUE),mar=c(0,0,0,0))
307         plot(1,type='n',xlim=c(0,28),ylim=c(10^-2,10^2),log='y',xlab='',ylab
                ='',axes=F)
308         cset <-  c('red','cornflowerblue')
309         for (jj in 1:27) {
310             col.tog <-  jj%%2+1
311             xseq    <-  jj+seq(-0.3,0.3,length.out=4)
312             ypts    <-  10^pars.kMST_fMST[jj,ii,1:4]
```

```
313           ylo      <-  10^(pars.kMST_fMST[jj,ii,1:4]-pars.kMST_fMST[jj,ii
                  ,5:8])
314           yhi      <-  10^(pars.kMST_fMST[jj,ii,1:4]+pars.kMST_fMST[jj,ii
                  ,5:8])
315           is.na(ypts) <-  is.na(pars.kMST_fMST[jj,ii,5:8])
316           arrows(x0=xseq,y0=ylo,y1=yhi,code=3,angle=90,length=0.03)
317           points(x=xseq,y=ypts,pch=21,col=cset[col.tog],cex=0.5,bg=cset[
                  col.tog])
318       }
319       axis(2,las=2)
320   }
321
322   x11(8,8)
323   xFigs   <-  seq(0.1,0.95,length=2)
324   yFigs   <-  seq(0.95,0.1,length=6)
325   for (ii in 1:5) {
326       par(fig=c(xFigs[1],xFigs[2],yFigs[ii+1],yFigs[ii]),new=ifelse(ii==1,
              FALSE,TRUE),mar=c(0,0,0,0))
327       plot(1,type='n',xlim=c(0,28),ylim=c(10^-3,10^2),log='y',xlab='',ylab
              ='',axes=F)
328       cset <-  c('red','cornflowerblue')
329       for (jj in 1:27) {
330           col.tog <-  jj%%2+1
331           xseq    <-  jj+seq(-0.3,0.3,length.out=4)
332           ypts    <-  10^pars.kMS_fMST[jj,ii,1:4]
333           ylo      <-  10^(pars.kMS_fMST[jj,ii,1:4]-pars.kMS_fMST[jj,ii
                  ,5:8])
334           yhi      <-  10^(pars.kMS_fMST[jj,ii,1:4]+pars.kMS_fMST[jj,ii
                  ,5:8])
335           is.na(ypts) <-  is.na(pars.kMS_fMST[jj,ii,5:8])
336           arrows(x0=xseq,y0=ylo,y1=yhi,code=3,angle=90,length=0.03)
337           points(x=xseq,y=ypts,pch=21,col=cset[col.tog],cex=0.5,bg=cset[
                  col.tog])
338       }
339       axis(2,las=2)
340   }
```

B.3.2 Linear/Langmuir split

```
1  #Linear/Langmuir Analysis
2  hplc.raw    <-  read.table('hplc_data.csv',header=TRUE, stringsAsFactor=
       FALSE,sep=',',as.is=TRUE)
3  prop.raw    <-  read.table('soil_properties.csv',header=TRUE,
       stringsAsFactors=FALSE,sep=',',as.is=TRUE)
4
5  foc         <-  prop.raw$TOC/100
6  fclay       <-  prop.raw$Clay/100
7
8  soil_list   <-  c('KA','ST','BT','BA','U','B','FT','SOU','W1','W2','SAS'
       ,'SSL','MPK','S2','W','AM','H','BOX','GUA','PO','BU','LCL','LCO','J'
       ,'R','Z','P')
9  soil_order  <-  prop.raw[prop.raw[,1] %in% soil_list,]
```

```
soil_order  <-  soil_order[order(soil_order$TOC),]$SoilCode
nSoil       <-  length(soil_order)

mc_list <-  c('HMX','RDX','NG','TNT','DNT')
nMC         <-  length(mc_list)
vial_list   <-  c(3,8,13,18)
nVial       <-  length(vial_list)

collist<-rev(c(rgb(0,seq(18,9,-1),0,8,maxColorValue =18),
               rgb(seq(0,8,1),seq(8,0,-1),0,8,maxColorValue =18),
               rgb(seq(9,18,1),0,0,8,maxColorValue =18)))

# Function to fit langmuir data
langmuir    <-  function(params,soilCode,dataset,munit)     {

    mc_elem <-  grep(munit,c('HMX','RDX','NG','TNT','DNT'))

    sub.soil<-  subset(dataset,dataset$SOILCODE==soilCode)
    c_obs   <-  sub.soil[,c('MC','VIAL','A.C','D1.C','D2.C','D3.C','D4.C
        ')]
    q_obs   <-  sub.soil[,c('MC','VIAL','Q.A','Q.D1','Q.D2','Q.D3','Q.D4
        ')]

    Kw      <-  exp(params[1])
    qT      <-  exp(params[2])
    fS      <-  exp(params[3])

    c_mc    <-  subset(c_obs,c_obs$MC==c('HMX','RDX','NG','TNT','DNT')[
        mc_elem])
    q_mc    <-  subset(q_obs,q_obs$MC==c('HMX','RDX','NG','TNT','DNT')[
        mc_elem])
    q_mc    <-  q_mc[,c('Q.A','Q.D1','Q.D2','Q.D3','Q.D4')]

    q_mod   <-  stm_lang(Kw,fS,qT,c_mc)
    q_ssq   <-  stm_ssq(q_mc,q_mod,0)

    return(q_ssq)
}

# Function to fit linear data
linear      <-  function(params,soilCode,dataset,munit)     {

    mc_elem <-  grep(munit,c('HMX','RDX','NG','TNT','DNT'))

    sub.soil<-  subset(dataset,dataset$SOILCODE==soilCode)
    c_obs   <-  sub.soil[,c('MC','VIAL','A.C','D1.C','D2.C','D3.C','D4.C
        ')]
    q_obs   <-  sub.soil[,c('MC','VIAL','Q.A','Q.D1','Q.D2','Q.D3','Q.D4
        ')]

    Kw      <-  exp(params[1])
```

```
55      fS        <-  exp(params[2])
56
57      c_mc      <-  subset(c_obs,c_obs$MC==c('HMX','RDX','NG','TNT','DNT')[
            mc_elem])
58      q_mc      <-  subset(q_obs,q_obs$MC==c('HMX','RDX','NG','TNT','DNT')[
            mc_elem])
59      q_mc      <-  q_mc[,c('Q.A','Q.D1','Q.D2','Q.D3','Q.D4')]
60
61      q_mod     <-  stm_linear(Kw,fS,c_mc)
62      q_ssq     <-  stm_ssq(q_mc,q_mod,0)
63
64      return(q_ssq)
65  }
66
67  linlang <-  matrix(NA,nrow=nSoil,ncol=5)
68  # Params = K,q,f
69  params <-  c(1,3.5,0.5)
70
71  # Threshold denotes break point for linear/langmuir split
72  cov_thresh  <-  0.9
73
74  lin_err <-  matrix(0,nrow=nSoil,ncol=nMC,dimnames=list(soil_order,mc_
        list))
75  lin_cov <-  matrix(0,nrow=nSoil,ncol=nMC,dimnames=list(soil_order,mc_
        list))
76
77  for (ii in 1:nSoil) {
78
79      for (jj in 1:5){
80
81          # Fit using langmuir on per mc/sorbent/adsorption time
82          lang_par    <-  optim(par=params,fn=langmuir,soilCode=soil_order
                [ii],dataset=hplc.raw,munit=mc_list[jj],method='L-BFGS-B',
                hessian=TRUE,control=list(maxit=300))
83
84          # Compute K/Q Covariance
85              vc  <- solve(matrix(NA,nrow=nrow(lang_par$hessian),ncol=ncol
                    (lang_par$hessian)))
86              try(vc  <-  solve(lang_par$hessian))
87
88          # Linear/Langmuir check
89              lin_cov[ii,jj]  <-  ifelse(abs(vc[1,2])>=cov_thresh | is.na(
                    vc[1,2]),1,0)
90      }
91  }
92
93  ## Output linear/langmuir table
94  lincov    <-  paste('../data/lin_cov_v1.csv',sep='')
95  write.table(lin_cov,file=lincov,sep=',',col.names=T,row.names=T)
```

B.3.3 STM model code

```
# Comparison of models

hplc.raw     <-  read.table(fil='../data/hplc_data.csv',header=TRUE,
    stringsAsFactor=FALSE,sep=',',as.is=TRUE)
prop.raw     <-  read.table(file='../data/soil_properties.csv',header=
    TRUE,stringsAsFactors=FALSE,sep=',',as.is=TRUE)
cov.lin      <-  read.table(file='../data/lin_covv2.csv',header=TRUE,
    stringsAsFactor=FALSE,sep=',',as.is=TRUE)
mbal.yesno   <-  read.table(file='../data/MB_yesno_v3.csv',header=TRUE,
    sep=',',as.is=TRUE,stringsAsFactors=FALSE)

soil_list    <-  c('KA','ST','BT','BA','U','B','FT','SOU','W1','W2','SAS'
    ,'SSL','MPK','S2','W','AM','H','BOX','GUA','PO','BU','LCL','LCO','J'
    ,'R','Z','P')

soil_order   <-  prop.raw[prop.raw[,1] %in% soil_list,]
soil_order   <-  soil_order[order(soil_order$TOC),]
nSoil        <-  length(soil_order$SoilCode)

mc_list      <-  c('HMX','RDX','NG','TNT','DNT')
nMC          <-  length(mc_list)

collist<-rev(c(rgb(0,seq(18,9,-1),0,8,maxColorValue =18),
            rgb(seq(0,8,1),seq(8,0,-1),0,8,maxColorValue =18),
            rgb(seq(9,18,1),0,0,8,maxColorValue =18)))

# 3 Models  -   k(M,S)_f(M,S,T) ==> mst_model
#           -   k(M,S)_f(M,S)   ==> ms_model
#           -   k(M,S)_f(S,T)   ==> st_model
mst_model_opt   <-  function(pars,Obs,Lin) {
    Kq       <-  10^pars[1]
    K        <-  10^pars[2]
    fS       <-  10^pars[3:6]

    KQfit    <-  rep(Kq,dim(Obs)[1])
    Kfit     <-  rep(K,dim(Obs)[1])
    fFit     <-  fS[Obs[,2]]
    linear   <-  Lin

    c.obs    <-  Obs[,3:7]
    q.obs    <-  Obs[,8:12]

    q.lan    <-  matrix(NA,nc=5,nr=length(Kfit))
    q.lin    <-  matrix(NA,nc=5,nr=length(Kfit))
    q.mod    <-  matrix(NA,nc=5,nr=length(Kfit))
    for (ii in 1:dim(Obs)[1]) {
        for (jj in 1:5){
            q.lan[ii,jj]   <-  KQfit[ii]*c.obs[ii,jj]/(1+Kfit[ii]*c.obs[
                ii,jj]) +
                               fFit[ii]*KQfit[ii]*c.obs[ii,1]/(1+Kfit[ii
                                   ]*c.obs[ii,1])
```

```
44
45              q.lin[ii,jj]    <-  KQfit[ii]*c.obs[ii,jj] +
46                                  fFit[ii]*KQfit[ii]*c.obs[ii,1]
47
48              q.mod[ii,jj]     <-  linear*q.lin[ii,jj]+(1-linear)*q.lan[ii,
                    jj]
49          }
50      }
51      qres     <-  (log10(q.obs)-log10(q.mod))^2
52      is.na(qres) <-  !is.finite(qres)
53      ssq      <-  sum(qres,na.rm=T)
54      return(ssq)
55  }
56  ms_model_opt   <-  function(pars,Obs,Lin) {
57      Kq       <-  10^pars[1]
58      K        <-  10^pars[2]
59      fS       <-  10^pars[3]
60
61      KQfit    <-  rep(Kq,dim(Obs)[1])
62      Kfit     <-  rep(K,dim(Obs)[1])
63      fFit     <-  rep(fS,dim(Obs)[1])
64      linear   <-  Lin
65
66      c.obs    <-  Obs[,3:7]
67      q.obs    <-  Obs[,8:12]
68
69      q.lan    <-  matrix(NA,nc=5,nr=length(Kfit))
70      q.lin    <-  matrix(NA,nc=5,nr=length(Kfit))
71      q.mod    <-  matrix(NA,nc=5,nr=length(Kfit))
72      for (ii in 1:dim(Obs)[1]) {
73          for (jj in 1:5){
74              q.lan[ii,jj]    <-  KQfit[ii]*c.obs[ii,jj]/(1+Kfit[ii]*c.obs[
                    ii,jj]) +
75                                  fFit[ii]*KQfit[ii]*c.obs[ii,1]/(1+Kfit[ii
                                        ]*c.obs[ii,1])
76
77              q.lin[ii,jj]    <-  KQfit[ii]*c.obs[ii,jj] +
78                                  fFit[ii]*KQfit[ii]*c.obs[ii,1]
79
80              q.mod[ii,jj]     <-  linear*q.lin[ii,jj]+(1-linear)*q.lan[ii,
                    jj]
81          }
82      }
83      qres     <-  (log10(q.obs)-log10(q.mod))^2
84      is.na(qres) <-  !is.finite(qres)
85      ssq      <-  sum(qres,na.rm=T)
86      return(ssq)
87  }
88  st_model_opt <-  function(pars,Obs,Lin) {
89      Kq       <-  10^pars[1:5]
90      K        <-  10^pars[6:10]
```

```
91      fS       <-  10^pars[11:14]
92
93      # KQfit   <-  ifelse(Obs[,1]==1,10^Kq[1],
94                    # ifelse(Obs[,1]==2,10^Kq[2],
95                    # ifelse(Obs[,1]==3,10^Kq[3],
96                    # ifelse(Obs[,1]==4,10^Kq[4],10^Kq[5]))))
97
98      # Kfit    <-  ifelse(Obs[,1]==1,10^K[1],
99                    # ifelse(Obs[,1]==2,10^K[2],
100                   # ifelse(Obs[,1]==3,10^K[3],
101                   # ifelse(Obs[,1]==4,10^K[4],10^K[5]))))
102
103     # fFit    <-  ifelse(Obs[,2]<6,10^fS[1],
104                   # ifelse(Obs[,2]<11,10^fS[2],
105                   # ifelse(Obs[,2]<16,10^fS[3],10^fS[4])))
106
107     # linear  <-  ifelse(Obs[,1]==1,Lin[1],
108                   # ifelse(Obs[,1]==2,Lin[2],
109                   # ifelse(Obs[,1]==3,Lin[3],
110                   # ifelse(Obs[,1]==4,Lin[4],Lin[5]))))
111
112     KQfit   <-  Kq[Obs[,1]]
113     Kfit    <-  K[Obs[,1]]
114     fFit    <-  fS[Obs[,2]]
115     linear  <-  Lin[Obs[,1]]
116
117     c.obs   <-  Obs[,3:7]
118     q.obs   <-  Obs[,8:12]
119
120     q.lan   <-  matrix(NA,nc=5,nr=length(Kfit))
121     q.lin   <-  matrix(NA,nc=5,nr=length(Kfit))
122     q.mod   <-  matrix(NA,nc=5,nr=length(Kfit))
123     for (ii in 1:length(Kfit)) {
124         for (jj in 1:5){
125             q.lan[ii,jj]   <-  KQfit[ii]*c.obs[ii,jj]/(1+Kfit[ii]*c.obs[
                    ii,jj]) +
126                               fFit[ii]*KQfit[ii]*c.obs[ii,1]/(1+Kfit[ii
                                  ]*c.obs[ii,1])
127
128             q.lin[ii,jj]   <-  KQfit[ii]*c.obs[ii,jj] +
129                               fFit[ii]*KQfit[ii]*c.obs[ii,1]
130
131             q.mod[ii,jj]    <-  linear[ii]*q.lin[ii,jj]+(1-linear[ii])*q
                    .lan[ii,jj]
132         }
133     }
134     qres    <-  (log10(q.obs)-log10(q.mod))^2
135     is.na(qres) <-  !is.finite(qres)
136     ssq     <-  sum(qres,na.rm=T)
137     return(ssq)
138 }
```

```
139 st_model_ssq <-  function(pars,Obs,Lin) {
140     Kq      <-  10^pars[1:5]
141     K       <-  10^pars[6:10]
142     fS      <-  10^pars[11:14]
143 
144     # KQfit   <-  ifelse(Obs[,1]==1,10^Kq[1],
145                   # ifelse(Obs[,1]==2,10^Kq[2],
146                   # ifelse(Obs[,1]==3,10^Kq[3],
147                   # ifelse(Obs[,1]==4,10^Kq[4],10^Kq[5]))))
148 
149     # Kfit    <-  ifelse(Obs[,1]==1,10^K[1],
150                   # ifelse(Obs[,1]==2,10^K[2],
151                   # ifelse(Obs[,1]==3,10^K[3],
152                   # ifelse(Obs[,1]==4,10^K[4],10^K[5]))))
153 
154     # fFit    <-  ifelse(Obs[,2]<6,10^fS[1],
155                   # ifelse(Obs[,2]<11,10^fS[2],
156                   # ifelse(Obs[,2]<16,10^fS[3],10^fS[4])))
157 
158     # linear  <-  ifelse(Obs[,1]==1,Lin[1],
159                   # ifelse(Obs[,1]==2,Lin[2],
160                   # ifelse(Obs[,1]==3,Lin[3],
161                   # ifelse(Obs[,1]==4,Lin[4],Lin[5]))))
162 
163     KQfit   <-  Kq[Obs[,1]]
164     Kfit    <-  K[Obs[,1]]
165     fFit    <-  fS[Obs[,2]]
166     linear  <-  Lin[Obs[,1]]
167 
168     c.obs   <-  Obs[,3:7]
169     q.obs   <-  Obs[,8:12]
170     m.obs   <-  Obs[,1]
171 
172     q.lan   <-  matrix(NA,nc=5,nr=length(Kfit))
173     q.lin   <-  matrix(NA,nc=5,nr=length(Kfit))
174     q.mod   <-  matrix(NA,nc=5,nr=length(Kfit))
175     for (ii in 1:length(Kfit)) {
176         for (jj in 1:5){
177             q.lan[ii,jj]   <-  KQfit[ii]*c.obs[ii,jj]/(1+Kfit[ii]*c.obs[
                    ii,jj]) +
178                               fFit[ii]*KQfit[ii]*c.obs[ii,1]/(1+Kfit[ii
                                  ]*c.obs[ii,1])
179 
180             q.lin[ii,jj]   <-  KQfit[ii]*c.obs[ii,jj] +
181                               fFit[ii]*KQfit[ii]*c.obs[ii,1]
182 
183             q.mod[ii,jj]    <-  linear[ii]*q.lin[ii,jj]+(1-linear[ii])*q
                    .lan[ii,jj]
184         }
185     }
186 
```

```
187       qres     <-  (log10(q.obs)-log10(q.mod))^2
188       #qres[!is.finite(qres)]     <-  log10(q.mod[!is.finite(qres)])^2
189       is.na(qres) <-  !is.finite(qres)
190       qres[is.na(qres)]     <-  0
191       ssq.chem=matrix(0,nc=5,nr=1)
192       for (ii in 1:length(m.obs)) {
193           ssq.chem[m.obs[ii]]     <-  ssq.chem[m.obs[ii]]+rowSums(qres)[ii]
194       }
195       #ssq      <-  sum(qres,na.rm=T)
196       return(ssq.chem)
197   }
198
199   # Prepare output matrices
200   mst.qk  <-  matrix(NA,nc=5,nr=nSoil)
201   mst.k   <-  matrix(NA,nc=5,nr=nSoil)
202   mst.fs  <-  array(NA,c(nSoil,5,4))
203   mst.ssq <-  array(NA,c(nSoil,5))
204   mst.n   <-  array(0,c(nSoil,5))
205
206   ms.qk   <-  matrix(NA,nc=5,nr=nSoil)
207   ms.k    <-  matrix(NA,nc=5,nr=nSoil)
208   ms.fs   <-  array(NA,c(nSoil,5))
209   ms.ssq  <-  array(NA,c(nSoil,5))
210   ms.n    <-  array(0,c(nSoil,5))
211
212   st.qk   <-  matrix(NA,nc=5,nr=nSoil)
213   st.qk.e <-  matrix(NA,nc=5,nr=nSoil)
214   st.k    <-  matrix(NA,nc=5,nr=nSoil)
215   st.k.e  <-  matrix(NA,nc=5,nr=nSoil)
216   st.fs   <-  array(NA,c(nSoil,4))
217   st.fs.e <-  array(NA,c(nSoil,4))
218   st.ssq  <-  array(NA,c(nSoil,5))
219   st.ssq.lin  <-  array(NA,c(nSoil,5))
220   st.n    <-  array(0,c(nSoil,5))
221
222   st.comp   <-  array(NA,c(nSoil,14))
223   colnames(st.comp)     <-  c(paste('KQ_',mc_list,sep=''),paste('K_',mc_
          list,sep=''),paste('fS_',c(2,48,240,720),sep=''))
224   rownames(st.comp)     <-  soil_order$SoilCode
225
226   st.e.comp   <-  array(NA,c(nSoil,14))
227   colnames(st.e.comp)     <-  c(paste('KQ_',mc_list,sep=''),paste('K_',mc_
          list,sep=''),paste('fS_',c(2,48,240,720),sep=''))
228   rownames(st.e.comp)     <-  soil_order$SoilCode
229
230   # Loop over soils
231   for (ii in 1:nSoil) {
232       print(paste('Soil_',ii,sep=''))
233       flush.console()
234       # Select Soil Data
235       sub.soil     <-  hplc.raw[hplc.raw[,2]==soil_order$SoilCode[ii],]
```

```
236
237     # remove bad mass balance data
238     for (jj in 1:dim(sub.soil)[1]) {
239         is.na(sub.soil[jj,4:32])    <- ifelse((sub.soil[jj,3]==4 | sub.
                soil[jj,3]==9 | sub.soil[jj,3]==14 | sub.soil[jj,3]==19) &
                sub.soil[jj,1]=='TNT',TRUE,ifelse((sub.soil[jj,3]==5 | sub.
                soil[jj,3]==10 | sub.soil[jj,3]==15 | sub.soil[jj,3]==20) &
                sub.soil[jj,1]!='TNT',TRUE,FALSE))
240         is.na(sub.soil[jj,4:32])    <- ifelse(mbal.yesno[mbal.yesno
                [,3]==sub.soil[jj,1] & mbal.yesno[,1]==soil_list[ii] & mbal.
                yesno[,2]==sub.soil[jj,3],4]==1,FALSE,TRUE)
241     }
242
243     # Generate indexing lists for MC, adsorption time
244     mtmp          <- data.matrix(sub.soil[,1])
245     M.List        <- ifelse(mtmp=='HMX',1,
246                       ifelse(mtmp=='RDX',2,
247                       ifelse(mtmp=='NG',3,
248                       ifelse(mtmp=='TNT',4,5))))
249     V.List        <- data.matrix(sub.soil[,3])
250     T.List        <- ifelse(V.List<6,1,
251                       ifelse(V.List<11,2,
252                       ifelse(V.List<16,3,4)))
253
254     # Select observed data
255     obs                 <- matrix(c(M.List,T.List,data.matrix(sub.soil
            [,6:10]),data.matrix(sub.soil[,28:32])),nc=12)
256     is.na(obs[,1])      <- obs[,3]==0
257     # Remove incomplete sets
258     obs                 <- obs[complete.cases(obs),]
259     m.obs               <- obs[,1]
260     t.obs               <- obs[,2]
261     c.obs               <- obs[,3:7]
262     q.obs               <- obs[,8:12]
263
264     st.obs              <- obs
265     lin.obs             <- data.matrix(cov.lin[ii,])
266
267     st.theta                <- c(rep(0,5),rep(0,5),rep(-3,4))
268
269     # Loop over MC for MST model
270     for (jj in 1:5) {
271         mst.theta       <- c(0,0,rep(-3,4))
272         mst.obs         <- st.obs[st.obs[,1]==jj,]
273         mst.linear      <- lin.obs[jj]
274
275         mst.fit         <- optim(par=mst.theta,fn=mst_model_opt,Lin=mst
                .linear,Obs=mst.obs,method='L-BFGS-B',hessian=TRUE,control=
                list(maxit=300))
276
277         mst.qk[ii,jj]   <- mst.fit$par[1]
```

```
278         mst.k[ii,jj]    <-  mst.fit$par[2]
279         mst.fs[ii,jj,]  <-  mst.fit$par[3:6]
280         mst.ssq[ii,jj]  <-  mst.fit$value
281         mst.n[ii,jj]    <-  sum(!is.na(mst.obs[,8:12]))
282     }
283     print('MST_OK')
284     flush.console()
285
286     # Loop over MC for MST model
287     for (jj in 1:5) {
288         ms.theta        <-  c(0,0,-3)
289         ms.obs          <-  st.obs[st.obs[,1]==jj,]
290         ms.linear       <-  lin.obs[jj]
291         ms.fit          <-  optim(par=ms.theta,fn=ms_model_opt,Lin=ms.
                linear,Obs=ms.obs,method='L-BFGS-B',hessian=TRUE,control=
                list(maxit=300))
292
293         ms.qk[ii,jj]    <-  ms.fit$par[1]
294         ms.k[ii,jj]     <-  ms.fit$par[2]
295         ms.fs[ii,jj]    <-  ms.fit$par[3]
296         ms.ssq[ii,jj]   <-  ms.fit$value
297         ms.n[ii,jj]     <-  sum(!is.na(ms.obs[,8:12]))
298     }
299     print('MS_OK')
300     flush.console()
301
302     # Fit all MC at once for ST model
303     st.fit              <-  optim(par=st.theta,fn=st_model_opt,Lin=lin.
            obs,Obs=st.obs,method='L-BFGS-B',hessian=TRUE,control=list(maxit
            =300))
304
305     # Set up hessian
306     hess.raw    <-  st.fit$hessian
307     c.del   <-  c()
308     par.v   <-  c(paste('KQ_',mc_list,sep=''),paste('K_',mc_list,sep='')
            ,paste('fS_',c(2,48,240,720),sep=''))
309
310     # Remove row/column for non-fit data (i.e. KL for linear fits)
311     for (kk in 1:dim(hess.raw)[2]) {
312         if (sum(abs(hess.raw[,kk]))==0) {
313             c.del   <-  c(c.del, kk)
314         }
315     }
316      if (length(c.del)>0) {
317         fit.fin     <-  tmpfits[-c.del]
318         hess.fin    <-  hess.raw[-c.del,-c.del]
319         par.fin     <-  par.v[-c.del]
320     }
321     vc          <- solve(matrix(NA,nrow=nrow(hess.fin),ncol=ncol(hess.
            fin)))
322     try(vc      <-  solve(hess.fin))
```

```
323       err.fin      <-  sqrt(diag(vc))
324
325       # Output parameters and SSQ
326       tmpfits      <-  st.fit$par
327       chem.ssq     <-  st_model_ssq(pars=tmpfits,Obs=st.obs,Lin=lin.obs)
328       st.ssq[ii,] <-  chem.ssq
329       is.na(tmpfits)  <-  tmpfits==st.theta
330
331       st.comp[soil_order$SoilCode[ii],par.fin]    <-  fit.fin
332       st.e.comp[soil_order$SoilCode[ii],par.fin]  <-  err.fin
333
334       # Count data for RMSE calculation
335       for (jj in 1:5) {
336           st.n[ii,jj]     <-  sum(!is.na(st.obs[st.obs[,1]==jj,8:12]))
337       }
338       print('ST_OK')
339       flush.console()
340  }
341
342  # Output MST model fit
343  mst.comp <- cbind(mst.qk,mst.k,mst.fs[,,1],mst.fs[,,2],mst.fs[,,3],mst.
         fs[,,4])
344  mst.fs.name <- paste('fS_',mc_list,sep='')
345  colnames(mst.comp)  <-  c(paste('KQ_',mc_list,sep=''),paste('K_',mc_list
         ,sep=''),paste(mst.fs.name,'_2',sep=''),paste(mst.fs.name,'_48',sep=
         ''),paste(mst.fs.name,'_240',sep=''),paste(mst.fs.name,'_720',sep=''
         ))
346  rownames(mst.comp)  <-  soil_order$SoilCode
347       # Replace values that are unchanged
348       is.na(mst.comp[,1:10])   <-  ifelse(mst.comp[,1:10]==0,TRUE,FALSE)
349       is.na(mst.comp[,11:30])   <-  ifelse(mst.comp[,11:30]==-3,TRUE,FALSE
              )
350  write.table(mst.comp,file=paste(out_path,'fit_mst_v4.csv',sep=''),sep=',
         ',col.names=T,row.names=T)
351
352  # Output MS model fit
353  ms.comp <- cbind(ms.qk,ms.k,ms.fs)
354  colnames(ms.comp)  <-  c(paste('KQ_',mc_list,sep=''),paste('K_',mc_list,
         sep=''),paste('fS_',mc_list,sep=''))
355  rownames(ms.comp)  <-  soil_order$SoilCode
356       # Replace values that are unchanged
357       is.na(ms.comp[,1:10])   <-  ifelse(ms.comp[,1:10]==0,TRUE,FALSE)
358       is.na(ms.comp[,11:15])   <-  ifelse(ms.comp[,11:15]==-3,TRUE,FALSE)
359  write.table(ms.comp,file=paste(out_path,'fit_ms_v4.csv',sep=''),sep=',',
         col.names=T,row.names=T)
360
361  # Output ST model fit and error
362  fitcor    <-  paste(out_path,'fit_st_v4.csv',sep='')
363  errcor    <-  paste(out_path,'err_st_v4.csv',sep='')
364       # Replace values that are unchanged
365       is.na(st.comp[,1:10])   <-  ifelse(st.comp[,1:10]==0,TRUE,FALSE)
```

```
366       is.na(st.comp[,11:14])    <-   ifelse(st.comp[,11:14]==-3,TRUE,FALSE)
367
368  write.table(st.comp, file=fitcor ,sep=',',col.names=T,row.names=T)
369  write.table(st.e.comp, file=errcor ,sep=',',col.names=T,row.names=T)
```

B.4 Model fit figures

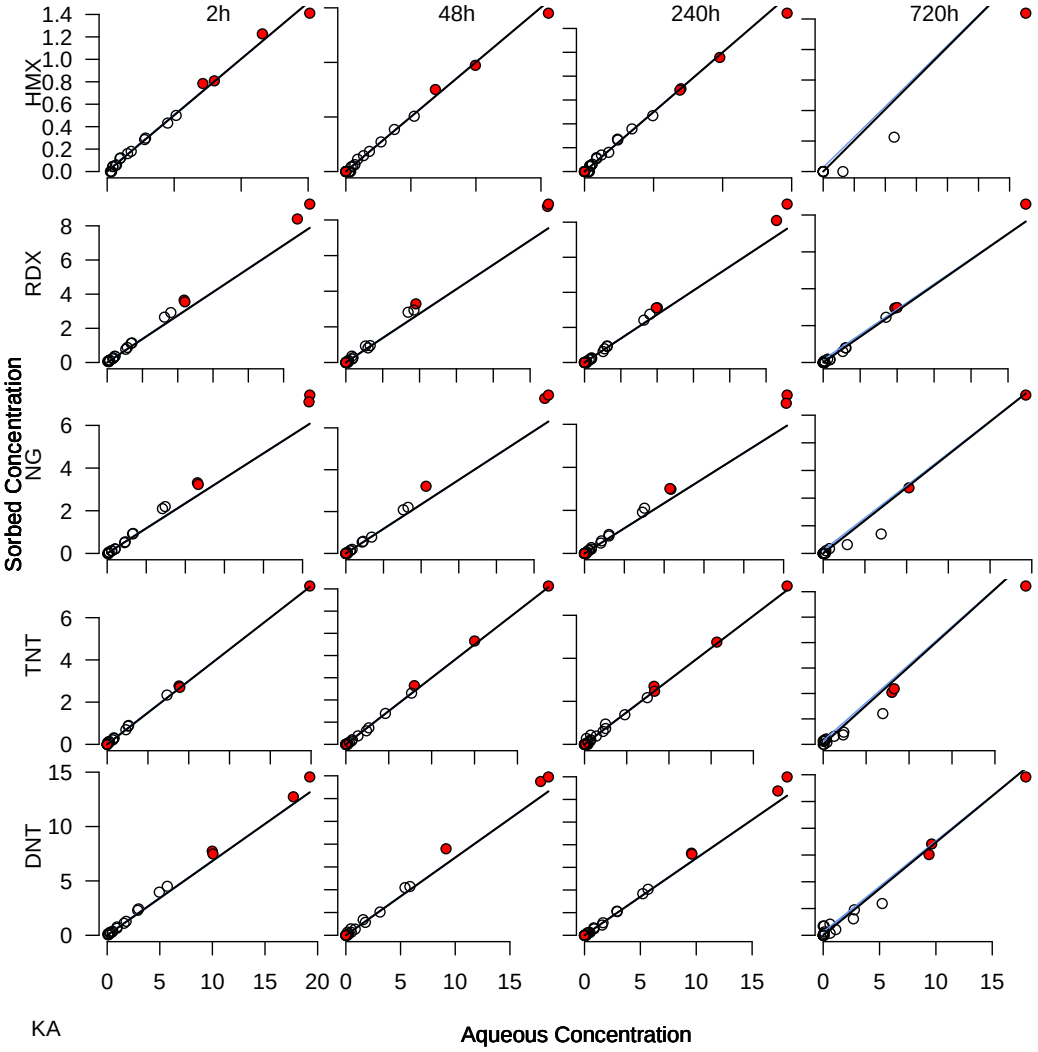
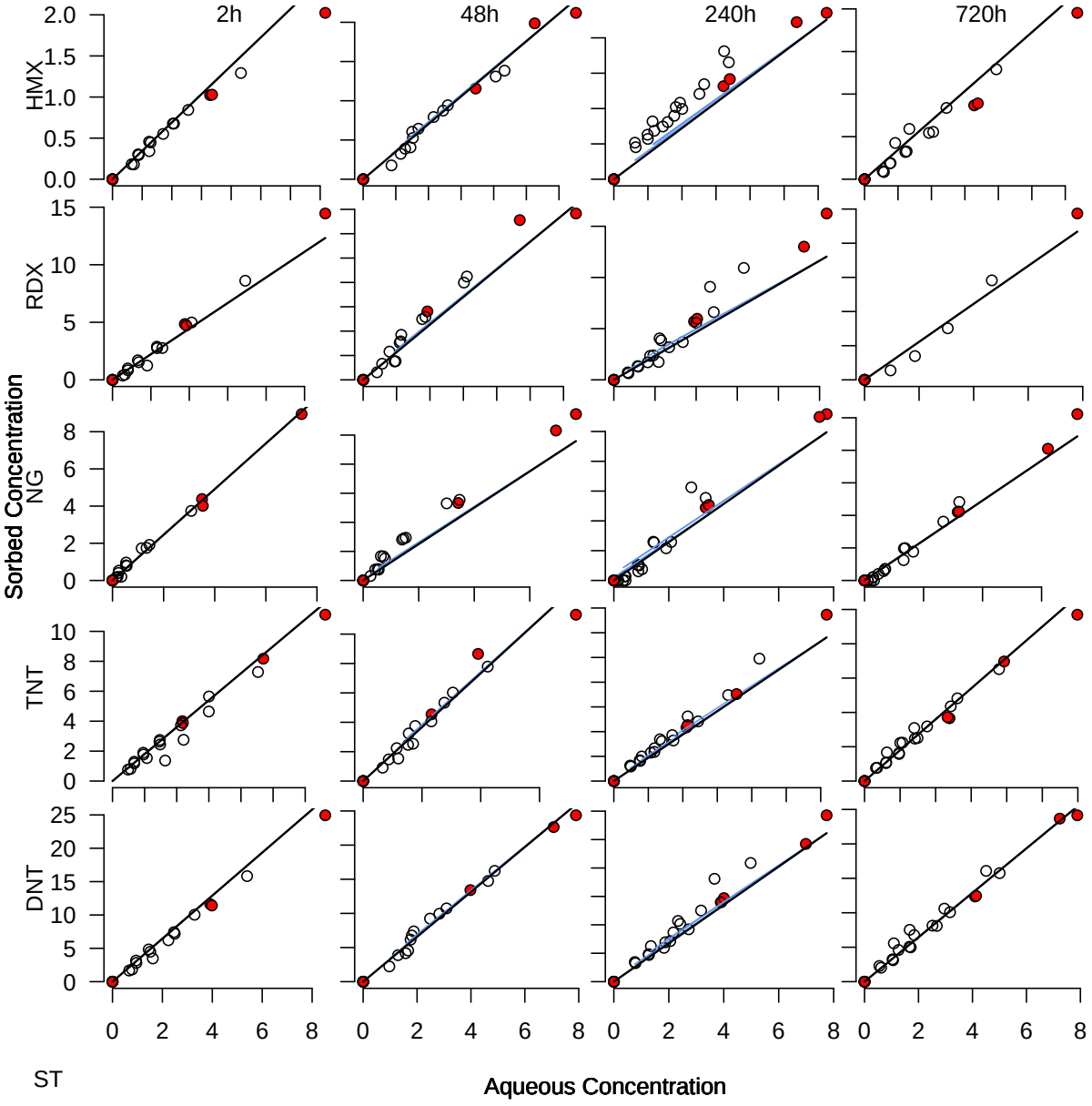
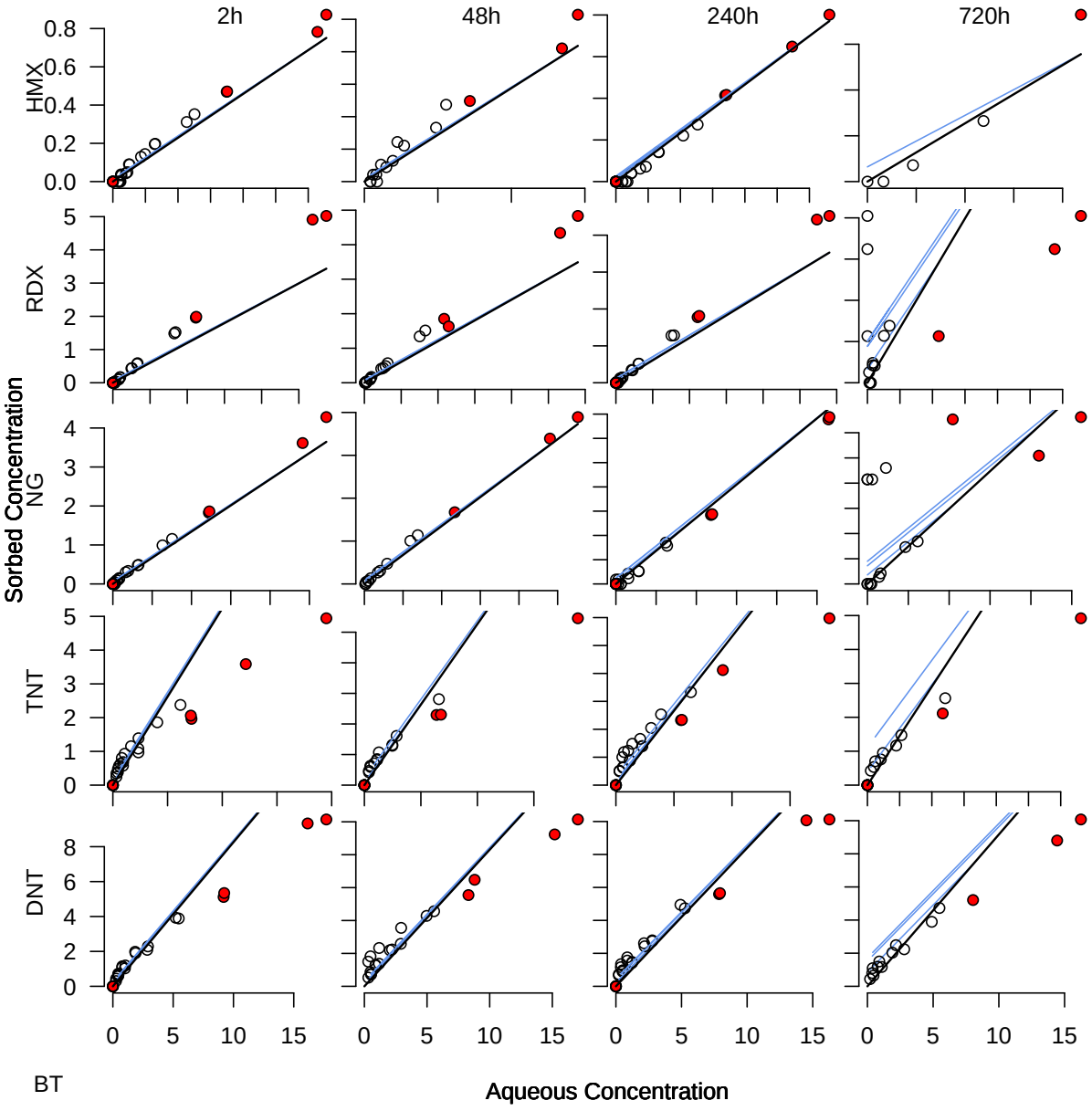
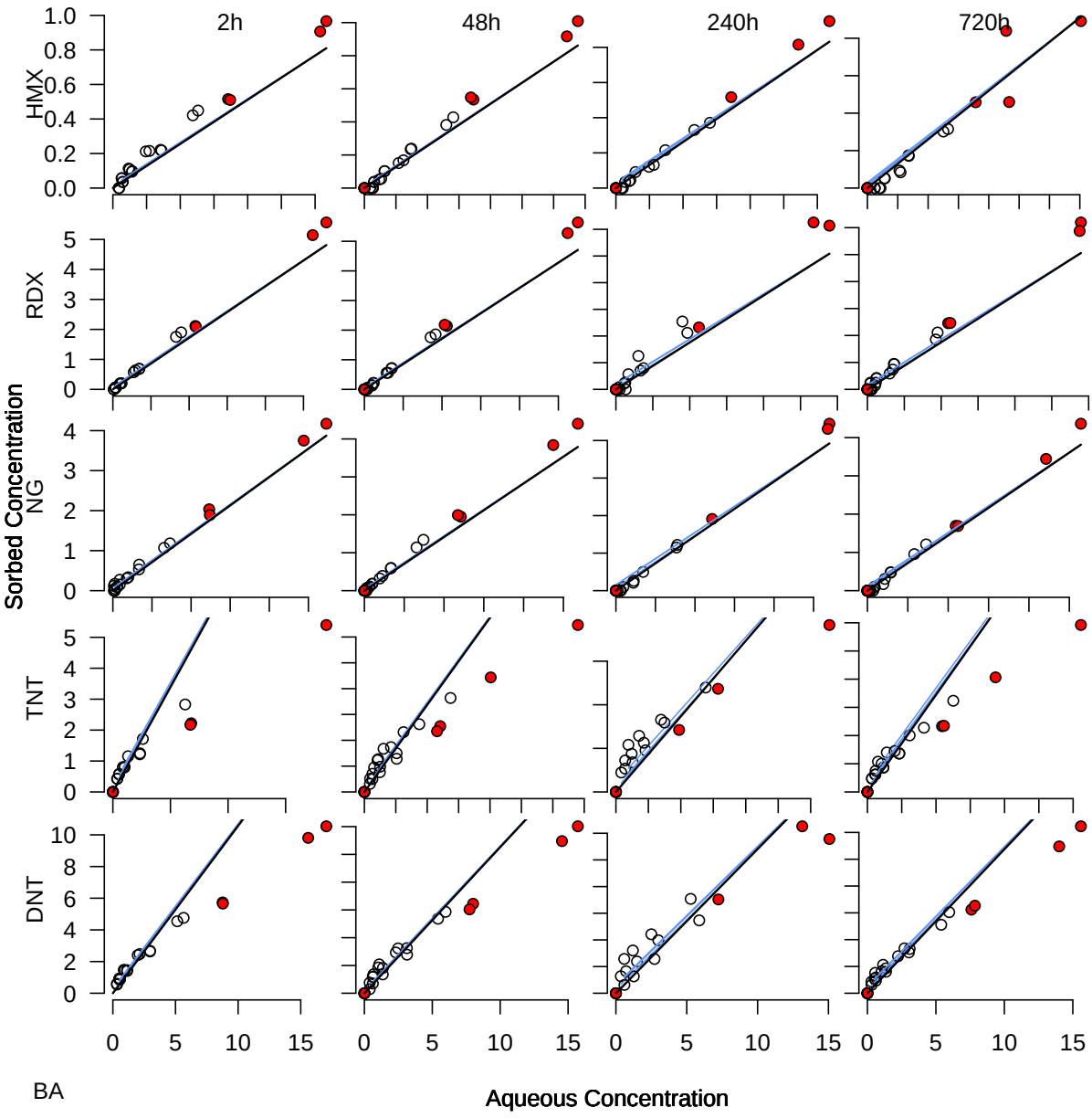
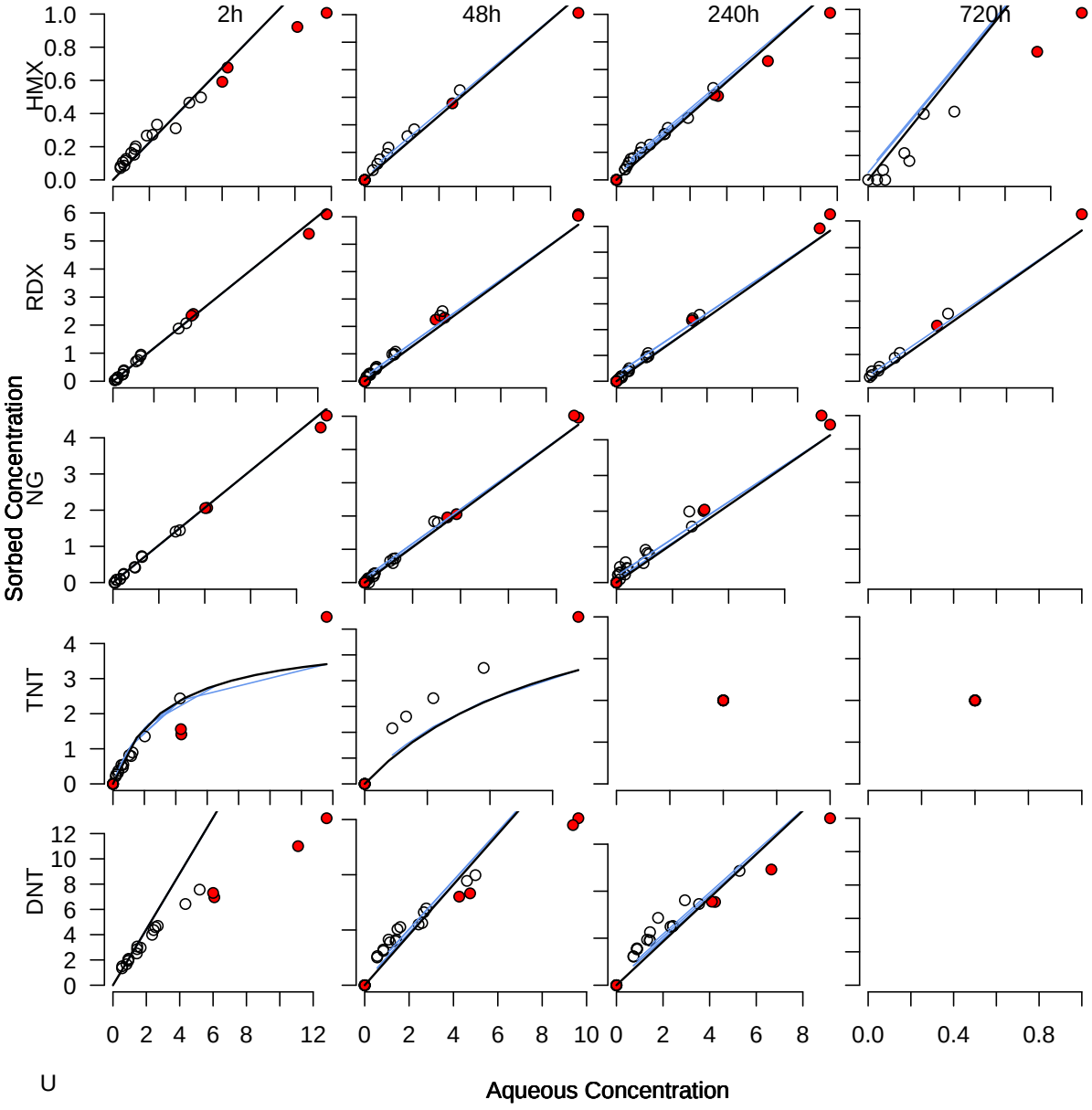


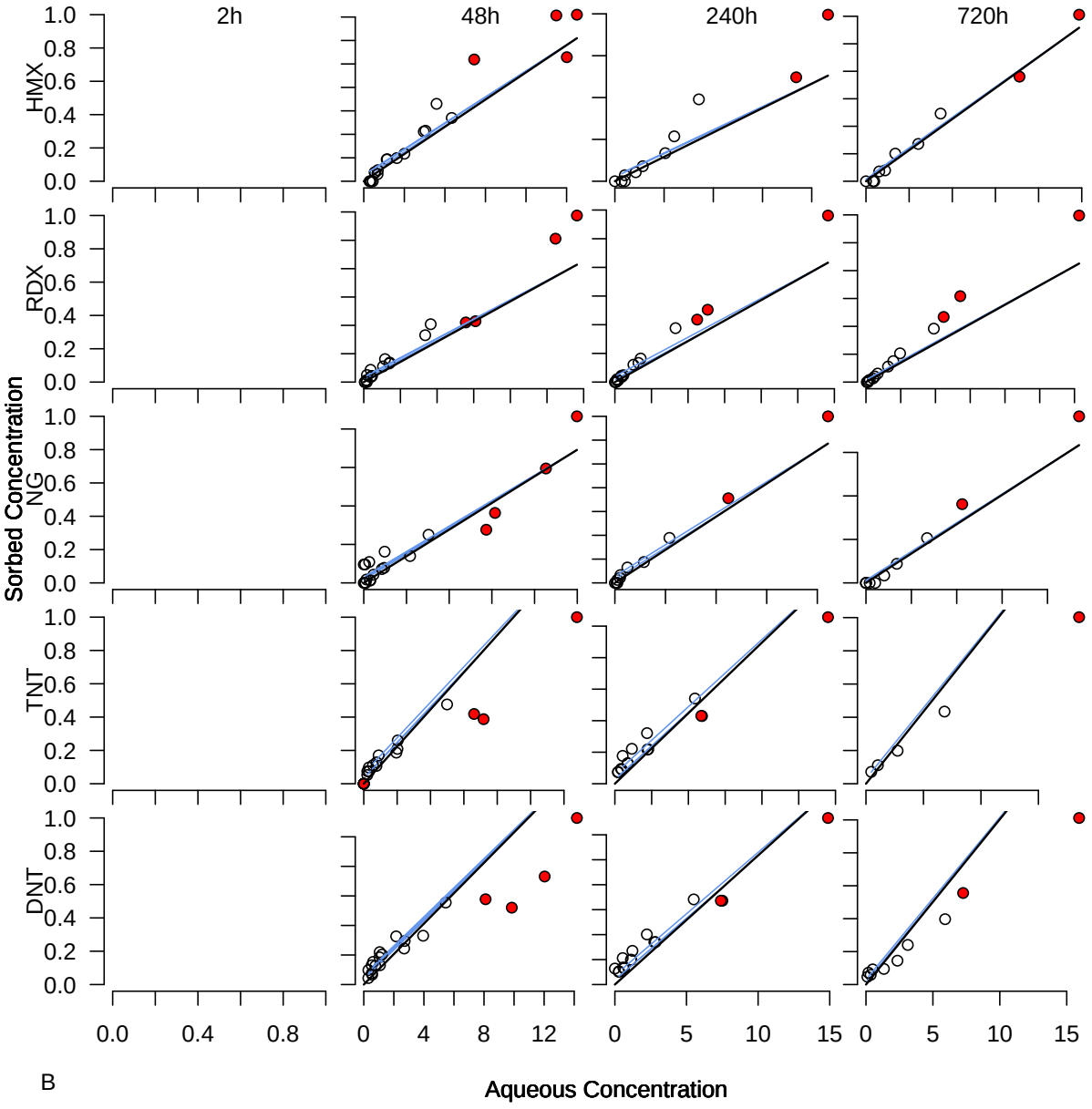
Figure B.2: Fit of STM to observed data. Black lines are adsorption, blue lines are desorption. Filled points are adsorption point, hollow points are desorption point.


2h
48h
240h
720h
HMX
RDX
NG
TNT
DNT
Sorbed Concentration
Aqueous Concentration
ST

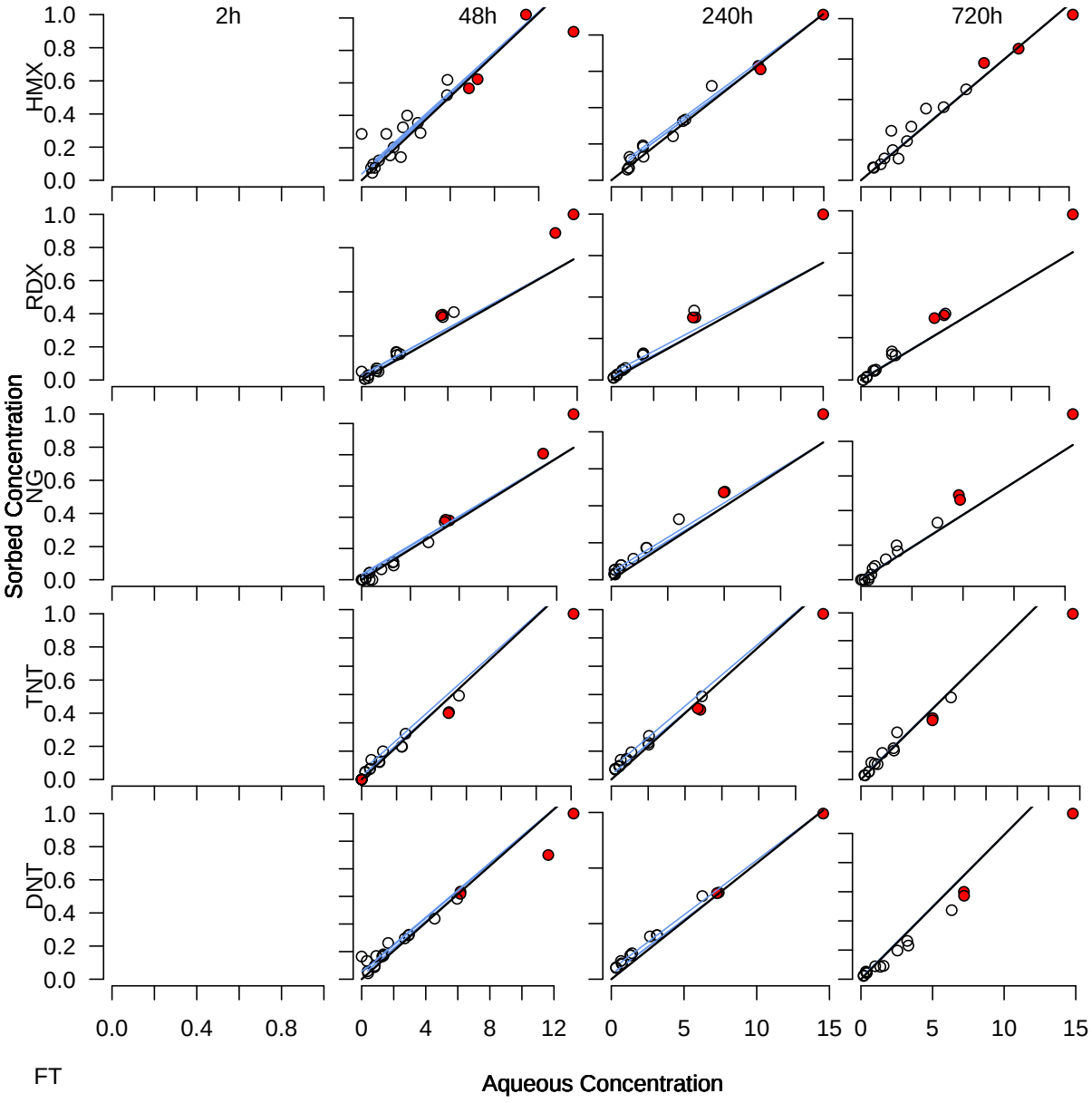

2h
48h
240h
720h
HMX
RDX
NG
TNT
DNT
Sorbed Concentration
Aqueous Concentration
BT

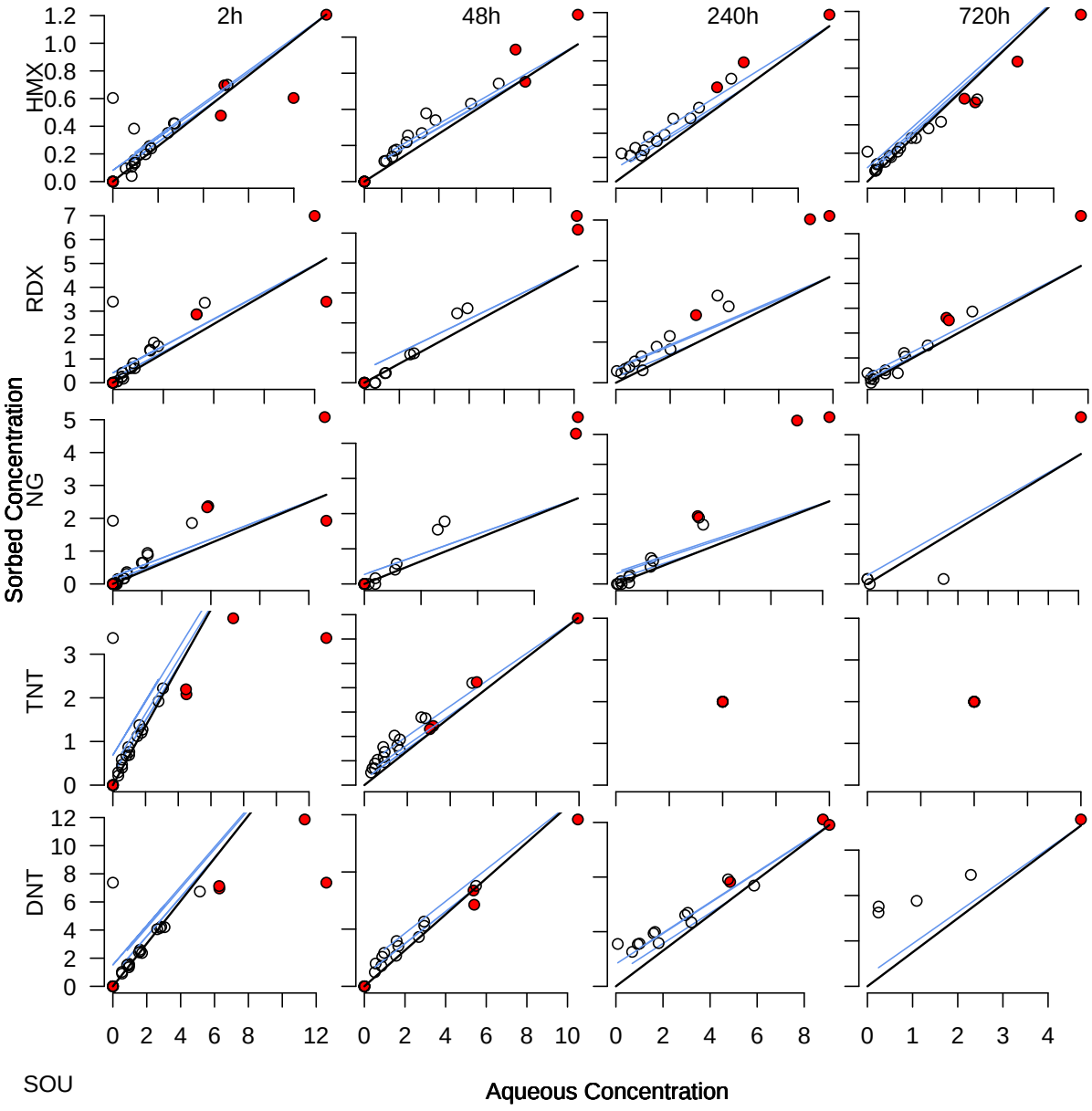

2h
48h
240h
720h
HMX
RDX
NG
TNT
DNT
Sorbed Concentration
Aqueous Concentration
BA

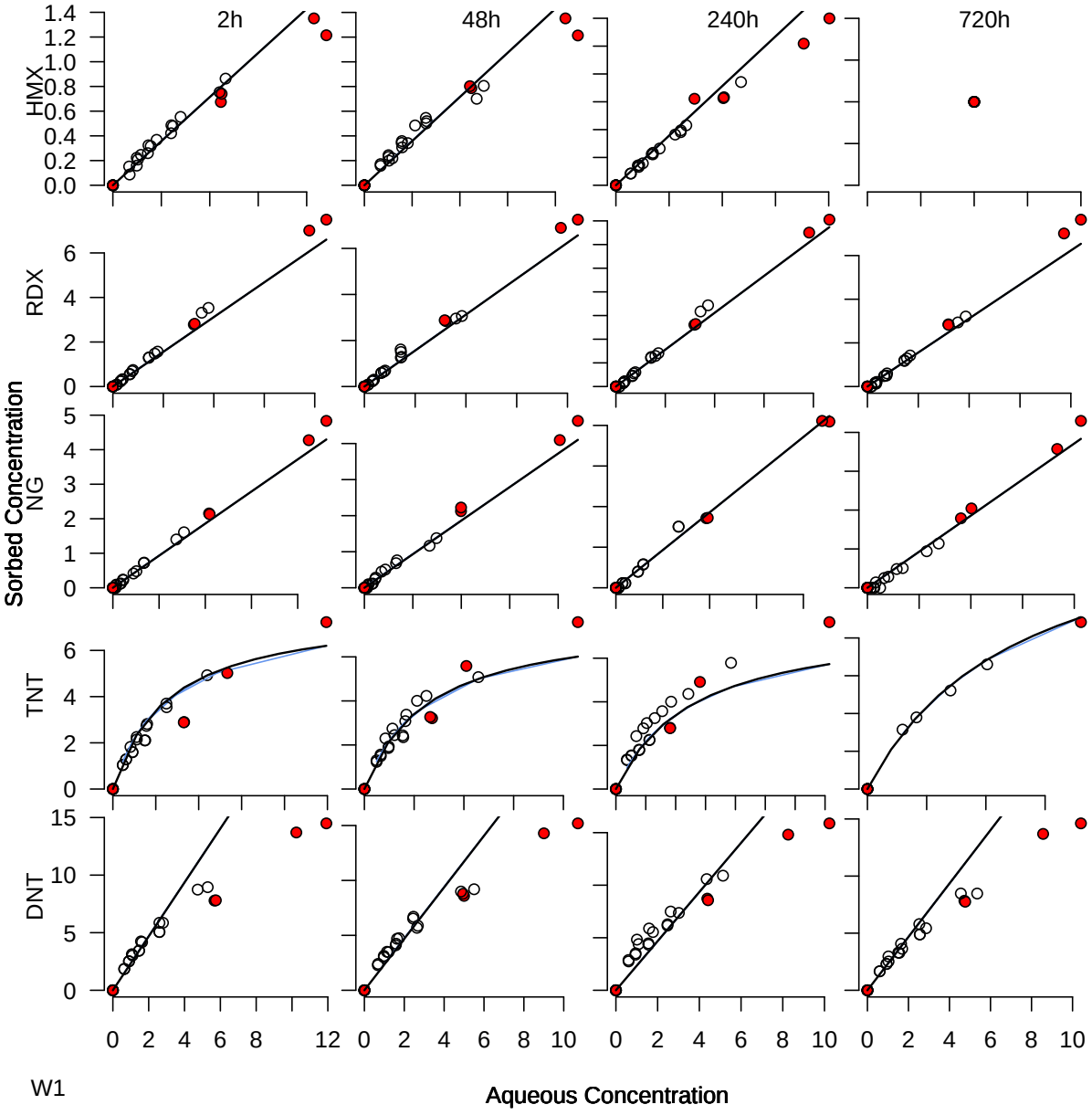

2h
48h
240h
720h
HMX
RDX
NG
TNT
DNT
Sorbed Concentration
Aqueous Concentration
U

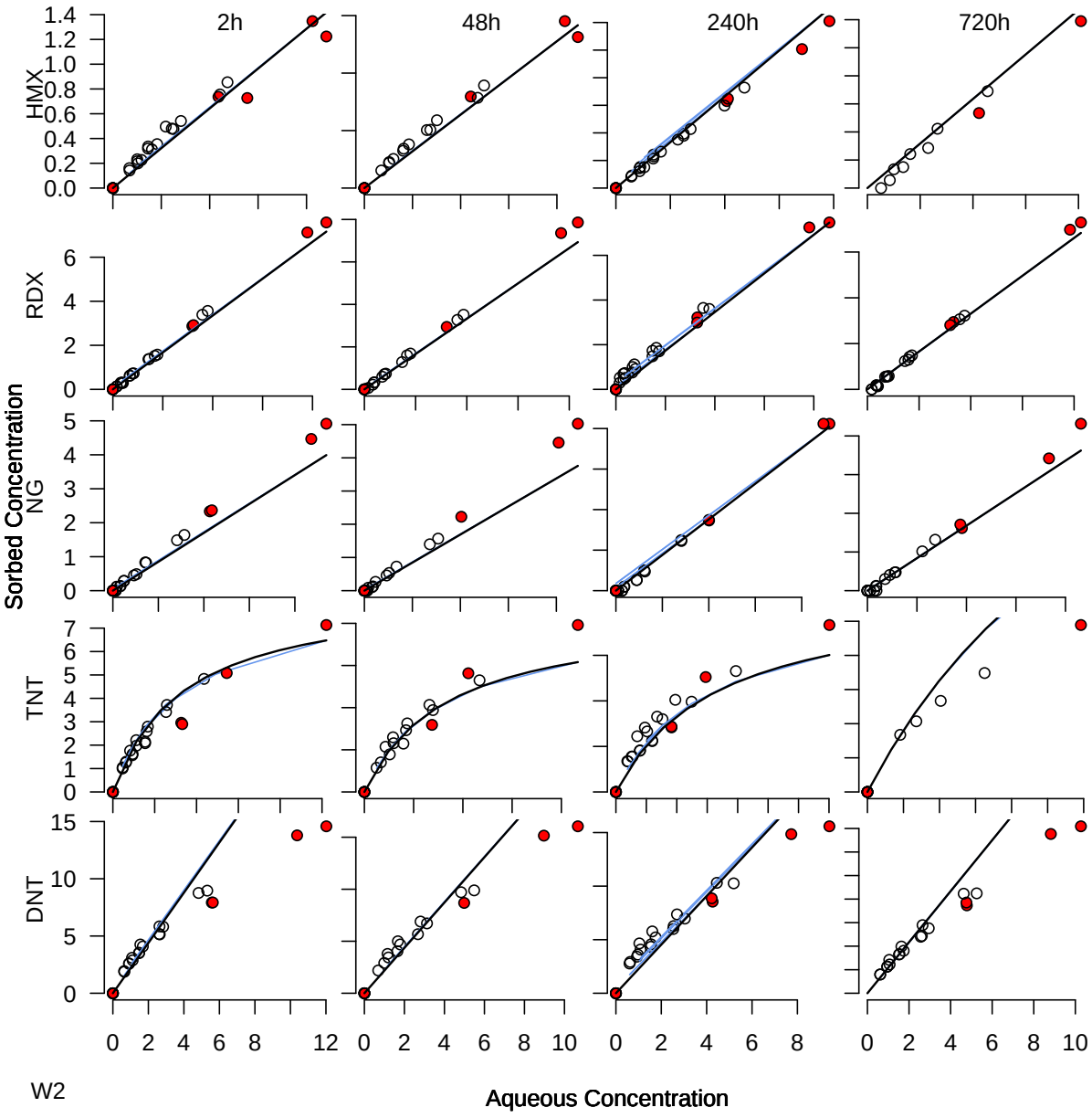

2h
48h
240h
720h
HMX
RDX
NG
TNT
DNT
Sorbed Concentration
Aqueous Concentration
0.0
0.2
0.4
0.6
0.8
1.0
0
4
8
12
5
10
15

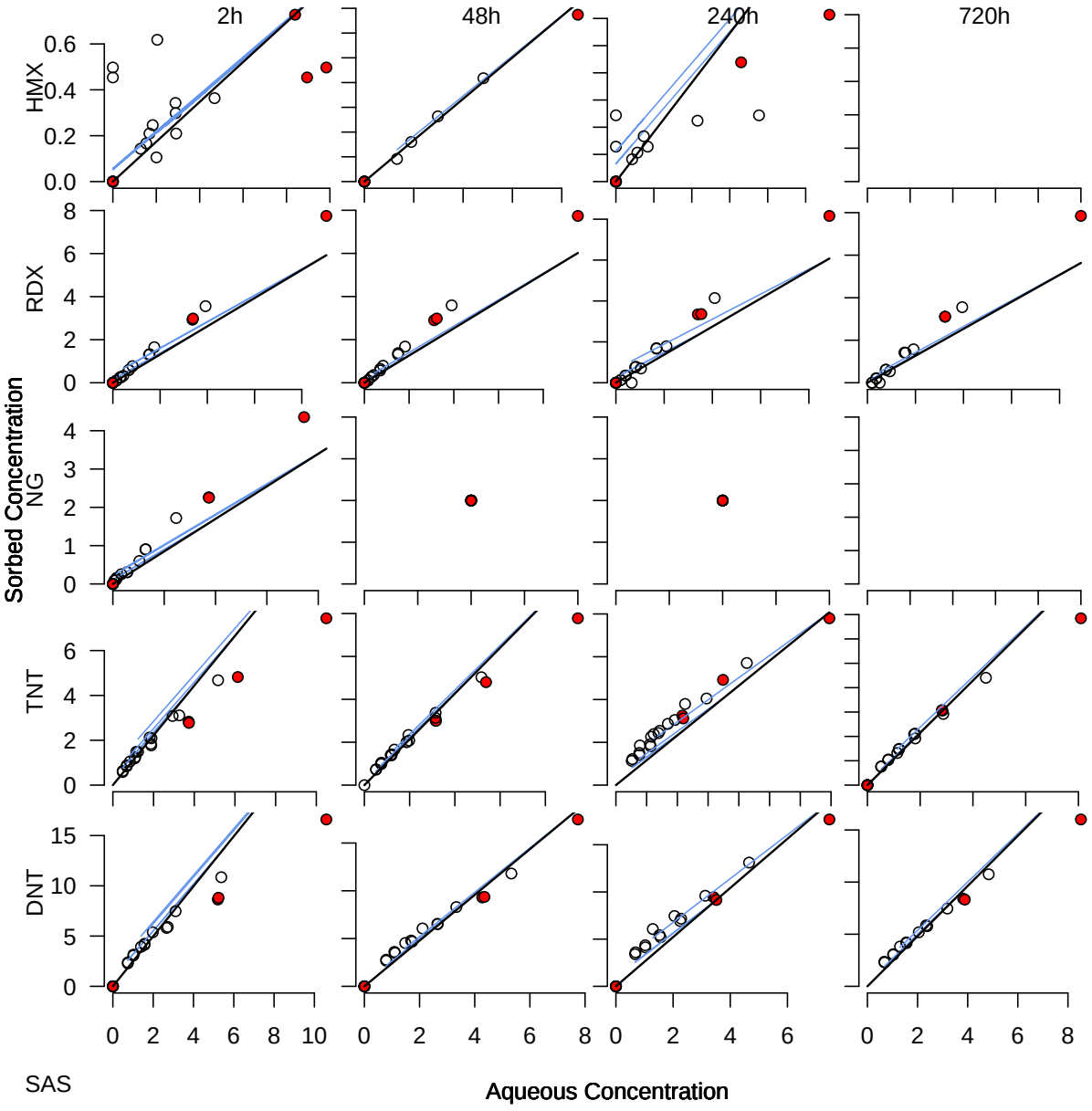
B

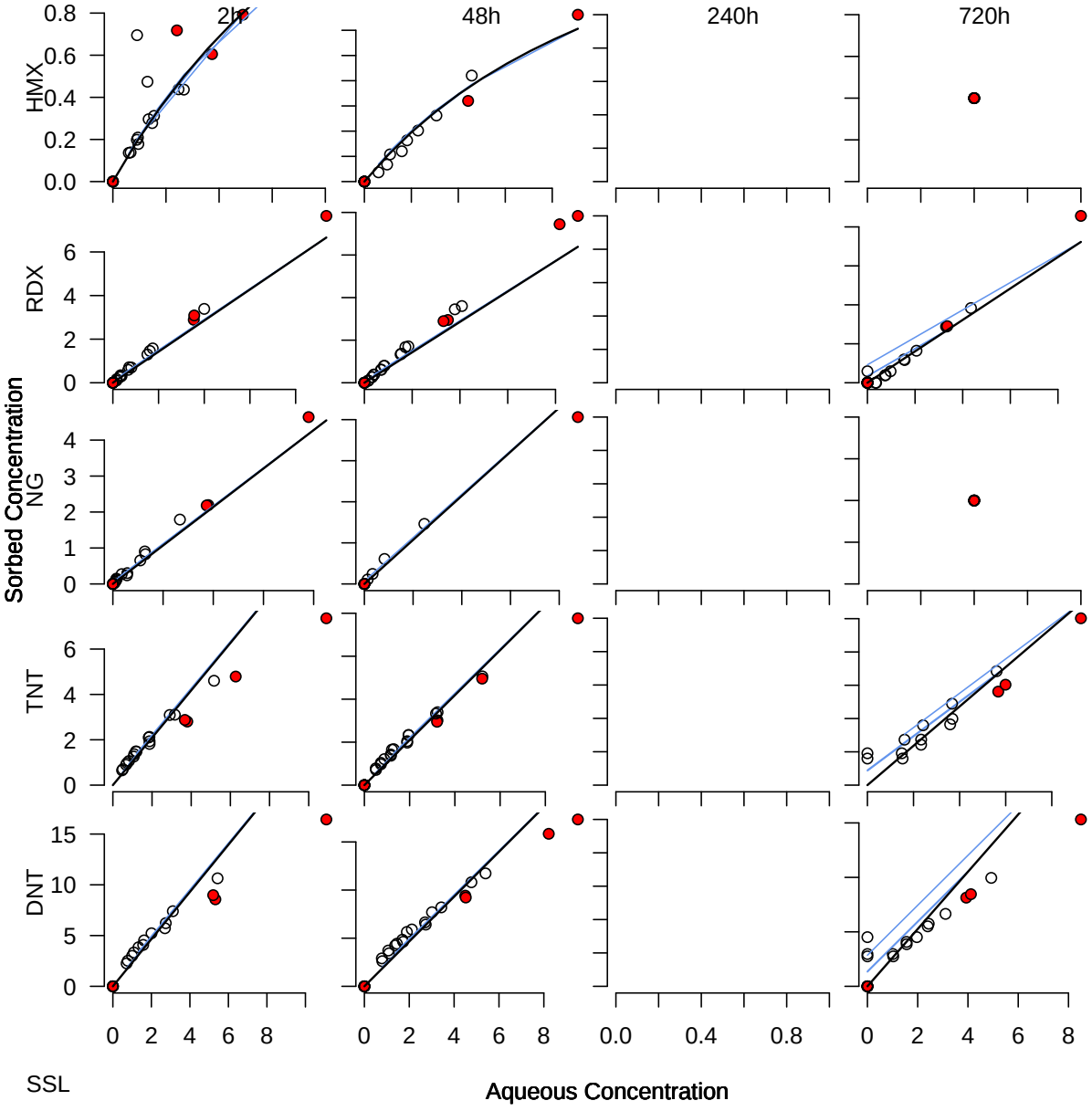

2h
48h
240h
720h
HMX
RDX
NG
TNT
DNT
Sorbed Concentration
Aqueous Concentration
FT

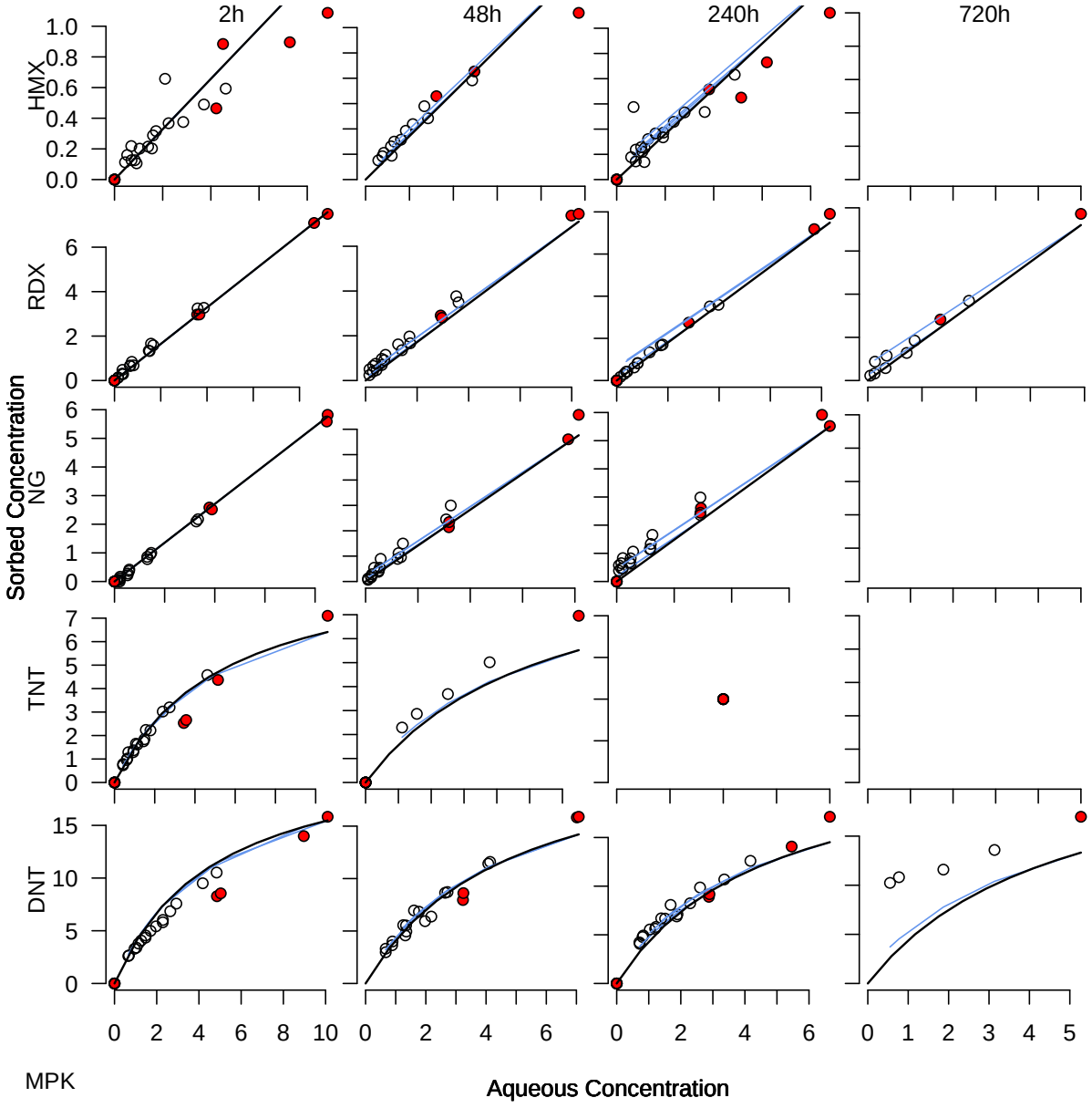

2h
48h
240h
720h
HMX
RDX
NG
TNT
DNT
Sorbed Concentration
Aqueous Concentration
SOU

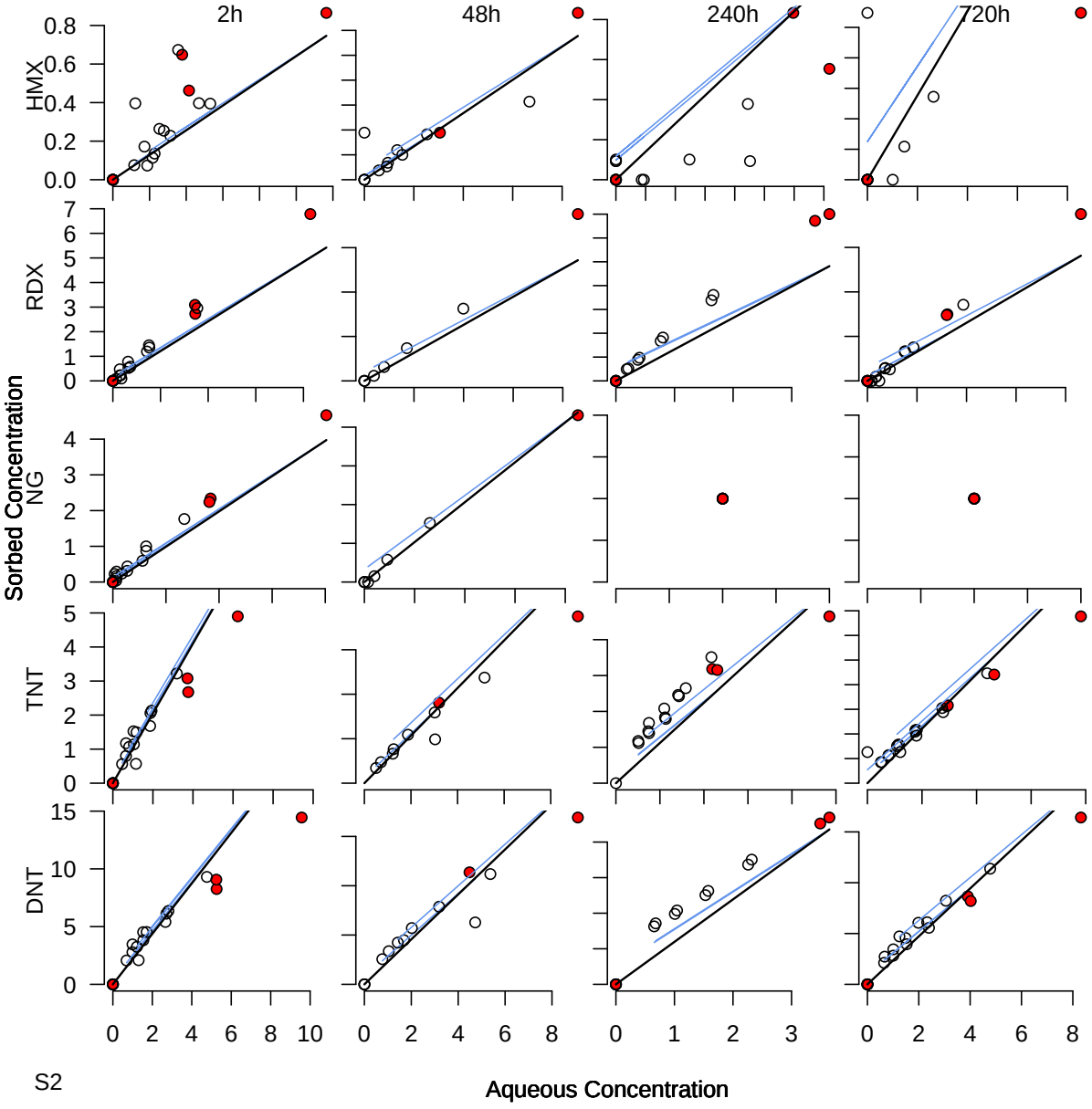

2h
48h
240h
720h
HMX
RDX
NG
TNT
DNT
Sorbed Concentration
Aqueous Concentration
W1

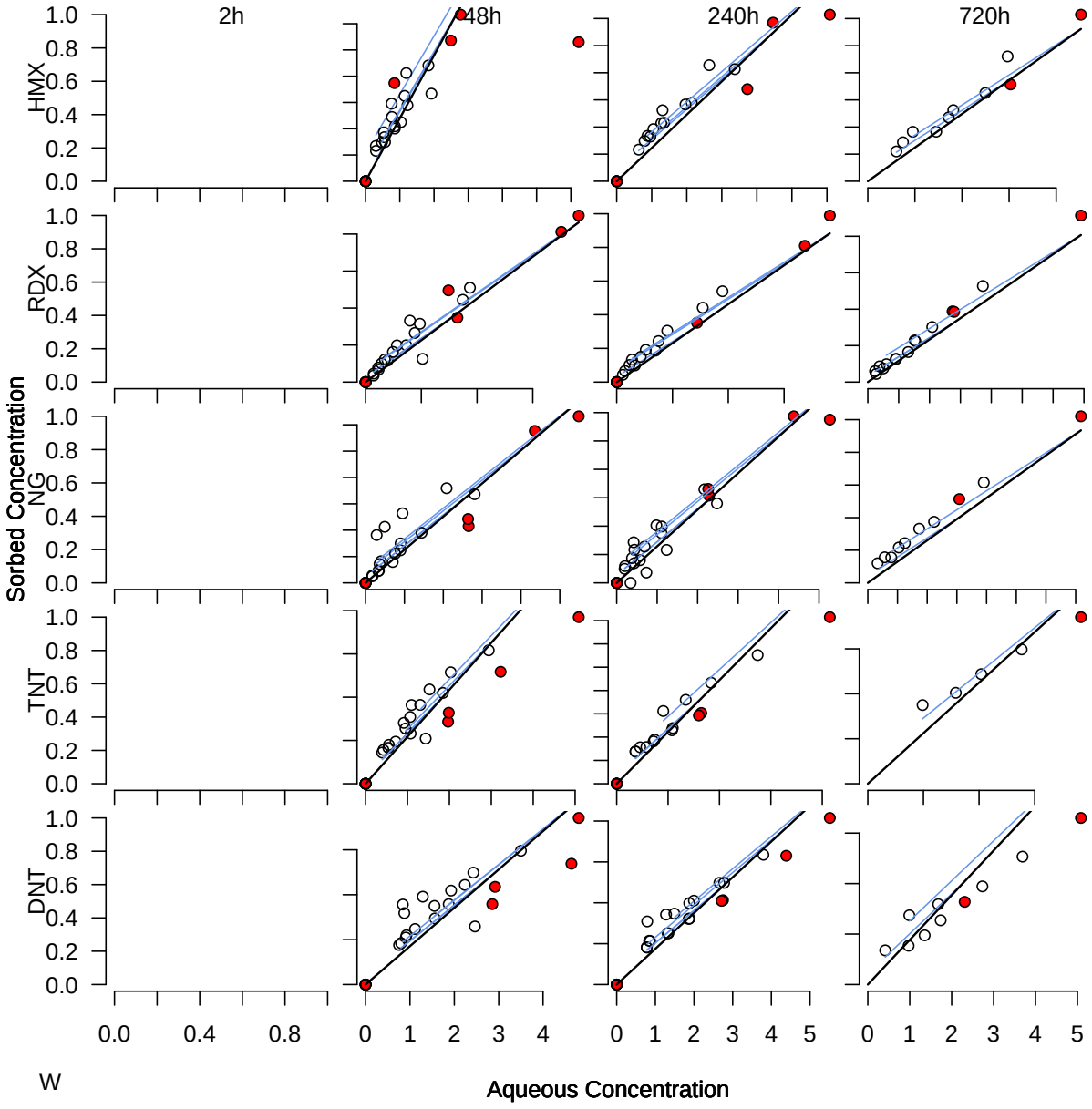

2h
48h
240h
720h
HMX
RDX
NG
TNT
DNT
Sorbed Concentration
Aqueous Concentration
W2

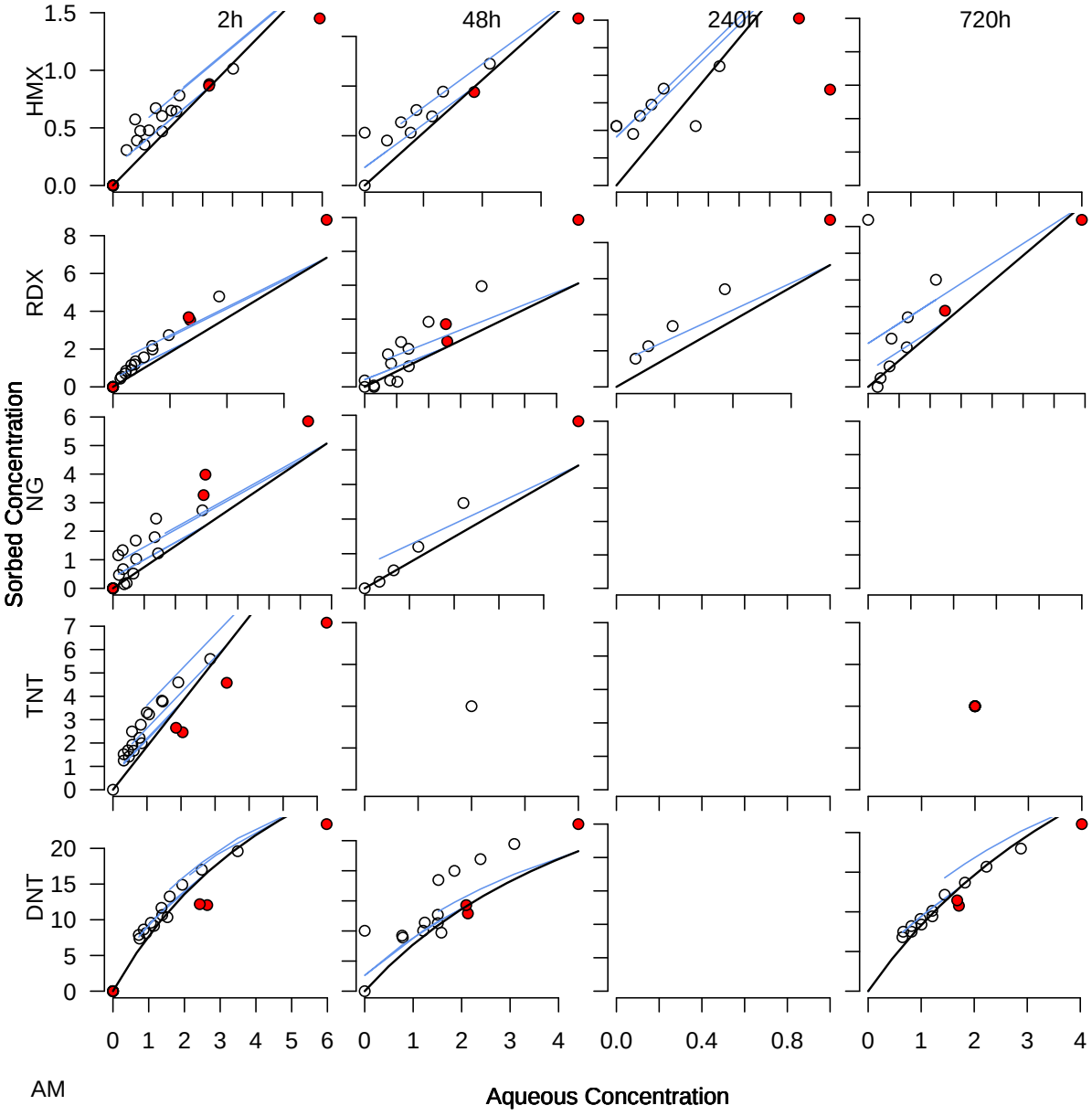

2h
48h
240h
720h
HMX
RDX
NG
TNT
DNT
Sorbed Concentration
Aqueous Concentration
SAS

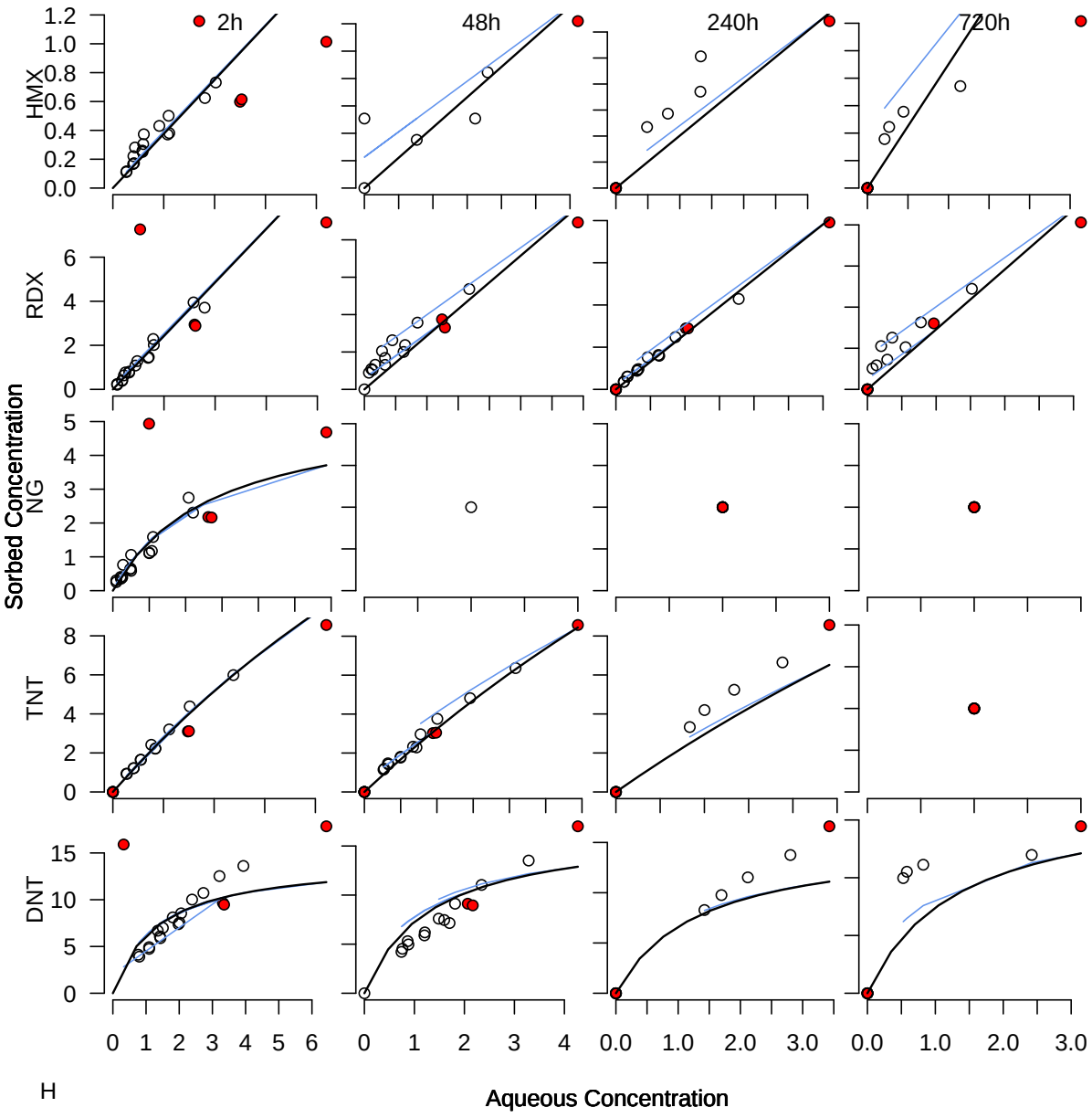

2h
48h
240h
720h
HMX
RDX
NG
TNT
DNT
Sorbed Concentration
Aqueous Concentration
SSL


2h
48h
240h
720h
HMX
RDX
NG
TNT
DNT
MPK
Sorbed Concentration
Aqueous Concentration

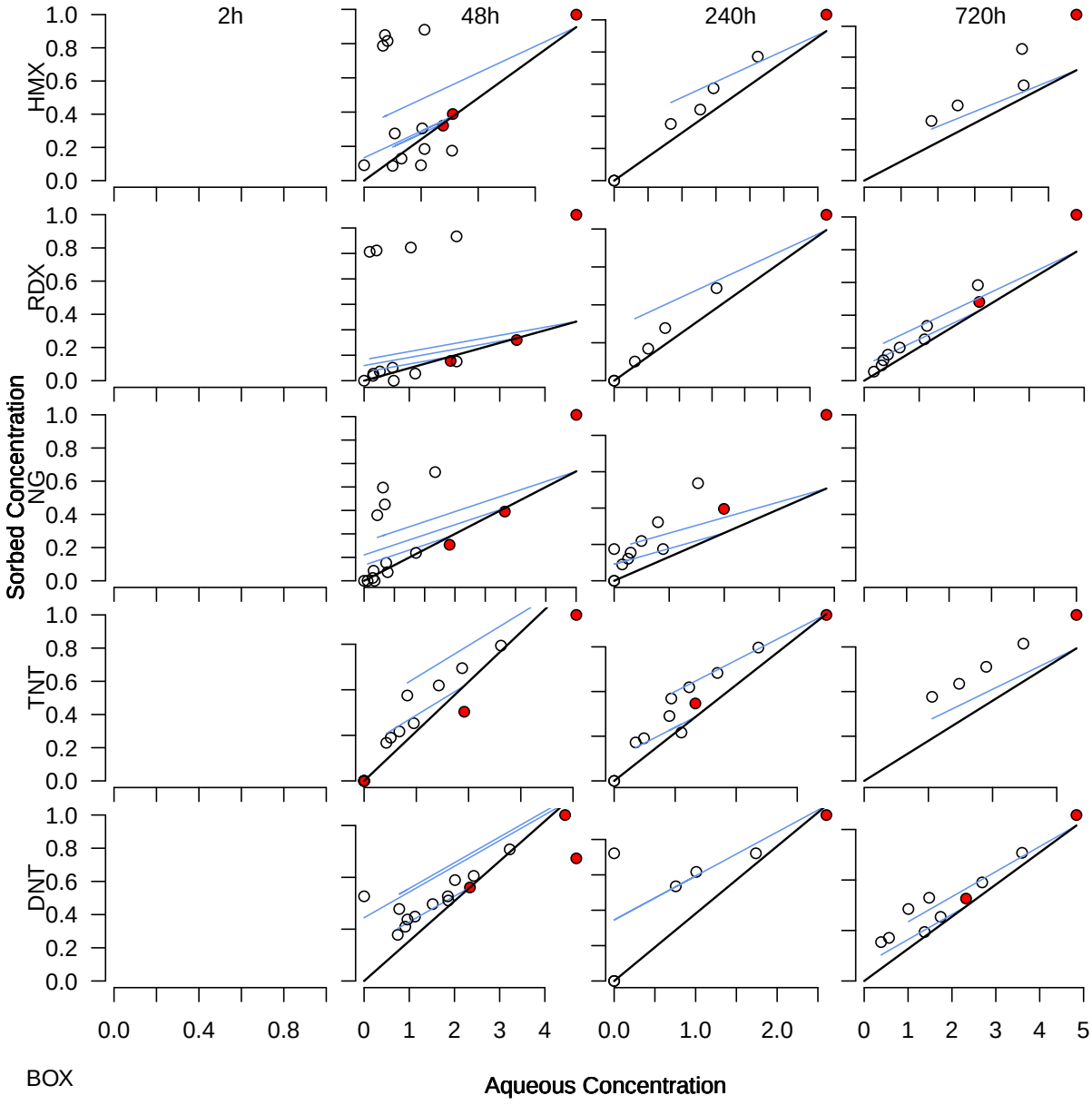

2h
48h
240h
720h
HMX
RDX
NG
TNT
DNT
Sorbed Concentration
Aqueous Concentration
S2

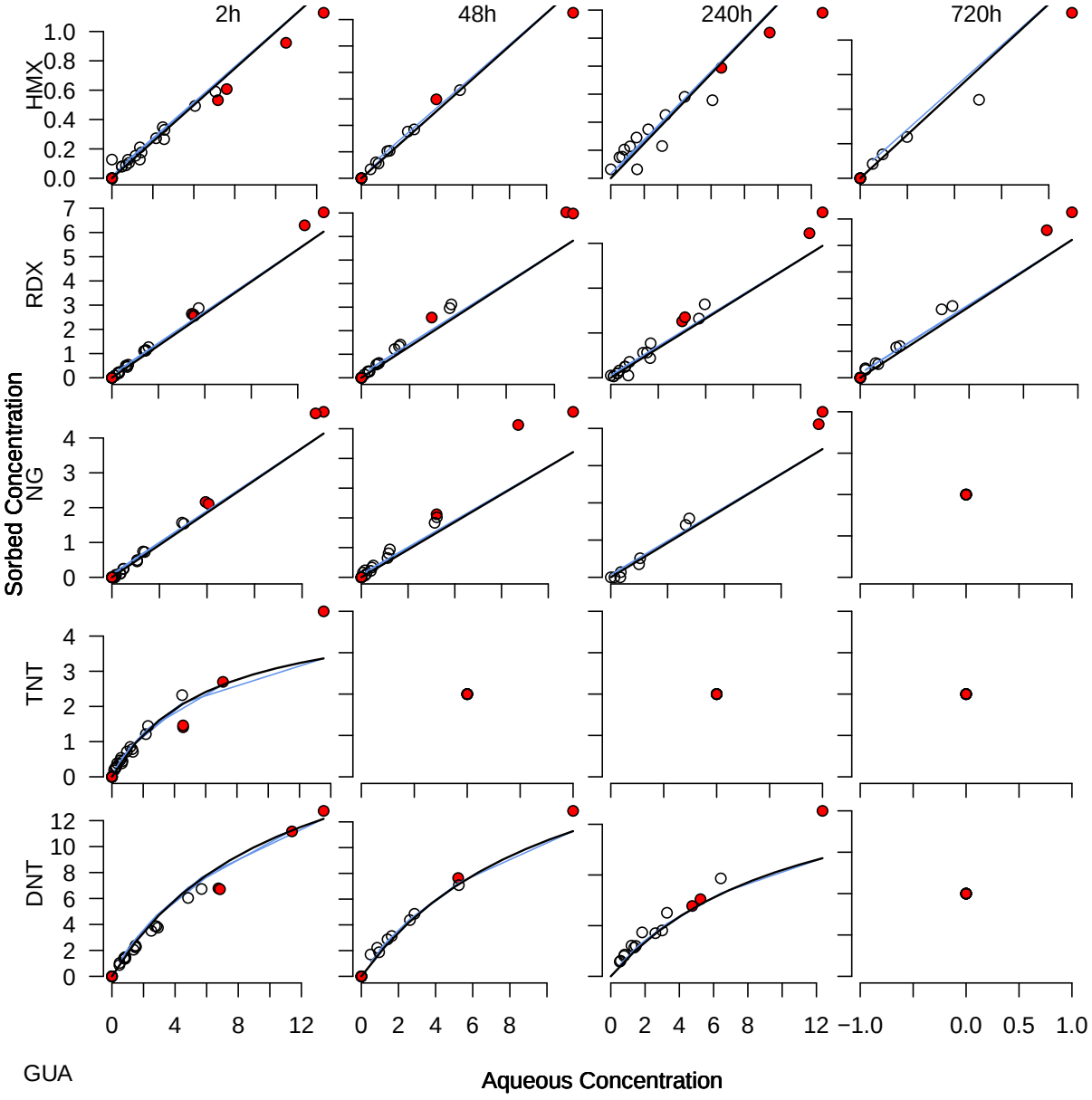

2h
48h
240h
720h
HMX
RDX
NG
TNT
DNT
Sorbed Concentration
Aqueous Concentration
W

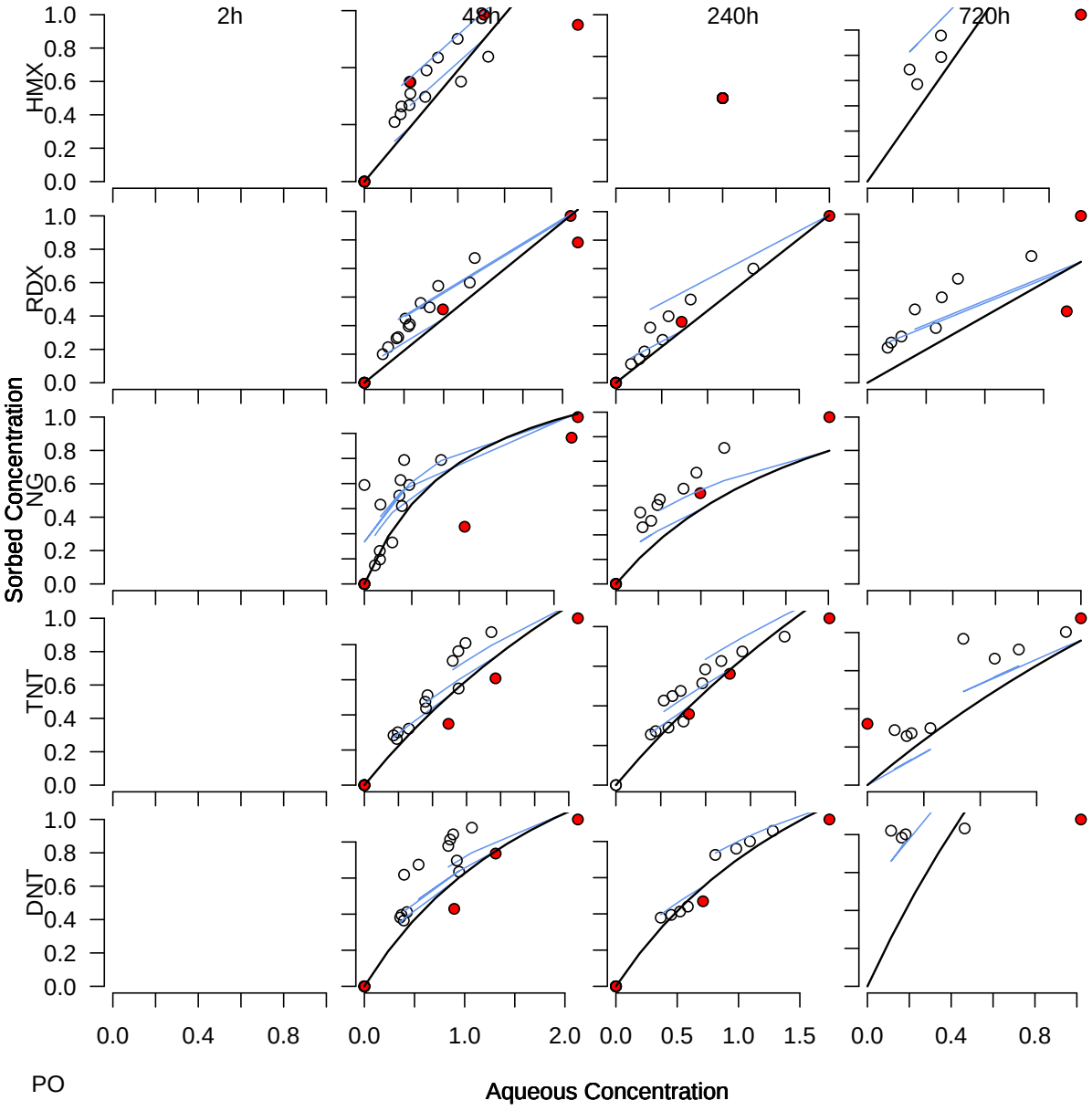

2h
48h
240h
720h
HMX
RDX
NG
TNT
DNT
Sorbed Concentration
Aqueous Concentration
AM

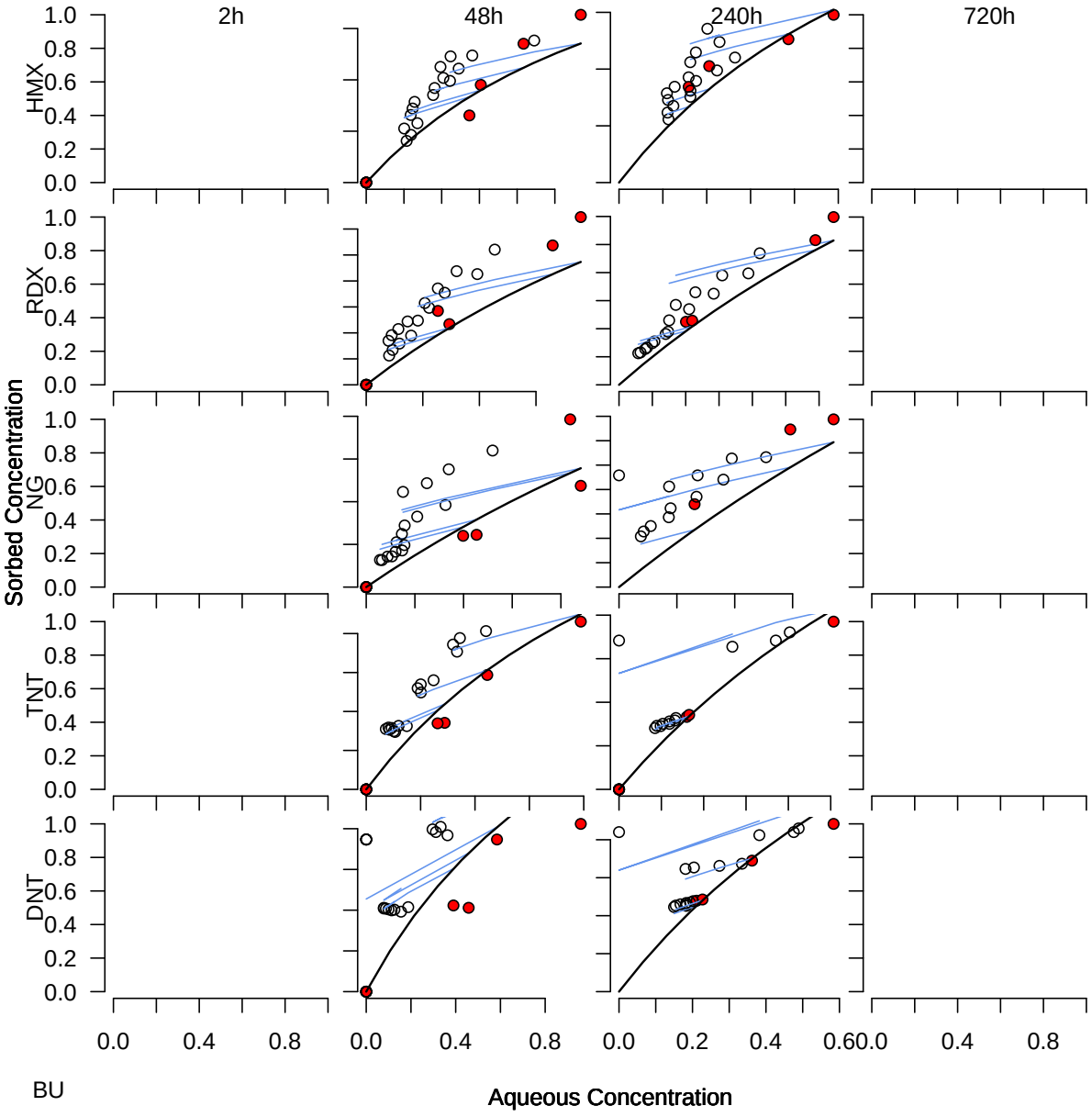

2h
48h
240h
720h
HMX
RDX
NG
TNT
DNT
Sorbed Concentration
Aqueous Concentration

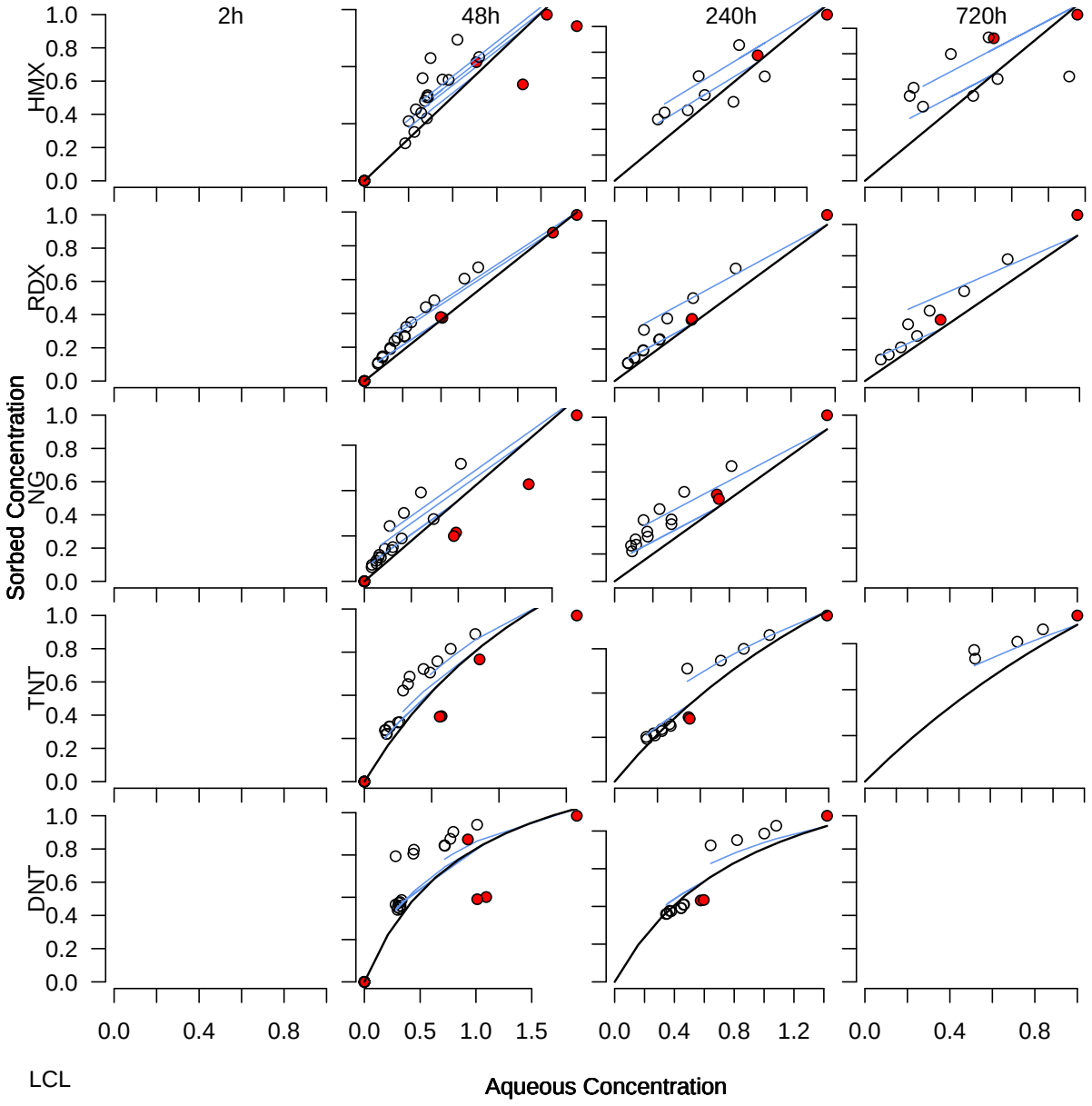
H

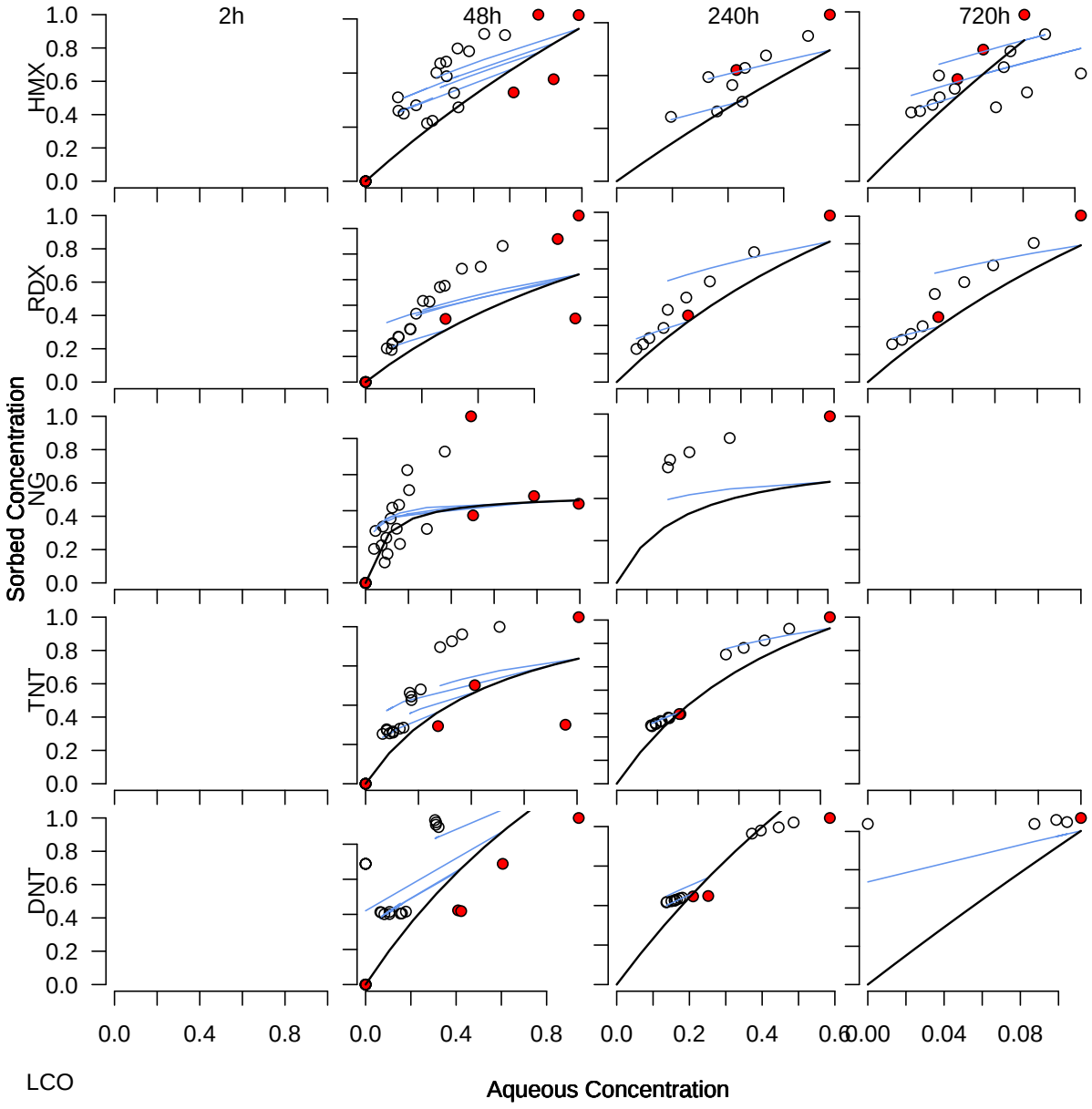

2h
48h
240h
720h
HMX
RDX
NG
TNT
DNT
Sorbed Concentration
Aqueous Concentration
BOX

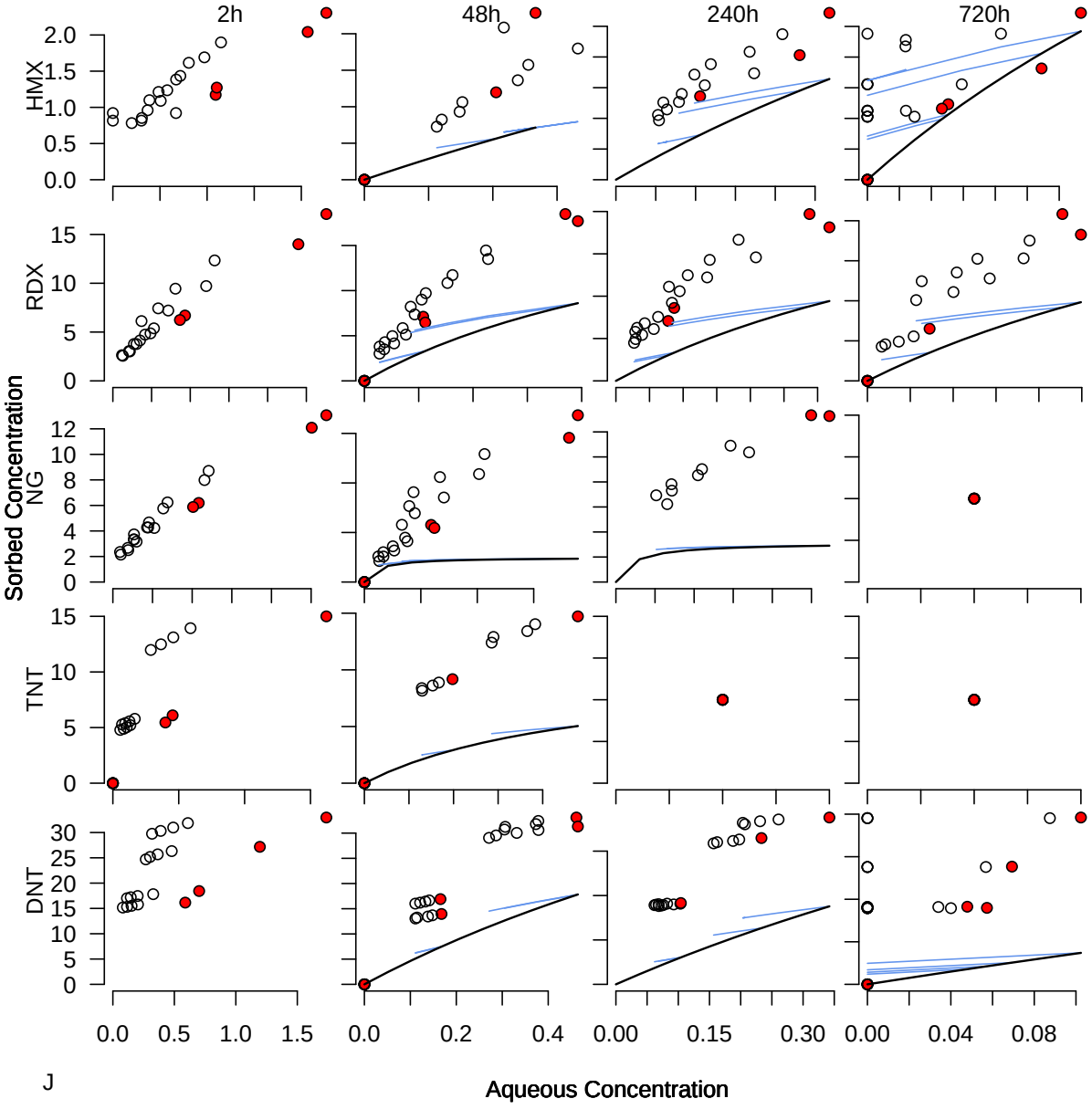

2h
48h
240h
720h
HMX
RDX
NG
TNT
DNT
Sorbed Concentration
Aqueous Concentration
GUA


2h
48h
240h
720h
HMX
RDX
NG
TNT
DNT
Sorbed Concentration
Aqueous Concentration
PO

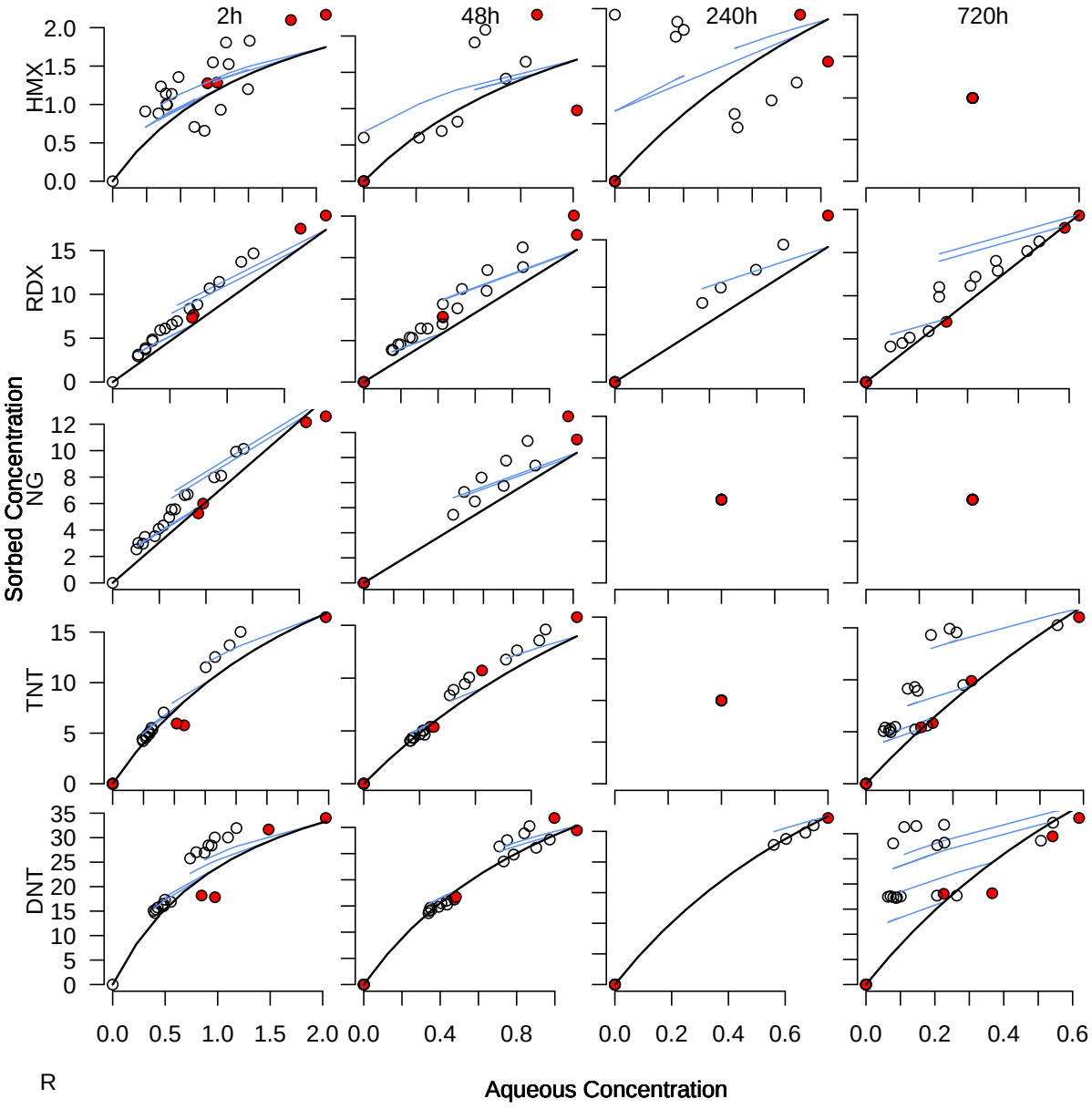

2h
48h
240h
720h
HMX
RDX
NG
TNT
DNT
Sorbed Concentration
Aqueous Concentration
BU

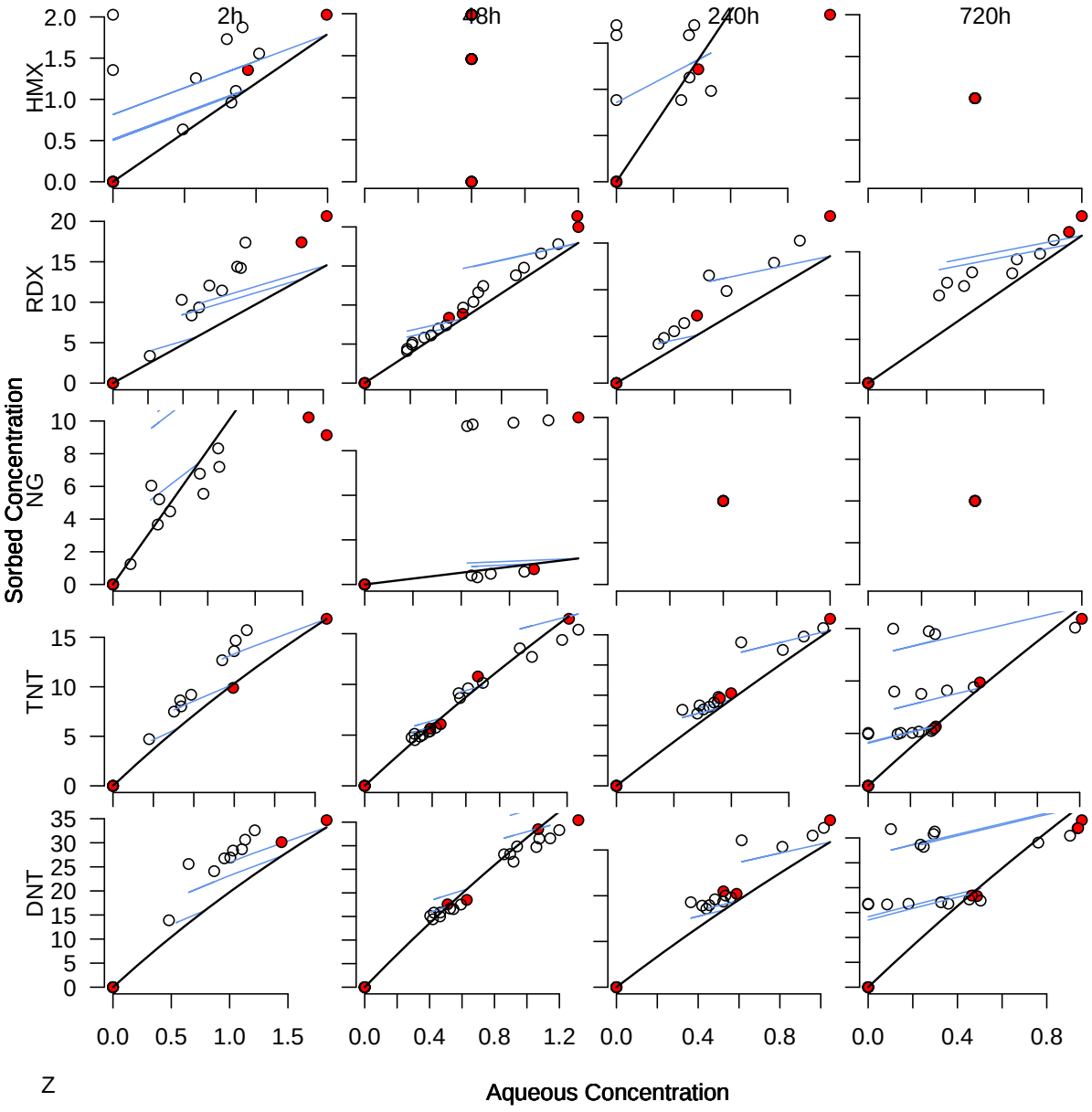

2h
48h
240h
720h
HMX
RDX
NG
TNT
DNT
Sorbed Concentration
Aqueous Concentration
LCL

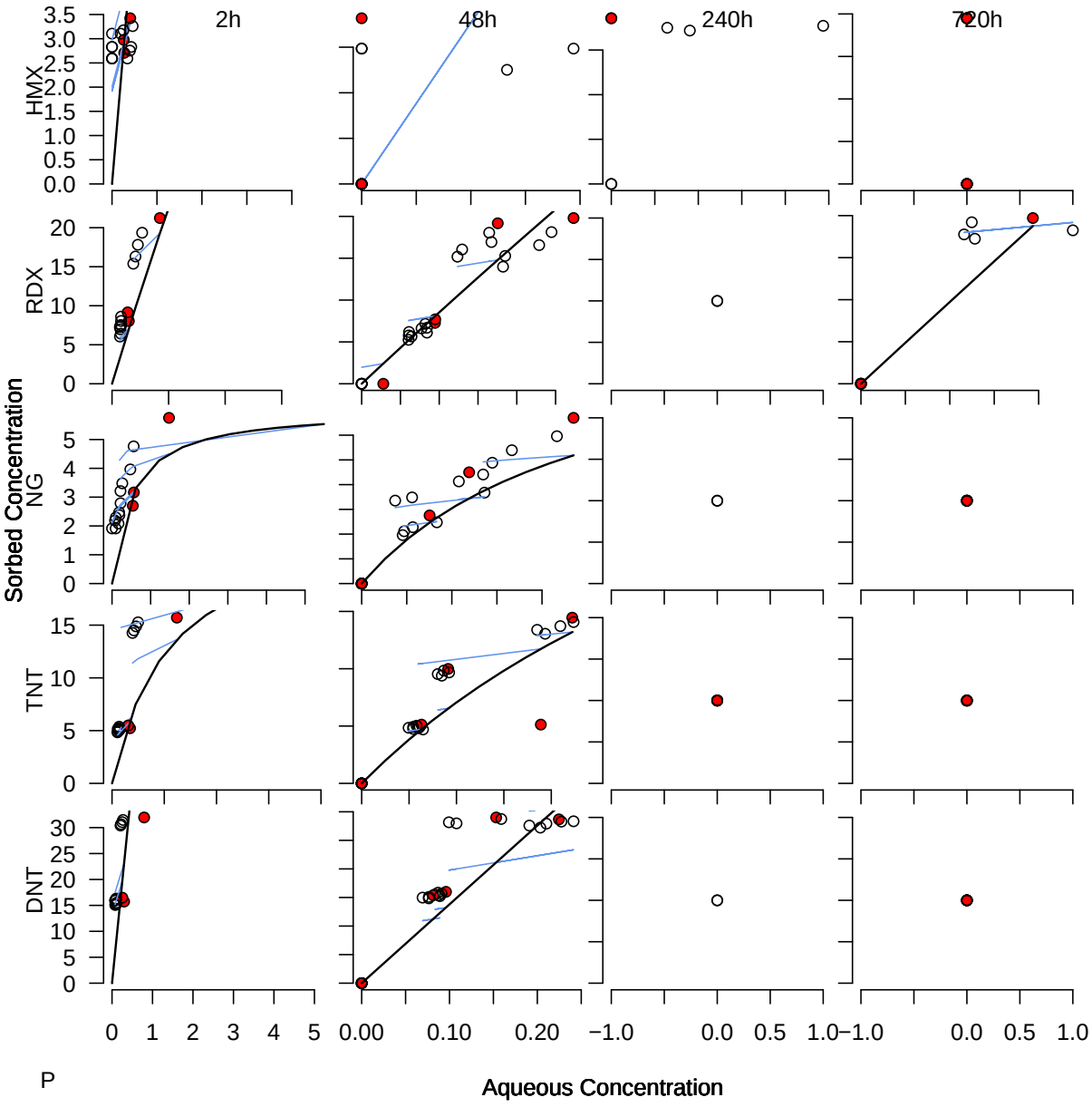

2h
48h
240h
720h
HMX
RDX
NG
TNT
DNT
Sorbed Concentration
Aqueous Concentration
LCO


2h
48h
240h
720h
HMX
RDX
NG
TNT
DNT
Sorbed Concentration
Aqueous Concentration
0.0 0.5 1.0 1.5
0.0 0.2 0.4
0.00 0.15 0.30
0.00 0.04 0.08

J


2h
48h
240h
720h
HMX
RDX
NG
TNT
DNT
Sorbed Concentration
Aqueous Concentration
R


2h
48h
240h
720h
HMX
RDX
NG
TNT
DNT
Sorbed Concentration
Aqueous Concentration
Z


2h
48h
240h
720h
HMX
RDX
NG
TNT
DNT
Sorbed Concentration
Aqueous Concentration
P

B.5 STM parameters

B.5.1 K_P and K_L

Table B.1: Parameters for STM derived K_P And K_L. NA indicates "Not Analyzed". For K_L NA indicates either linear or "Not Analyzed".

Soil	**MC**	$log_{10}K_p$	$log_{10}K_L$
KA	HMX	-0.000381	
ST	HMX	0.538	
BT	HMX	-0.25	
BA	HMX	-0.202	
U	HMX	0.0518	
B	HMX	-0.256	
FT	HMX	0.092	
SOU	HMX	0.0712	
W1	HMX	0.251	
W2	HMX	0.201	
SAS	HMX	0.21	
SSL	HMX	0.345	-0.122
MPK	HMX	0.215	
S2	HMX	0.0924	
W	HMX	0.347	
AM	HMX	0.336	
H	HMX	0.267	
BOX	HMX	0.288	
GUA	HMX	0.0851	
PO	HMX	0.565	
BU	HMX	0.556	0.41
LCL	HMX	0.482	
LCO	HMX	0.492	-0.0628
J	HMX	0.492	-0.0628
R	HMX	0.946	0.595
Z	HMX	0.812	
P	HMX	1.25	

Table B.1 – continued from previous page

Soil	MC	$log_{10}K_p$	$log_{10}K_L$
KA	RDX	-0.165	
ST	RDX	0.347	
BT	RDX	-0.532	
BA	RDX	-0.374	
U	RDX	-0.23	
B	RDX	-0.468	
FT	RDX	-0.273	
SOU	RDX	-0.247	
W1	RDX	-0.109	
W2	RDX	-0.0826	
SAS	RDX	-0.214	
SSL	RDX	-0.153	
MPK	RDX	-0.0852	
S2	RDX	-0.234	
W	RDX	0.0197	
AM	RDX	-0.127	
H	RDX	0.0779	
BOX	RDX	-0.0987	
GUA	RDX	-0.189	
PO	RDX	0.229	
BU	RDX	0.173	-1.02
LCL	RDX	0.173	
LCO	RDX	0.252	-0.836
J	RDX	0.252	-0.836
R	RDX	0.52	
Z	RDX	0.414	-4.99
P	RDX	0.596	-1.4

Table B.1 – continued from previous page

Soil	**MC**	$log_{10}K_p$	$log_{10}K_L$
KA	NG	-0.234	
ST	NG	0.0892	
BT	NG	-0.482	
BA	NG	-0.457	
U	NG	-0.287	
B	NG	-0.48	
FT	NG	-0.331	
SOU	NG	-0.542	
W1	NG	-0.333	
W2	NG	-0.377	
SAS	NG	-0.402	
SSL	NG	-0.278	
MPK	NG	-0.169	
S2	NG	-0.322	
W	NG	0.0665	
AM	NG	-0.217	
H	NG	0.289	-0.441
BOX	NG	-0.367	
GUA	NG	-0.344	
PO	NG	0.544	-0.0331
BU	NG	0.137	-0.958
LCL	NG	0.168	
LCO	NG	0.772	0.662
J	NG	0.772	0.662
R	NG	0.637	
Z	NG	0.649	
P	NG	0.588	0.295

Table B.1 – continued from previous page

Soil	**MC**	$log_{10}K_p$	$log_{10}K_L$
KA	TNT	-0.127	
ST	TNT	0.556	
BT	TNT	0.109	
BA	TNT	0.222	
U	TNT	0.402	-0.227
B	TNT	0.0274	
FT	TNT	0.0431	
SOU	TNT	0.0967	-2.4
W1	TNT	0.781	-0.111
W2	TNT	0.704	-0.225
SAS	TNT	0.316	
SSL	TNT	0.314	
MPK	TNT	0.553	-0.433
S2	TNT	0.296	
W	TNT	0.605	
AM	TNT	0.482	
H	TNT	0.464	-1.14
BOX	TNT	0.447	
GUA	TNT	0.189	-0.491
PO	TNT	0.955	-0.467
BU	TNT	0.913	-0.0893
LCL	TNT	0.938	-0.283
LCO	TNT	1.03	0.295
J	TNT	1.03	0.295
R	TNT	1.2	-0.21
Z	TNT	1.02	-0.708
P	TNT	1.18	0.262

Table B.1 – continued from previous page

Soil	**MC**	$log_{10}K_p$	$log_{10}K_L$
KA	DNT	-0.167	
ST	DNT	0.509	
BT	DNT	-0.0911	
BA	DNT	0.0166	
U	DNT	0.344	
B	DNT	-0.00682	
FT	DNT	-0.00694	
SOU	DNT	0.145	
W1	DNT	0.369	
W2	DNT	0.336	
SAS	DNT	0.366	
SSL	DNT	0.36	
MPK	DNT	0.679	-0.678
S2	DNT	0.324	
W	DNT	0.598	
AM	DNT	0.866	-0.796
H	DNT	1.03	-0.12
BOX	DNT	0.395	
GUA	DNT	0.294	-1.04
PO	DNT	1.23	-0.35
BU	DNT	1.35	-0.0863
LCL	DNT	1.43	0.0223
LCO	DNT	1.41	-0.222
J	DNT	1.41	-0.222
R	DNT	1.49	-0.0938
Z	DNT	1.08	-0.917
P	DNT	1.4	

B.5.2 f_{ST}

Table B.2: f_{ST} parameter for STM. NA indicates "Not Analyzed"

Soil	$log_{10} f_{ST}^{2h}$	$log_{10} f_{ST}^{48h}$	$log_{10} f_{ST}^{240h}$	$log_{10} f_{ST}^{720h}$
KA	-2.38	-2.53	-3.83	-1.68
ST	-6.54	-1.73	-1.33	-6.09
BT	-1.74	-1.62	-1.45	-0.884
BA	-1.77	-1.9	-1.39	-1.47
U	-8.12	-1.51	-1.3	-1.45
B	NA	-1.33	-1.29	-1.71
FT	NA	-1.37	-1.22	-2.24
SOU	-1.06	-0.901	-0.78	-1.14
W1	-2.93	-2.57	-5.5	-8.57
W2	-1.9	-2.25	-1.33	-6.95
SAS	-1.14	-1.51	-0.911	-1.44
SSL	-1.88	-1.81	NA	-0.835
MPK	-5.37	-1.35	-1.02	-0.944
S2	-1.44	-1.09	-0.878	-0.927
W	NA	-1.1	-0.979	-0.931
AM	-0.656	-0.648	-0.632	-0.5
H	-1.84	-0.708	-1.05	-0.66
BOX	NA	-0.258	-0.273	-0.551
GUA	-1.62	-1.57	-1.68	-1.44
PO	NA	-0.484	-0.309	-0.401
BU	NA	0.11	0.259	NA
LCL	NA	-0.676	-0.445	-0.241
LCO	NA	-0.0314	0.156	0.304
J	NA	-0.0314	0.156	0.304
R	-0.388	-0.168	-0.0398	0.254
Z	-0.0745	0.291	0.265	0.407
P	0.318	0.652	NA	0.949

Appendix C

TRANSPORT OF MC IN A COLUMN

C.1 MATLAB code

The column model was written as a group of 3 functions for MATLAB R2013b. It was built to take advantage of 3 parallel tasks and fit against the SSQ of linear residauls. **column_1D_DEG_v3** is the actual model. It returns a matrix containing aqueous concentrations for a singe chemical. **column_run_DEG_v1** runs the model for all three chemicals simultaneously, then calculates a linear SSQ residual. **column_psearch_DEG** controls the pattern search and submits the fitting to the workers.

column_1D_DEG_v3

```
1  function [ct] = column_1D_DEG_v3(Cinput,D,Q,K,kr,nLayer,A,texp,tzero,dt_
       print)
2      %ct=1;
3      %%% --- UNITS --- %%%
4      %   C     [=] mg/cm3
5      %   D     [=] cm2/s
6      %   v     [=] cm/s
7      %   K     [=] unitless
8      %   A     [=] cm2
9      %   texp  [=] s
10     %   tzero[=] s
11         %        kr        [=] s^-1
12
13     dt = 0.1;
14     trk=0;
15     LoR = texp;
16     lcolumn = 10; %10 cm column
17
18     Kx = K(1);
19     K0 = K(2);
20
21     % Define some bookkeeping variables
22     QC    = zeros(nLayer,1);   % Advective transport
23     EC    = zeros(nLayer+1,1); % Diffusive transport - Not used
24     dL    = lcolumn/nLayer;    % Diffusive length (equivalent to layer
           thickness)
25     VdCdt = zeros(nLayer,1);   % Instantaneous mass change
```

```
26      dC    = zeros(nLayer,1);   % Concentration change
27      ct.t  = zeros(nLayer,floor(LoR/dt_print));
28      ct.d  = zeros(nLayer,floor(LoR/dt_print));
29      ct.x  = zeros(nLayer,floor(LoR/dt_print));
30      ct.o  = zeros(nLayer,floor(LoR/dt_print));
31      ca  = zeros(nLayer,floor(LoR/dt_print));
32
33      % Calculate V (each layer is same size, so only one V)
34      Vol = A*dL;
35
36      % Transfer between layers can occur via advection (down only) or
37      % diffusion (either direction)
38
39      % Define concentrations inside column (input concentration is C(1)
            and
40      % output concentration is C(nlayer)
41      C.t   = zeros(nLayer,1);
42      C.d   = zeros(nLayer,1);
43      C.x   = zeros(nLayer,1);
44      C.o   = zeros(nLayer,1);
45      C.a   = zeros(nLayer,1);
46
47      Cdin=Cinput;
48
49      % Begin time loop
50      for t=0:dt:LoR
51          if t==tzero
52              Cdin=0;
53          end
54
55          if mod(t,dt_print)==0
56              trk=trk+1;
57              ct.t(:,trk)=C.d(:)+C.x(:)+C.o(:);
58              ct.d(:,trk)=C.d(:);
59              ct.x(:,trk)=C.x(:);
60              ct.o(:,trk)=C.o(:);
61              ca(:,trk)=C.a(:);
62          end
63
64          for ii = 1:nLayer
65              % Calculate advective transport
66              QC(ii) = Q.*C.d(ii);
67          end
68
69          VdCdt(1) = Q.*Cdin-QC(1)+...
70                      (D*A/dL)*(C.d(2)-C.d(1))-kr*C.d(1)*Vol;
71          for ii = 2:nLayer-1
72              % Determine overall layer transport
73              VdCdt(ii) = QC(ii-1)-QC(ii)+...
74                          (D*A/dL)*(C.d(ii-1)-C.d(ii))+...
75                          (D*A/dL)*(C.d(ii+1)-C.d(ii))-...
```

```
                                                    kr*C.d(ii)*Vol;
        end
        VdCdt(nLayer) = QC(nLayer-1)-QC(nLayer)+...
                        (D*A/dL).*(C.d(nLayer-1)-C.d(nLayer))-...
                                                    kr*C.d(nLayer)*Vol;


        % Update concentrations
        dC    = VdCdt*dt/Vol;
        C.t= C.t+dC;

        % Determine if mass is being added to soil, or being removed
        % if C.t(t+dt) > C.t(t) then mass added, otherwise, removed or
        % remains the same
        for ii = 1:nLayer

            if dC(ii) >= 0
                C.d(ii) = C.t(ii)/(1+Kx+K0);

                C.a(ii) = C.d(ii);
                C.o(ii) = K0*C.t(ii)/(1+Kx+K0);
                C.x(ii) = Kx*C.t(ii)/(1+Kx+K0);
            else
                C.o(ii) = K0*C.a(ii);
                C.d(ii) =(C.t(ii)-K0*C.a(ii))/(1+Kx);
                C.x(ii) = Kx*(C.t(ii)-K0*C.a(ii))/(1+Kx);
            end
        end
    end
end
```

column_run_DEG_v1

```
% Column FrontEnd for pattern search
% For chloride run, no sorption, find diffusion rate
function[ssq] = column_run_DEG_v1(psearch_var)
    chem_no = 3;
%%% Set known variables
    psearch_var=10.^psearch_var;

  % Initial concentration (ug/cm3)
    C0  = [10,5.5,9];
    % C0 = [Cl, RDX, TNT]

  % Flow rate of input stream (cm3/s)
    Q = 0.2/60;
  % Diffusion rate (cm2/s)
  % 1cm2/d ~ 2e-4cm2/s
    D_CL    =   psearch_var(1);
    D_RDX   =   psearch_var(1);
    D_TNT   =   psearch_var(1);

```

```
20    % Partition coefficients (Kx, K0) (unitless..for now)
21      K_CL(1:2)  = [1e-9,1e-9];
22      K_RDX(1:2) = [psearch_var(2),psearch_var(3)];
23      K_TNT(1:2) = [psearch_var(4),psearch_var(5)];
24
25    % Degradation rates [s^-1]
26      kr_CL      = 0;
27      kr_RDX     = psearch_var(6);
28      kr_TNT     = psearch_var(7);
29
30    % Number of effective layers in model
31      nLayer = 200;
32    % Cross sectional area of column (cm2)
33      A = 3.14159*1.1^2;
34    % Total runtime of column (s)
35      texp = 48*60*60;
36    % Time until Cinput = 0
37      tzero=24*60*60;
38    % Output every 'x' seconds of model time
39      dt_print = 60*30;
40
41      %column_run_DEG_v1(ans(2:8))
42
43  %%% Run the model
44  %[a_cl,b_cl]   = column_1D_v2(C0(1),D_CL, Q,K_CL, nLayer,A,texp,tzero,dt
        _print);
45  %[a_rdx,b_rdx] = column_1D_v2(C0(2),D_RDX,Q,K_RDX,nLayer,A,texp,tzero,dt
        _print);
46  %[a_tnt,b_tnt] = column_1D_v2(C0(3),D_TNT,Q,K_TNT,nLayer,A,texp,tzero,dt
        _print);
47
48  cl_par = parfeval(@column_1D_DEG_v1,2,C0(1),D_CL, Q,K_CL,kr_CL, nLayer,A
        ,texp,tzero,dt_print);
49  rdx_par= parfeval(@column_1D_DEG_v1,2,C0(2),D_RDX,Q,K_RDX,kr_RDX,nLayer,
        A,texp,tzero,dt_print);
50  tnt_par= parfeval(@column_1D_DEG_v1,2,C0(3),D_TNT,Q,K_TNT,kr_TNT,nLayer,
        A,texp,tzero,dt_print);
51
52  [a_cl,b_cl]   = fetchOutputs(cl_par);
53  [a_rdx,b_rdx]= fetchOutputs(rdx_par);
54  [a_tnt,b_tnt]= fetchOutputs(tnt_par);
55
56  %fprintf(1,'%f\t%f\t%f\t%f\n',Cinput,K,kr)
57
58  %%% Calculate SSQ or other forcing function
59    % Only observed values are at column exit (i.e. C(nlayer))
60    fid=fopen('D:\Users\Dropbox\Research\SERDP_1\Project_4-Column\USARMY_
          ECBC_Data\breakthrough.csv');
61    fdat=textscan(fid,'%f%f%f%f%[^\n\r]','Delimiter',',','HeaderLines',1);
62    obs=[fdat{1:end-1}];
63    fclose(fid);
```

```
64
65    % First run uses chloride, so we need columns 1 and 2 of the file
66    ssq_chem=zeros(3,1);
67    for qq = 1:3
68        tobs=obs(:,1);
69        cobs=obs(:,1+qq);
70
71        nvals=size(tobs,1);
72        % Get the values required from model output
73        if qq==1
74            chem_a=a_cl;
75        elseif qq==2
76            chem_a=a_rdx;
77        else
78            chem_a=a_tnt;
79        end
80
81        idex=tobs(:)*3600/dt_print;
82        cmod=chem_a.d(nLayer,idex+1);
83
84        ssq_indev = zeros(nvals,1);
85        dy = zeros(nvals,1);
86        for ii=1:nvals
87              if cobs(ii)==-9999
88                  ssq_indev(ii)=0;
89                  dy(ii) = 0;
90              else
91                  %if (cobs(ii) == 0) || (cmod(ii) == 0)
92                      ssq_indev(ii)=(cmod(ii)-cobs(ii))^2;
93                  %else
94                  %    ssq_indev(ii)=(log10(cmod(ii))-log10(cobs(ii)))^2;
95                  %end
96                  dy(ii) = abs(cmod(ii)-cobs(ii));
97              end
98        end
99        ssq_chem(qq) = sum(ssq_indev);
100
101
102      %%% Plot of dissolved conc as a function of time
103      subplot(3,1,qq,'replace')
104      plot(linspace(0,texp,texp/dt_print+1)/3600,chem_a.d(nLayer,:))
105      hold on;
106      plot(tobs,cobs,'or')
107      axis([0 texp/3600 0 C0(qq)+0.1*C0(qq)])
108      hold off;
109
110    end
111    ssq=sum(ssq_chem);
112    fprintf(1,'%2.2f\t%2.2f\t%2.2f\t%2.2f\t%2.2f\t%2.2f\t%2.2f%3.3f\n',
           log10(psearch_var),ssq);
113  end
```

column_psearch_DEG

```
%%% Psearch for column model
function[ps_fit] = column_psearch_DEG()
if matlabpool('size')==0
    parpool(3);
end

% Set initial value(s) for par variable - input at log10(par)
%theta = [-2.8];
theta = [-2,-4,-8,-2,-0.0223,-8,-1];
Kx = log10(3.5);
K0 = log10(5.5-10^Kx);
theta = [-2.4    -0.1     -9.00    Kx  K0       -12.00        -12.0];

% Set bound(s) for par varibale
UB = [9,9,0,9,0,0,0];
%UB = [-2.3];
LB = [-9,-9,-9,-9,-9,-12,-12];
%LB = [-4];

%%% From Experimental Setup
m_sw = 45.43/18.33; %g/mL = kg/L

% Set psearch algo parameters
options = psoptimset('UseParallel', 'always', 'CompletePoll', 'off', '
    Vectorized', 'off','Display','iter','MaxIter',400);

% Perform pattern search
[xfit,fval] = patternsearch(@column_run_DEG_v1,theta,[],[],[],[],LB,UB,
    options);
ps_fit=[fval,xfit];

fprintf(1,'%s\n','DONE');


end
```

Appendix D

DIFFUSION MODEL

D.1 2-layer model

```
## Normalized Concentration plots
## One Soil Per Page

graphics.off()
rm(list=ls(all=TRUE))

name     <-  'two_layer'
vrs      <-  'v6_logResid'

dat_path     <-  '../data/'
out_path     <-  '../output/'
fig_path     <-  '../figs/'

hplc.raw     <-  read.table(paste(dat_path,'hplc_data.csv', sep=''),
    header=TRUE, stringsAsFactor=FALSE,sep=',',as.is=TRUE)
prop.raw     <-  read.table(file=paste(dat_path,'soil_properties.csv',sep
    =''),header=TRUE,stringsAsFactors=FALSE,sep=',',as.is=TRUE)

foc          <-  prop.raw$TOC/100
fclay        <-  prop.raw$Clay/100

soil_order   <-  prop.raw[prop.raw[,1] %in% unique(hplc.raw[,2]),]
soil_foc     <-  soil_order[order(soil_order$TOC),]
foc_order    <-  soil_order[order(soil_order$TOC),]$TOC/100
fcl_order    <-  soil_order[order(soil_order$TOC),]$Clay/100
soil_order   <-  soil_order[order(soil_order$TOC),]$SoilCode
nSoil        <-  length(soil_order)

mc_list      <-  c('HMX','RDX','NG','TNT','DNT')
nMC          <-  length(mc_list)

hplc.raw$MTOT   <-  hplc.raw$A.C*hplc.raw$V.A+
                    hplc.raw$D1.C*hplc.raw$V.D1+
                    hplc.raw$D2.C*hplc.raw$V.D2+
                    hplc.raw$D3.C*hplc.raw$V.D3+
                    hplc.raw$D4.C*hplc.raw$V.D4+
                    hplc.raw$E1.C*hplc.raw$V.E1+
                    hplc.raw$E2.C*hplc.raw$V.E2+
```

```
                        hplc.raw$E3.C*hplc.raw$V.E3

hplc.raw$M.EXT  <-  hplc.raw$E1.C*hplc.raw$V.E1+
                    hplc.raw$E2.C*hplc.raw$V.E2+
                    hplc.raw$E3.C*hplc.raw$V.E3

vList   <-  matrix(c(1, 6, 11, 16, 2, 7, 12, 17, 3, 8, 13, 18, 4, 9, 14,
    19, 5, 10, 15, 20),ncol=4,byrow=T)

collist<-rev(c(rgb(0,seq(nSoil,round(nSoil*2/5)+1,-1),0,8,maxColorValue
    =nSoil),
            rgb(seq(0,round(nSoil*2/5),1),seq(round(nSoil*2/5),0,-1),0,8,
                maxColorValue =nSoil),
            rgb(seq(round(nSoil*2/5)+1,nSoil,1),0,0,8,maxColorValue =
                nSoil)))

ct1<-   function(tv,fd1,fd2,ct1.0,ct2.0,vd,fcl,fsl,hv) {
    Vaq =   5       #ml
    ms  =   5       #g
    Vhv =   hv
    rho =   1.300   #g/mL

    h1  =   (Vaq + fcl*(Vhv+ms/rho))/(Vaq + Vhv + ms/rho -(1-fcl-fsl)*(
        Vhv + ms/rho))
    h2  =   (fsl*(Vhv+ms/rho))/(Vaq + Vhv + ms/rho -(1-fcl-fsl)*(Vhv +
        ms/rho))

    #h1 =       0.4+fcl*0.6
        #h2     =       1-h1

    vh1=vd/h1
    vh2=vd/h2

    s1 = fd1*vh1
    s2 = fd2*vh2

    c1  <-  ct1.0*((s1/(s1+s2))*exp(-(s1+s2)*tv)+s2/(s1+s2))-ct2.0*(h2/
        h1)*(s2/(s1+s2))*(exp(-(s1+s2)*tv)-1)
    return(c1)
}

ct2<-   function(tv,fd1,fd2,ct1.0,ct2.0,vd,fcl,fsl,hv) {
    Vaq =   5       #ml
    ms  =   5       #g
    Vhv =   hv
    rho =   1.300   #g/mL

    h1  =   (Vaq + fcl*(Vhv+ms/rho))/(Vaq + Vhv + ms/rho -(1-fcl-fsl)*(
        Vhv + ms/rho))
    h2  =   (fsl*(Vhv+ms/rho))/(Vaq + Vhv + ms/rho -(1-fcl-fsl)*(Vhv +
        ms/rho))
```

```
79
80      #h1 =         0.4+fcl*0.6
81          #h2       =         1-h1
82
83          vh1=vd/h1
84      vh2=vd/h2
85
86      s1 = fd1*vh1
87      s2 = fd2*vh2
88
89      c2  <-  ct2.0*((s2/(s1+s2))*exp(-(s1+s2)*tv)+s1/(s1+s2))-ct1.0*(h1/
            h2)*(s1/(s1+s2))*(exp(-(s1+s2)*tv)-1)
90      return(c2)
91  }
92
93  two_layer_v2    <-  function(tpts,tads,fd1,fd2,vd,fcl,fsl,hv,plt=FALSE)
        {
94      t.zero  <-  c(tads,tads+1,tads+2,tads+3,tads+4)
95
96      # Compute a non-desorbing solution for all times in tpts
97      # Arguments are:
98      #   tpts-   points to compute solution,
99      #   fd1 -   dissolved fraction in layer 1,
100     #   fd2 -   dissolved fraction in layer 2,
101     #   1   -   Total initial concentration in layer 1,
102     #   0   -   Total initial concentration in layer 2,
103     #   h1  -   depth of layer 1,
104     #   h2  -   depth of layer 2
105
106     CT.1    <-  ct1(tpts,fd1,fd2,1,0,vd,fcl,fsl,hv)
107     CT.2    <-  ct2(tpts,fd1,fd2,1,0,vd,fcl,fsl,hv)
108
109     # Compute dissolved concentration at adsorption time
110     Cd.ADS  <-  fd1*ct1(t.zero[1],fd1,fd2,1,0,vd,fcl,fsl,hv)
111
112     # Time shift solution for negative dissolved concentration (used for
            superposition)
113     CT.1.D1 <-  ct1(ifelse((tpts-t.zero[1])<=0,0,tpts-t.zero[1]),fd1,fd2
            ,ifelse((tpts-t.zero[1])<=0,0,-Cd.ADS),0,vd,fcl,fsl,hv)
114     CT.2.D1 <-  ct2(ifelse((tpts-t.zero[1])<=0,0,tpts-t.zero[1]),fd1,fd2
            ,ifelse((tpts-t.zero[1])<=0,0,-Cd.ADS),0,vd,fcl,fsl,hv)
115
116     # Compute dissolved concentration after first desorption (
            Superposition of ads+d1)
117     Cd.D1   <-  fd1*(ct1(t.zero[2],fd1,fd2,1,0,vd,fcl,fsl,hv) +
118                      ct1(1,fd1,fd2,-Cd.ADS,0,vd,fcl,fsl,hv))
119
120     # Time shift solution for negative dissolved concentration (used for
            superposition)
121     CT.1.D2 <-  ct1(ifelse((tpts-t.zero[2])<=0,0,tpts-t.zero[2]),fd1,fd2
            ,ifelse((tpts-t.zero[2])<=0,0,-Cd.D1),0,vd,fcl,fsl,hv)
```

```
122     CT.2.D2 <-  ct2(ifelse((tpts-t.zero[2])<=0,0,tpts-t.zero[2]),fd1,fd2
            ,ifelse((tpts-t.zero[2])<=0,0,-Cd.D1),0,vd,fcl,fsl,hv)
123
124     # Compute dissolved concentration after second desorption (
            Superposition of ads+d1+d2)
125     Cd.D2   <-  fd1*(ct1(t.zero[3],fd1,fd2,1,0,vd,fcl,fsl,hv) +
126                      ct1(2,fd1,fd2,-Cd.ADS,0,vd,fcl,fsl,hv) +
127                      ct1(1,fd1,fd2,-Cd.D1,0,vd,fcl,fsl,hv))
128
129     # Time shift solution for negative dissolved concentration (used for
            superposition)
130     CT.1.D3 <-  ct1(ifelse((tpts-t.zero[3])<=0,0,tpts-t.zero[3]),fd1,fd2
            ,ifelse((tpts-t.zero[3])<=0,0,-Cd.D2),0,vd,fcl,fsl,hv)
131     CT.2.D3 <-  ct2(ifelse((tpts-t.zero[3])<=0,0,tpts-t.zero[3]),fd1,fd2
            ,ifelse((tpts-t.zero[3])<=0,0,-Cd.D2),0,vd,fcl,fsl,hv)
132
133     # Compute dissolved concentration after third desorption (
            Superposition of ads+d1+d2+d3)
134     Cd.D3   <-  fd1*(ct1(t.zero[4],fd1,fd2,1,0,vd,fcl,fsl,hv) +
135                      ct1(3,fd1,fd2,-Cd.ADS,0,vd,fcl,fsl,hv) +
136                      ct1(2,fd1,fd2,-Cd.D1,0,vd,fcl,fsl,hv) +
137                      ct1(1,fd1,fd2,-Cd.D2,0,vd,fcl,fsl,hv))
138
139     # Time shift solution for negative dissolved concentration (used for
            superposition)
140     CT.1.D4 <-  ct1(ifelse((tpts-t.zero[4])<=0,0,tpts-t.zero[4]),fd1,fd2
            ,ifelse((tpts-t.zero[4])<=0,0,-Cd.D3),0,vd,fcl,fsl,hv)
141     CT.2.D4 <-  ct2(ifelse((tpts-t.zero[4])<=0,0,tpts-t.zero[4]),fd1,fd2
            ,ifelse((tpts-t.zero[4])<=0,0,-Cd.D3),0,vd,fcl,fsl,hv)
142
143     # Compute dissolved concentration after third desorption (
            Superposition of ads+d1+d2+d3)
144     Cd.D4   <-  fd1*(ct1(t.zero[5],fd1,fd2,1,0,vd,fcl,fsl,hv) +
145                      ct1(4,fd1,fd2,-Cd.ADS,0,vd,fcl,fsl,hv) +
146                      ct1(3,fd1,fd2,-Cd.D1,0,vd,fcl,fsl,hv) +
147                      ct1(2,fd1,fd2,-Cd.D2,0,vd,fcl,fsl,hv) +
148                      ct1(1,fd1,fd2,-Cd.D3,0,vd,fcl,fsl,hv))
149
150     ## Output the superposition of all solutions
151     C.Layer1    <-  CT.1 + CT.1.D1 + CT.1.D2 + CT.1.D3 + CT.1.D4
152     C.Layer2    <-  CT.2 + CT.2.D1 + CT.2.D2 + CT.2.D3 + CT.2.D4
153
154     C.out       =   matrix(c(C.Layer1,C.Layer2),ncol=2)
155
156     if (plt==1) {
157         plot(tpts,CT.1,type='l',ylim=c(-1,1))
158         lines(tpts,CT.1.D1,col='red')
159         lines(tpts,CT.1.D2,col='blue')
160         lines(tpts,CT.1.D3,col='green')
161         lines(tpts,CT.1.D4,col='purple')
```

```
162         points(x=t.zero,y=c(Cd.ADS,Cd.D1,Cd.D2,Cd.D3,Cd.D4),pch=21,bg=NA
                ,cex=2)
163     } else if (plt==2) {
164         plot(CT.2,type='l',ylim=c(-1,1))
165         lines(CT.2.D1,col='grey50')
166         lines(CT.2.D2,col='grey60')
167         lines(CT.2.D3,col='grey70')
168         lines(CT.2.D4,col='grey80')
169     }
170
171     return(C.out)
172 }
173
174 two_layer_plot_v2<- function(tads,mKp1,mKp2,obs,sname,mc,vd,fcl,fsl,hv)
        {
175     fd1 <- 1/(1+mKp1)
176     fd2 <- 1/(1+mKp2)
177
178     xFigs   <- seq(0.1,0.95,length.out=5)
179     yFigs   <- rev(seq(0.1,0.95,length.out=6))
180     out.mar <- c(0,0,0,0)
181
182     # Generate 4x3 plot
183     for (ii in 1:4) {
184         tpts    <- tads[ii]
185         pt.loc  <- c(100,150,200,250,300)
186
187         tseq    <- c(seq(0,1.5,length.out=75),
188                      seq(1.5,tpts,length.out=25),
189                      seq(tpts,tpts+1,length.out=50),
190                      seq(tpts+1,tpts+2,length.out=50),
191                      seq(tpts+2,tpts+3,length.out=50),
192                      seq(tpts+3,tpts+4,length.out=50),
193                      seq(tpts+4,tpts+5,length.out=50))
194         yvals<-two_layer_v2(tseq,tads[ii],fd1,fd2,vd,fcl,fsl,hv)
195
196         # Plot Dissolved Concentrations
197         par(fig=c(xFigs[ii],xFigs[ii+1],yFigs[mc+1],yFigs[mc]),mar=out.
                mar,new=ifelse(mc==1 & ii==1,FALSE,TRUE))
198         plot(1,type='n',xlim=c(0,400),ylim=c(0,1),axes=F,xlab='',ylab=''
                )
199         rect(xleft=-900,xright=900,ybottom=-1,ytop=2,col='grey90',border
                =NA)
200         abline(h=seq(0,1,length.out=5),col='white',lwd=2)
201         abline(v=c(0,pt.loc),col='white',lwd=2)
202         abline(h=0,lwd=4,col='cornflowerblue')
203
204         lines(x=seq(1,350,1),y=fd1*yvals[,1],col='black',lwd=2)
205         #lines(x=seq(1,350,1),y=fd2*yvals[,2],col='red',lwd=2)
206
207         if (ii==1) {
```

```
208             axis(2,at=seq(0,1,length.out=5),las=2)
209         }
210         if (ii==4) {
211             legend('topright',bg='white',legend=c(paste(sname,mc_list[mc
                ],sep='_______')))
212         }
213
214         mod <- two_layer_v2(c(0,seq(tpts,by=1,length.out=5)),tpts,fd1,
            fd2,vd,fcl)
215         points(x=c(0,pt.loc),y=fd1*mod[,1],pch=21,col='blue',cex=1.5,bg=
            NA)
216
217         # Plot observed data
218         for (kk in 2:6) {
219             points(x=rep(pt.loc[kk-1],length(obs[(1+5*(ii-1)):(5*(ii)),
                kk])),y=obs[(1+5*(ii-1)):(5*(ii)),kk],pch=4)
220         }
221         axis(1,at=c(0,pt.loc),labels=c('t=0','A','D1','D2','D3','D4'))
222     }
223 }
224
225 two_layer_plot_v3<- function(tads,mKp1,mKp2,obs,sname,mc,vd,fcl,fsl,hv)
        {
226     fd1 <- 1/(1+mKp1)
227     fd2 <- 1/(1+mKp2)
228
229     xFigs   <- seq(0.1,0.9,length.out=6)
230     yFigs   <- rev(seq(0.1,0.95,length.out=6))
231     out.mar <- c(0,0,0,0)
232
233     mext.mod    <- matrix(NA,ncol=1,nrow=4)
234     mext.obs    <- matrix(NA,ncol=5,nrow=4)
235
236     # Generate 4x3 plot
237     for (ii in 1:4) {
238         yl <- 1e-4
239         yu <- 1
240
241         tpts    <- tads[ii]
242         pt.loc  <- c(100,150,200,250,300)
243
244         tseq    <- c(seq(tpts-1,tpts,length.out=50),
245                      seq(tpts,tpts+1,length.out=50),
246                      seq(tpts+1,tpts+2,length.out=50),
247                      seq(tpts+2,tpts+3,length.out=50),
248                      seq(tpts+3,tpts+4,length.out=50),
249                      seq(tpts+4,tpts+5,length.out=50))
250
251         yvals<-two_layer_v2(tseq,tads[ii],fd1,fd2,vd,fcl,fsl,hv)
252
253         # Plot Dissolved Concentrations
```

```
254         par(fig=c(xFigs[ii],xFigs[ii+1],yFigs[mc+1],yFigs[mc]),mar=out.
                mar,new=ifelse(mc==1 & ii==1,FALSE,TRUE))
255         plot(1,type='n',xlim=c(75,325),ylim=c(yl,yu),axes=F,xlab='',ylab
                ='',log='y')
256         rect(xleft=-900,xright=900,ybottom=1e-5,ytop=2,col='grey90',
                border=NA)
257         abline(h=10^seq(-4,0,length.out=5),col='white',lwd=2)
258         abline(v=c(pt.loc),col='white',lwd=2)
259         abline(h=0,lwd=4,col='cornflowerblue')
260
261         mtext(side=2,at=(yFigs[mc]+yFigs[mc+1])/2,outer=T,line=-1,text=
                mc_list[mc])
262
263         lines(x=seq(51,350,1),y=fd1*yvals[,1],col='blue',lwd=2)
264         #lines(x=seq(1,350,1),y=fd2*yvals[,2],col='red',lwd=2)
265
266         if (ii==1) {
267             axis(2,at=log_axis(yl,yu)[[2]],labels=log_axis(yl,yu)[[3]],
                    las=2)
268             legend('bottomleft',bg='white',legend=c(paste('fd1=',signif(
                    fd1,4),sep=''),paste('fd2=',signif(fd2,4),sep='')))
269         }
270
271         mod <-  two_layer_v2(c(seq(tpts,by=1,length.out=5)),tpts,fd1,fd2
                ,vd,fcl,fsl,hv)
272         #points(x=c(pt.loc),y=fd1*mod[,1],pch=21,col='blue',cex=1.5,bg=
                NA)
273
274         # Plot observed data
275         for (kk in 2:6) {
276             points(x=rep(pt.loc[kk-1],length(obs[(1+5*(ii-1)):(5*(ii)),
                    kk])),y=obs[(1+5*(ii-1)):(5*(ii)),kk],pch=4,bg=rgb
                    (255,255,255,alpha=75,maxColorValue=255),cex=1.5)
277         }
278         axis(1,at=c(pt.loc),labels=c('A','D1','D2','D3','D4'))
279
280         ypts    <-  obs[(1+5*(ii-1)):(5*(ii)),7]
281         ypts    <-  ifelse(ypts==0,yl,ypts)
282
283         Vaq =   5       #ml
284         ms  =   5       #g
285         Vhv =   hv
286         rho =   1.300   #g/mL
287
288         V1  =   (Vaq + fcl*(Vhv+ms/rho))
289         V2  =   (fsl*(Vhv+ms/rho))
290
291         h1  =   (Vaq + fcl*(Vhv+ms/rho))/(Vaq + Vhv + ms/rho -(1-fcl-fsl
                )*(Vhv + ms/rho))
292         h2  =   (fsl*(Vhv+ms/rho))/(Vaq + Vhv + ms/rho -(1-fcl-fsl)*(Vhv
                + ms/rho))
```

```
293
294         mext.mod[ii]     <-  (1-fd1)*mod[5,1]*h1+mod[5,2]*h2
295         mext.obs[ii,]    <-  ypts
296     }
297     par(fig=c(xFigs[5],xFigs[6],yFigs[mc+1],yFigs[mc]),mar=out.mar,new=
            TRUE)
298     plot(1,type='n',xlab='',ylab='',xlim=c(0,5),ylim=c(-1,1),axes=F,log=
            '')
299     for (ii in 1:4) {
300         resd    <-  log10(mext.obs[ii,])-log10(mext.mod[ii])
301         is.na(resd) <-  !is.finite(resd)
302         resd    <-  ifelse(mext.obs[ii,]!=0,resd,0.45)
303         points(x=rep(ii,5),y=resd,pch=ifelse(mext.obs[ii,]!=0,21,8))
304
305         if (any(resd > 1,na.rm=T)) {
306             arrows(x0=ii,y0=0.69897,y1=0.95,length=0.05)
307             text(x=ii,y=0.6,labels=signif(min(resd[resd > 1],na.rm=T),2)
                    ,cex=0.5)}
308         if (any(resd < -1,na.rm=T)) {
309             arrows(x0=ii,y0=-0.69897,y1=-0.95,length=0.05)
310             text(x=ii,y=-0.6,labels=signif(max(resd[resd < -1],na.rm=T)
                    ,2),cex=0.5)}
311     }
312     abline(h=c(-0.69897,-0.30103,0,0.30103,0.69897),col='cornflowerblue'
            ,lty=c(3,2,1,2,3))
313     axis(4,at=c(-1,-0.69897,-0.30103,0,0.30103,0.69897,1),labels=c('1/10
            ','1/5','1/2','1','2','5','10'),las=2,cex.axis=0.75)
314     if (mc == nMC) {axis(1,at=seq(1,4,1),labels=c('2h','48h','240h','720
            h'),las=2)}
315     box()
316     if (mc == 3) {
317         mtext(side=3,at=(xFigs[1]+xFigs[5])/2,outer=T,line=-2,text='
                Normalized Aq.')
318         mtext(side=3,at=(xFigs[5]+xFigs[6])/2,outer=T,line=-2,text='
                Extraction')
319         mtext(side=4,at=0.5,outer=T,line=-1,text='log10(obs/mod)')
320         mtext(side=1,at=0.05,line=-2,text=sname,outer=T)
321     }
322 }
323
324 ssq_calc        <-  function(tads,pars,vd,cobs,fcl,fsl,hv){
325     lin=FALSE
326
327     fd1     <-  1/(1+10^pars[1])
328     fd2     <-  1/(1+10^pars[2])
329
330     tpts    <-  matrix(c(tads,tads+1,tads+2,tads+3,tads+4),ncol=5)
331     ssq=0
332     # Cobs is Ads, D1, D2, D3, D4 + extractant
333
334     for (ii in 1:length(tads) ){
```

```
335         mod <- two_layer_v2(c(0,tpts[ii,]),tpts[ii,1],fd1,fd2,vd,fcl,
                fsl,hv)
336         # Subset data
337         if (tads[ii]==2) {
338             vl <- 0
339             vu <- 6
340         } else if (tads[ii]==48) {
341             vl <- 5
342             vu <- 11
343         } else if (tads[ii]==240) {
344             vl <- 10
345             vu <- 16
346         } else {
347             vl <- 15
348             vu <- 21
349         }
350
351         obs <- cobs[cobs[,1]>vl & cobs[,1]<vu,]
352
353         # Calculate a SSQ
354         ssq.tmp <- 0
355         for (jj in 1:dim(obs)[1]) {
356             logmod <- log10(c(fd1*mod[2:6,1]))
357             linmod <- c(fd1*mod[2:6,1])
358             logobs <- log10(obs[jj,2:6])
359             logobs <- ifelse(is.finite(logobs) | is.na(logobs),logobs
                    ,-9)
360             linobs <- obs[jj,2:6]
361             is.na(linobs) <- ifelse(linobs<0,TRUE,FALSE)
362
363             Vaq = 5          #ml
364             ms = 5           #g
365             Vhv = hv
366             rho = 1.300      #g/mL
367
368             V1 = (Vaq + fcl*(Vhv+ms/rho))
369             V2 = (fsl*(Vhv+ms/rho))
370
371             h1 = (Vaq + fcl*(Vhv+ms/rho))/(Vaq + Vhv + ms/rho -(1-fcl
                    -fsl)*(Vhv + ms/rho))
372             h2 = (fsl*(Vhv+ms/rho))/(Vaq + Vhv + ms/rho -(1-fcl-fsl)*
                    (Vhv + ms/rho))
373
374             linobs.mext <- obs[jj,7]
375             linmod.mext <- (1-fd1)*mod[6,1]*h1+mod[6,2]*h2
376
377             logobs.mext <- log10(linobs.mext)
378             logobs.mext <- ifelse(is.finite(linobs.mext) | is.na(linobs
                    .mext),linobs.mext,-9)
379             logmod.mext <- log10(linmod.mext)
380
```

```
381                 ssq.tmp <-  ssq.tmp +   sum((ifelse(lin==TRUE,linobs,logobs)
                        -ifelse(lin==TRUE,linmod,logmod))^2,na.rm=T)# + ifelse(
                        lin==TRUE,1,0)*(ifelse(is.na(linobs.mext),linmod.mext,
                        linobs.mext)-linmod.mext)^2
382             }
383             ssq <-  ssq+ssq.tmp
384         }
385         return(ssq)
386 }
387
388 # pdf(file='Two-Layer_boundary_cases2.pdf',paper='special',height=10,
        width=10,onefile=T)
389 # ### Test Case ###
390 # tseq     <-  seq(0,1000,length.out=10000)
391
392 # for (ii in 1:4) {
393     # fd1      <-  c(1,1e-9,1,1e-9)[ii]
394     # fd2      <-  rev(c(1e-9,1,1,1e-9))[ii]
395     # tads     <-  200
396     # vd=1e-1
397     # fcl                 <-  0.5
398
399     # mods     <-  two_layer_v2(tseq,tads,fd1,fd2,vd,fcl,fsl,hv)
400     # plot(mods[,1],type='l',ylim=c(0,1),xlab='index',ylab='Normalized
          Caq')
401     # legend('topright',legend=c(paste('fd1 = ',fd1,'      fd2 = ',fd2,
          sep=''),'Outer','Inner'),lty=1,col=c(NA,'black','red'))
402     # lines(mods[,2],col='red')
403
404     # plot((mods[,1]+mods[,2]),col='cornflowerblue')
405 # }
406 # dev.off()
407
408 ##########-------####################-------##########
409 # Fit using Optim package to normalized concentrations
410 ##########-------####################-------##########
411 library(ANMmisc)
412 ## Read data
413 ## Generate Normalized Data
414 ## Fit to data
415 psize    <-  read.table(file=paste(dat_path,'lnorm_fit.csv',sep=''),sep='
        ,',as.is=TRUE,stringsAsFactors=FALSE)
416 colnames(psize) <-  c('SOIL','MU','SIGMA','deltaMU','deltaSIGMA')
417
418 fit.out <-  matrix(NA,ncol=6,nrow=nMC*nSoil)
419
420 mbal.yesno  <-  read.table(file='D:/Users/Dropbox/Research/SERDP_1/
        Project_3-Rapid_Sorption/data/MB_yesno_v1.csv',sep=',',as.is=TRUE,
        stringsAsFactors=FALSE)
421
```

```
422 pdf(file='Two-Layer_optim_v6_logResid.pdf',paper='special',height=8.5,
    width=11,onefile=T)
423 for (ii in 1:nSoil) {
424 sub.soil    <- hplc.raw[hplc.raw$SOILCODE==soil_order[ii],]
425     for (jj in 1:nMC) {
426         sub.MC      <- sub.soil[sub.soil$MC==mc_list[jj],]
427
428         tmp         <- matrix(c(sub.MC[,'VIAL'],
429                                 sub.MC$A.C*sub.MC$V.A/sub.MC$MTOT,
430                                 sub.MC$D1.C*sub.MC$V.D1/sub.MC$MTOT,
431                                 sub.MC$D2.C*sub.MC$V.D2/sub.MC$MTOT,
432                                 sub.MC$D3.C*sub.MC$V.D3/sub.MC$MTOT,
433                                 sub.MC$D4.C*sub.MC$V.D4/sub.MC$MTOT,
434                                 sub.MC$M.EXT/sub.MC$MTOT),ncol=7)
435
436         mb.ok   <- mbal.yesno[mbal.yesno[,1]==soil_order[ii] & mbal.
                yesno[,3]==mc_list[jj],]
437         for (kk in 1:20) {
438             is.na(tmp[tmp[,1]==kk,2:7]) <- ifelse(mb.ok[kk,4]==1,FALSE,
                    TRUE)
439             is.na(tmp[tmp[,1]==kk,2:7]) <- is.nan(tmp[tmp[,1]==kk,2:7])
440         }
441
442         fcl             <-      prop.raw[prop.raw$SoilCode==soil_order[
                ii],]$Clay/100
443         fsl     <- prop.raw[prop.raw$SoilCode==soil_order[ii],]$Silt/
                100
444         hv      <- prop.raw[prop.raw$SoilCode==soil_order[ii],]$HV
445
446         Dm      <- 1            #cm2/d
447         Dm      <- Dm/24        #cm2/hr
448         radius  <- exp(psize[psize[,1]==soil_order[ii],'MU'])     #um
449         radius  <- radius/1e4
450         vd      <- Dm/radius
451         theta   <- c(0.5,0.5)
452         opt.fit <- optim(par=theta,fn=ssq_calc,fcl=fcl,fsl=fsl,hv=hv,
                tads=c(2,48,240,720),vd=vd,cobs=tmp,method='L-BFGS-B',lower=
                c(-4,-4),upper=c(4,4))
453
454         tseq    <- seq(0,800,length.out=10000)
455         mKp1    <- 10^opt.fit$par[1]
456         mKp2    <- 10^opt.fit$par[2]
457         tads    <- c(2,48,240,720)
458
459
460         two_layer_plot_v3(tads,mKp1,mKp2,tmp,soil_order[ii],jj,vd,fcl,
                fsl,hv)
461         fit.out[jj+nMC*(ii-1),]   <- matrix(c(ii,jj,opt.fit$value,mKp1,
                mKp2,vd),nrow=1)
462     }
463 }
```

```
464 dev.off()
465 write.table(x=fit.out,file='Two-Layer_optim_v6_logResid.csv',sep=',')
466
467
468 ## Residuals point-by-point
469 fit.out <- read.table(paste('Two-Layer_optim_v6_logResid.csv',sep=''),
        header=TRUE,as.is=TRUE,stringsAsFactors=FALSE,sep=',')
470 psize <- read.table(file=paste(dat_path,'lnorm_fit.csv',sep=''),sep='
        ',as.is=TRUE,stringsAsFactors=FALSE)
471 colnames(psize) <- c('SOIL','MU','SIGMA','deltaMU','deltaSIGMA')
472 mbal.yesno <- read.table(file='D:/Users/Dropbox/Research/SERDP_1/
        Project_3-Rapid_Sorption/data/MB_yesno_v1.csv',sep=',',as.is=TRUE,
        stringsAsFactors=FALSE)
473
474 xFigs <- seq(0.15,0.9,length.out=6)
475 yFigs <- seq(0.95,0.1,length.out=nMC+1)
476 library(ANMmisc)
477
478 linear=FALSE
479 ylin=c(1e-5,1)
480 ylin=c(-0.1,0.1)
481 ylog=c(-1,1)
482
483
484 pdf(file='Two-Layer_resid_points_v6.pdf',paper='special',height=8.5,
        width=11,onefile=T)
485 for (ii in 1:nSoil) {
486 sub.soil <- hplc.raw[hplc.raw$SOILCODE==soil_order[ii],]
487   for (jj in 1:nMC) {
488     sub.MC <- sub.soil[sub.soil$MC==mc_list[jj],]
489
490     tmp <- matrix(c(sub.MC[,'VIAL'],
491                     sub.MC$A.C*sub.MC$V.A/sub.MC$MTOT,
492                     sub.MC$D1.C*sub.MC$V.D1/sub.MC$MTOT,
493                     sub.MC$D2.C*sub.MC$V.D2/sub.MC$MTOT,
494                     sub.MC$D3.C*sub.MC$V.D3/sub.MC$MTOT,
495                     sub.MC$D4.C*sub.MC$V.D4/sub.MC$MTOT,
496                     sub.MC$M.EXT/sub.MC$MTOT),ncol=7)
497
498     mb.ok <- mbal.yesno[mbal.yesno[,1]==soil_order[ii] & mbal.
            yesno[,3]==mc_list[jj],]
499     for (kk in 1:20) {
500       is.na(tmp[tmp[,1]==kk,2:7]) <- ifelse(mb.ok[kk,4]==1,FALSE,
              TRUE)
501       is.na(tmp[tmp[,1]==kk,2:7]) <- is.nan(tmp[tmp[,1]==kk,2:7])
502     }
503
504     fcl <- prop.raw[prop.raw$SoilCode==soil_order[
            ii],]$Clay/100
505     fsl <- prop.raw[prop.raw$SoilCode==soil_order[ii],]$Silt/
            100
```

```
506         hv      <-  prop.raw[prop.raw$SoilCode==soil_order[ii], ]$HV
507
508         Dm      <-  1           #cm2/d
509         Dm      <-  Dm/24       #cm2/hr
510         radius  <-  exp(psize[psize[,1]==soil_order[ii],'MU'])    #um
511         radius  <-  radius/1e4
512         vd      <-  Dm/radius
513
514         mKp1    <-  fit.out[jj+nMC*(ii-1),4]
515         mKp2    <-  fit.out[jj+nMC*(ii-1),5]
516
517         tads    <-  c(2,48,240,720)
518
519         fd1      <-  1/(1+mKp1)
520         fd2      <-  1/(1+mKp2)
521
522         xFigs   <-  seq(0.1,0.9,length.out=6)
523         yFigs   <-  rev(seq(0.1,0.95,length.out=6))
524         out.mar <-  c(0,0,0,0)
525
526         mext.mod    <-  matrix(NA,ncol=1,nrow=4)
527         mext.obs    <-  matrix(NA,ncol=5,nrow=4)
528
529
530         for (kk in 1:4) {
531             par(fig=c(xFigs[kk],xFigs[kk+1],yFigs[jj+1],yFigs[jj]),mar=c
                    (0,0,0,0),new=ifelse(kk==1 & jj == 1,FALSE,TRUE))
532             plot(1,type='n',xlab='',ylab='',xlim=c(0,5.5),ylim=c(ylog
                    [1],ylog[2]),axes=F)
533
534             tpts=seq(c(2,48,240,720)[kk],c(2,48,240,720)[kk]+4,length.
                    out=5)
535             mod.soil    <-  fd1*two_layer_v2(tpts,tads[kk],fd1,fd2,vd,
                    fcl,fsl,hv,plt=FALSE)[,1]
536             obs.soil    <-  tmp[tmp[,1]>c(0,5,10,15)[kk] & tmp[,1]<c
                    (6,11,16,21)[kk],2:6]
537
538             mod.soil    <-  log10(mod.soil)
539             obs.soil    <-  log10(obs.soil)
540
541             is.na(obs.soil)    <-  !is.finite(obs.soil)
542
543             resids      <-  apply(obs.soil,1,'-',mod.soil)
544             for (ij in 1:5) {
545                 points(x=rep(ij,5),y=resids[ij,],pch=21,bg=NA)
546                 if (any(resids[ij,] > ylog[2],na.rm=T)) {
547                     arrows(x0=ij,y0=0.69897,y1=ylog[2]-0.05*ylog[2],
                            length=0.05)
548                     text(x=ij,y=0.6,labels=signif(min(resids[ij,resids[
                            ij,] > ylog[2]],na.rm=T),2),cex=0.5)}
549                 if (any(resids[ij,] < ylog[1],na.rm=T)) {
```

```
550                     arrows(x0=ij,y0=-0.69897,y1=ylog[1]+0.05*ylog[1],
                            length=0.05)
551                     text(x=ij,y=-0.6,labels=signif(max(resids[ij,resids[
                            ij,] < ylog[1]],na.rm=T),2),cex=0.5)}
552             }
553
554             abline(h=c(-0.69897,-0.30103,0,0.30103,0.69897),col='
                    cornflowerblue',lty=c(3,2,1,2,3))
555             abline(h=c(-1,1),col='black')
556
557             if (kk == 1) {
558                 if (linear) {
559                     axis(2,tcl=-0.25,las=2)
560                     mtext(side=2,at=0,outer=F,line=2.5,text=mc_list[jj])
561                 } else {
562                     #axis(2,at=log_axis(1e-4,1)[[1]],labels=F,tcl=-0.25)
563                     #axis(2,at=log_axis(1e-4,1)[[2]],labels=log_axis(1e
                            -4,1)[[3]],las=2)
564                     axis(2,at=c
                            (-1,-0.69897,-0.30103,0,0.30103,0.69897,1),
                            labels=c('1/10','1/5','1/2','1','2','5','10'),
                            las=2,cex.axis=0.75)
565                     mtext(side=2,at=1e-2,outer=F,line=2.5,text=mc_list[
                            jj])
566                 }
567             }
568             if (jj == nMC) {
569                 axis(1,at=seq(1,5,1),labels=c('A','D1','D2','D3','D4'))
570             }
571
572             mext.obs[kk,1:5]      <-  tmp[tmp[,1]>c(0,5,10,15)[kk] & tmp
                    [,1]<c(6,11,16,21)[kk],7]
573
574             Vaq =   5       #ml
575             ms  =   5       #g
576             Vhv =   hv
577             rho =   1.300   #g/mL
578
579             V1  =   (Vaq + fcl*(Vhv+ms/rho))
580             V2  =   (fsl*(Vhv+ms/rho))
581
582             h1  =   (Vaq + fcl*(Vhv+ms/rho))/(Vaq + Vhv + ms/rho -(1-fcl
                    -fsl)*(Vhv + ms/rho))
583             h2  =   (fsl*(Vhv+ms/rho))/(Vaq + Vhv + ms/rho -(1-fcl-fsl)*
                    (Vhv + ms/rho))
584             mod     <-  two_layer_v2(tpts,tads[kk],fd1,fd2,vd,fcl,fsl,hv
                    ,plt=FALSE)
585             mext.mod[kk,1]      <-  (1-fd1)*mod[5,1]*h1+mod[5,2]*h2
586         }
587         par(fig=c(xFigs[5],xFigs[6],yFigs[jj+1],yFigs[jj]),mar=c
                (0,0,0,0),new=TRUE)
```

```
588           plot(1,type='n',xlab='',ylab='',xlim=c(0,5),ylim=c(ylog[1],ylog
                  [2]),axes=F)
589
590           for (kk in 1:4) {
591               #log_mext     <-  apply(mext.obs,2,'-',mext.mod)
592
593               resd         <-  log10(mext.obs[kk,])-log10(mext.mod[kk])
594               is.na(resd) <-  !is.finite(resd)
595               resd         <-  ifelse(mext.obs[kk,]!=0,resd,0.5*ylog[2])
596
597               points(x=rep(kk,5),y=resd,pch=ifelse(mext.obs[kk,]!=0,21,8))
598
599               if (any(resd > ylog[2],na.rm=T)) {
600                   arrows(x0=kk,y0=0.69897,y1=ylog[2]-0.05*ylog[2],length
                          =0.05)
601                   text(x=kk,y=0.6,labels=signif(min(resd[resd > ylog[2]],
                          na.rm=T),2),cex=0.5)}
602               if (any(resd < ylog[1],na.rm=T)) {
603                   arrows(x0=kk,y0=-0.69897,y1=ylog[1]+0.05*ylog[1],length
                          =0.05)
604                   text(x=kk,y=-0.6,labels=signif(max(resd[resd < ylog[1]],
                          na.rm=T),2),cex=0.5)}
605           }
606
607           if (jj==nMC) {
608               axis(1,at=seq(1,4,1),labels=c('2hr','48hr','240hr','720hr'))
609           }
610           abline(h=c(-0.69897,-0.30103,0,0.30103,0.69897),col='
                  cornflowerblue',lty=c(3,2,1,2,3))
611
612           axis(4,at=c(-1,-0.69897,-0.30103,0,0.30103,0.69897,1),labels=c('
                  1/10','1/5','1/2','1','2','5','10'),las=2,cex.axis=0.75)
613
614           box()
615           if (jj == 3) {
616               mtext(side=3,at=(xFigs[1]+xFigs[5])/2,outer=T,line=-2,text='
                      Normalized␣Aq.')
617               mtext(side=3,at=(xFigs[5]+xFigs[6])/2,outer=T,line=-2,text='
                      Extraction')
618               mtext(side=4,at=0.5,outer=T,line=-1,text='log10(obs/mod)')
619           }
620           if (jj == nMC) {mtext(side=1,at=0.05,line=-2,text=soil_order[ii
                  ],outer=T)}
621       }
622   }
623   dev.off()
624
625   ## Plot resulting variables vs. foc
626   fit.out <-  read.table(paste('Two-Layer_optim_v5_logResid.csv',sep=''),
          header=TRUE,as.is=TRUE,stringsAsFactors=FALSE,sep=',')
627   yFigs   <-  rev(seq(0.1,0.95,length.out=4))
```

```
xFigs    <-   seq(0.1,0.95,length.out=6)

pdf(file='two_layer_fitparam_v5_logResid.pdf',paper='special',height=12,
    width=12,onefile=T)
for (jj in 1:nMC) {
    par(fig=c(xFigs[jj],xFigs[jj+1],yFigs[2],yFigs[1]),mar=c(0,0,0,0),
        new=ifelse(jj==1,FALSE,TRUE))
    plot(1,type='n',xlim=c(1e-4,0.3),ylim=c(1e-4,1e4),log='xy',axes=F)
    for (ii in 1:nSoil) {
        m    =    (5+soil_foc[soil_foc$SoilCode==soil_order[ii],]$HV)/7
        foc  =    soil_foc[soil_foc$SoilCode==soil_order[ii],]$TOC/100
        mKp  =    fit.out[jj+nMC*(ii-1),4]
        kp   =    mKp/0.6
        fd   =    1/(1+kp)
        points(x=foc,y=mKp,pch=21,col=collist[ii],bg=ifelse(mKp==10^-4 |
            mKp==10^4,NA,collist[ii]),cex=1.75)
    }
    box()
    if (jj==1) {
        mtext(side=2,at=(yFigs[2]+yFigs[1])/2,outer=T,line=-1,text='mKp_
            outer')
        axis(2,at=log_axis(1e-3,1e3)[[1]],labels=F,tcl=-0.4)
        axis(2,at=log_axis(1e-3,1e3)[[2]],labels=log_axis(1e-3,1e3)
            [[3]],tcl=-0.8,las=2)
    }

    par(fig=c(xFigs[jj],xFigs[jj+1],yFigs[3],yFigs[2]),mar=c(0,0,0,0),
        new=TRUE)
    plot(1,type='n',xlim=c(1e-4,0.3),ylim=c(1e-1,1),log='xy',axes=F)
    for (ii in 1:nSoil) {
        m    =    (5+soil_foc[soil_foc$SoilCode==soil_order[ii],]$HV)/7
        foc  =    soil_foc[soil_foc$SoilCode==soil_order[ii],]$TOC/100
        mKp[ii] =     fit.out[jj+nMC*(ii-1),4]
        kp   =    mKp/0.4
        fd   =    1/(1+kp)
        #h1   =     0.4+soil_foc$Clay*0.6/100
        #points(x=foc,y=h1,pch=21,col=collist[ii],bg=ifelse(mKp==10^-4 |
            mKp==10^4,NA,collist[ii]),cex=1.75)
    }
    foc  =    soil_foc$TOC/100
    h1   =         0.4+soil_foc$Clay*0.6/100
    h2   =    1-h1
    #vd   =    log10(h1)-log10(h2)
    points(x=foc,y=h1,pch=21,col=collist,bg=ifelse(mKp==10^-4 | mKp
        ==10^4,NA,collist),cex=1.75)
    box()
    if (jj==1) {
        mtext(side=2,at=(yFigs[3]+yFigs[2])/2,outer=T,line=-1,text='h1')
        axis(2,at=log_axis(1e-1,1e1)[[1]],labels=F,tcl=-0.4)
        axis(2,at=log_axis(1e-1,1e1)[[2]],labels=log_axis(1e-1,1e1)
            [[3]],tcl=-0.8,las=2)
```

```
670       }
671
672       par(fig=c(xFigs[jj],xFigs[jj+1],yFigs[4],yFigs[3]),mar=c(0,0,0,0),
              new=TRUE)
673       plot(1,type='n',xlim=c(1e-4,0.3),ylim=c(1e-1,1),log='xy',axes=F)
674       for (ii in 1:nSoil) {
675           m   =   (5+soil_foc[soil_foc$SoilCode==soil_order[ii],]$HV)/7
676           foc =    soil_foc[soil_foc$SoilCode==soil_order[ii],]$TOC/100
677           vd  =    fit.out[jj+nMC*(ii-1),6]
678           mKp[ii] =    fit.out[jj+nMC*(ii-1),4]
679           #points(x=foc,y=vd,pch=21,col=collist[ii],bg=ifelse(vd==10^-4 |
                  vd==10^3,NA,collist[ii]))
680       }
681       foc =    soil_foc$TOC/100
682       h1  =         0.4+soil_foc$Clay*0.6/100
683       h2  =    1-h1
684       #vd  =    log10(h1)-log10(h2)
685       points(x=foc,y=h2,pch=21,col=collist,bg=ifelse(mKp==10^-4 | mKp
              ==10^4,NA,collist),cex=1.75)
686       box()
687       axis(1,at=log_axis(1e-4,1)[[1]],labels=F,tcl=-0.4)
688       axis(1,at=log_axis(1e-4,1)[[2]],labels=log_axis(1e-4,1)[[3]],tcl
              =-0.8,las=2)
689       if (jj==1) {
690           mtext(side=2,at=(yFigs[4]+yFigs[3])/2,outer=T,line=-1,text='h2')
691           axis(2,at=log_axis(1e-1,1e1)[[1]],labels=F,tcl=-0.4)
692           axis(2,at=log_axis(1e-1,1e1)[[2]],labels=log_axis(1e-1,1e1)
                  [[3]],tcl=-0.8,las=2)
693           #axis(2)
694       }
695       mtext(side=3,at=(xFigs[jj]+xFigs[jj+1])/2,outer=T,line=-1.5,text=mc_
              list[jj])
696       mtext(side=1,at=(xFigs[jj]+xFigs[jj+1])/2,outer=T,line=-1.5,text='
              foc')
697   }
698   dev.off()
699
700   ## Plot residuals for each MC/soil combo
701   fit.out <-  read.table(paste('Two-Layer_optim_v5_logResid.csv',sep=''),
          header=TRUE,as.is=TRUE,stringsAsFactors=FALSE,sep=',')
702
703   xFigs   <-  c(0.1,0.95)
704   yFigs   <-  seq(0.95,0.1,length.out=6)
705   omar    <-  c(0,0,0,0)
706
707
708   pdf(file='two_layer_resids_v5_logResid.pdf',paper='special',width=10,
          height=8,onefile=T)
709   for (kk in 1:4) {
710       #sub.mc  <-  hplc.raw[hplc.raw$MC==mc_list[jj],]
711       for (jj in 1:nMC) {
```

```
712         par(fig=c(xFigs[1],xFigs[2],yFigs[jj+1],yFigs[jj]),mar=omar,new=
                ifelse(jj==1, FALSE, TRUE))
713         plot(1,type='n',ylim=c(-0.5,0.5),xlim=c(0,nSoil+1),axes=F,xlab='
                ',ylab='')
714
715         abline(h=0,col='cornflowerblue')
716         abline(h=c(-0.25,0.25),col='cornflowerblue',lty=2)
717
718         sub.tads    <-  hplc.raw[hplc.raw$MC==mc_list[jj] & hplc.raw$
                VIAL>(5*(kk-1)) & hplc.raw$VIAL<(1+5*kk),]
719         tads    =   c(2,48,240,720)[kk]
720         tpts    =   tads+c(-tads,0,1,2,3,4)
721         for (ii in 1:nSoil) {
722             sub.soil    <-  sub.tads[sub.tads$SOILCODE==soil_order[ii],]
723
724             #obs.soil    <-  sub.soil[,6:10]*sub.soil[,c('V.A','V.D1','V
                    .D2','V.D3','V.D4')]/sub.soil$MTOT
725
726             obs.soil    <-  matrix(c(sub.soil$A.C*sub.soil$V.A/sub.soil$
                    MTOT,
727                                      sub.soil$D1.C*sub.soil$V.D1/sub.
                                             soil$MTOT,
728                                      sub.soil$D2.C*sub.soil$V.D2/sub.
                                             soil$MTOT,
729                                      sub.soil$D3.C*sub.soil$V.D3/sub.
                                             soil$MTOT,
730                                      sub.soil$D4.C*sub.soil$V.D4/sub.
                                             soil$MTOT),ncol=5)
731             #is.na(obs.soil) <-  ifelse(obs.soil==0,TRUE,FALSE)
732
733             mb.ok   <-  mbal.yesno[mbal.yesno[,1]==soil_order[ii] & mbal
                    .yesno[,3]==mc_list[jj] & mbal.yesno[,2]>(5*(kk-1)) &
                    mbal.yesno[,2]<(1+5*kk),]
734             for (ij in 1:5) {
735                 is.na(obs.soil[ij,1:5]) <-  ifelse(mb.ok[ij,4]==1,FALSE,
                        TRUE)
736                 is.na(obs.soil[ij,])    <-  is.nan(obs.soil[ij,])
737             }
738             fcl         <-      prop.raw[prop.raw$SoilCode==soil_order[
                    ii], ]$Clay/100
739             fsl     <-  prop.raw[prop.raw$SoilCode==soil_order[ii], ]$
                    Silt/100
740             hv      <-  prop.raw[prop.raw$SoilCode==soil_order[ii], ]$HV
741
742             mKp1        <-  fit.out[jj+nMC*(ii-1),4]
743                 fd1     <-  1/(1+mKp1)
744             mKp2        <-  fit.out[jj+nMC*(ii-1),5]
745                 fd2     <-  1/(1+mKp2)
746
747             Dm      <-  1           #cm2/d
748             Dm      <-  Dm/24       #cm2/hr
```

```
749                 radius  <-  exp(psize[psize[,1]==soil_order[ii],'MU'])     #
                        um
750                 radius  <-  radius/1e4
751                 vd      <-  Dm/radius
752
753                 fd2 <-  fd1
754
755                 mod.soil    <-  fd1*two_layer_v2(tpts,tads,fd1,fd2,vd,fcl,
                        fsl,hv)[,1]
756
757                 resd        <-  log10(c(data.matrix(obs.soil))/rep(mod.soil
                        [2:6],5))
758                 #resd        <-  c(data.matrix(obs.soil)) - rep(mod.soil
                        [2:6],5)
759                 #is.na(resd)       <-  !is.finite(resd)
760
761                 colr        <-  ifelse(ii%%2==0,'grey70','white')
762                 bx  <-  boxplot(x=resd,add=TRUE,ylim=c(-2,2),xlim=c(0,nSoil
                        +1),at=ii,col=colr,axes=FALSE)
763                 if (!is.na(bx$stats[1,1])) {
764                     if (bx$stats[5,1]<=-2) {arrows(x0=ii,y0=-1,y1=-1.75,
                            length=0.1)}
765                     if (bx$stats[1,1]>=2) {arrows(x0=ii,y0=1,y1=1.75,length
                            =0.1)}
766                     text(x=ii,y=0.5,labels=bx$n,cex=0.5)
767                 }
768             }
769             axis(2,at=seq(-0.5,0.5,length.out=5),las=2)
770             mtext(side=2,at=(yFigs[jj+1]+yFigs[jj])/2,line=-2,outer=T,text=
                    mc_list[jj])
771         }
772         axis(1,at=seq(1,nSoil,1),labels=soil_order,las=2)
773         mtext(side=3,at=0.2,line=-1,text=paste('tads = ',c('2hr','48hr','240
                hr','720hr')[kk],sep=''),outer=T)
774         mtext(side=2,at=0.525,line=-1,text='log (obs / mod)',outer=T)
775         #mtext(side=2,at=0.525,line=-1,text='obs - mod',outer=T)
776     }
777     dev.off()
778
779     xFigs   <-  c(0.1,0.95)
780     yFigs   =   seq(0.95,0.1,length.out=nMC+1)
781     pdf(file='two_layer_overallresids_v5_logResid.pdf',paper='special',width
            =10,height=8,onefile=T)
782     for (jj in 1:nMC) {
783         sub.mc  <-  hplc.raw[hplc.raw$MC==mc_list[jj],]
784
785         par(fig=c(xFigs[1],xFigs[2],yFigs[jj+1],yFigs[jj]),mar=omar,new=
                ifelse(jj==1, FALSE, TRUE))
786         plot(1,type='n',ylim=c(-0.5,0.5),xlim=c(0,nSoil+1),axes=F,xlab='',
                ylab='')
787         abline(h=0,col='cornflowerblue')
```

```
788     abline(h=c(-0.5,0.5),col='cornflowerblue',lty=2)
789
790     for (ii in 1:nSoil) {
791         sub.soil    <- sub.mc[sub.mc$SOILCODE==soil_order[ii],]
792         mKp1        <- fit.out[jj+nMC*(ii-1),4]
793             fd1     <- 1/(1+mKp1)
794         mKp2        <- fit.out[jj+nMC*(ii-1),5]
795             fd2     <- 1/(1+mKp2)
796         #vd          <- 4e2
797         fd2 <- fd1
798
799         fcl             <-      prop.raw[prop.raw$SoilCode==soil_order[
                ii],]$Clay/100
800         fsl     <- prop.raw[prop.raw$SoilCode==soil_order[ii],]$Silt/
                100
801         hv      <- prop.raw[prop.raw$SoilCode==soil_order[ii],]$HV
802
803         Dm      <- 1            #cm2/d
804         Dm      <- Dm/24        #cm2/hr
805         radius  <- exp(psize[psize[,1]==soil_order[ii],'MU'])     #um
806         radius  <- radius/1e4
807         vd      <- Dm/radius
808
809         mod.soil    <- fd1*two_layer_v2(tpts,tads,fd1,fd2,vd,fcl,fsl,hv
                )[,1]
810
811         resd    <- c()
812
813         for (kk in 1:4) {
814             sub.tads    <- sub.soil[sub.soil$VIAL>(5*(kk-1)) & sub.soil
                    $VIAL<(1+5*kk),]
815             tads    =   c(2,48,240,720)[kk]
816             tpts    =   tads+c(-tads,0,1,2,3,4)
817
818             obs.soil    <- matrix(c(sub.tads$A.C*sub.tads$V.A/sub.tads$
                    MTOT,
819                                     sub.tads$D1.C*sub.tads$V.D1/sub.
                                        tads$MTOT,
820                                     sub.tads$D2.C*sub.tads$V.D2/sub.
                                        tads$MTOT,
821                                     sub.tads$D3.C*sub.tads$V.D3/sub.
                                        tads$MTOT,
822                                     sub.tads$D4.C*sub.tads$V.D4/sub.
                                        tads$MTOT),ncol=5)
823             mb.ok   <- mbal.yesno[mbal.yesno[,1]==soil_order[ii] & mbal
                    .yesno[,3]==mc_list[jj] & mbal.yesno[,2]>(5*(kk-1)) &
                    mbal.yesno[,2]<(1+5*kk),]
824             for (ij in 1:5) {
825                 is.na(obs.soil[ij,1:5]) <- ifelse(mb.ok[ij,4]==1,FALSE,
                        TRUE)
826                 is.na(obs.soil[ij,])    <- is.nan(obs.soil[ij,])
```

```
827                 }
828                 #tmp.res          <-    c(data.matrix(obs.soil))-rep(mod.soil
                        [2:6],5)
829                 tmp.res           <-  log10(c(data.matrix(obs.soil))/rep(mod.
                        soil[2:6],5))
830                 is.na(tmp.res)          <-  !is.finite(tmp.res)
831                 tmp.res <-  tmp.res[!is.na(tmp.res)]
832                 resd      <-  c(resd,tmp.res)
833
834           }
835
836           colr          <-  ifelse(ii%%2==0,'grey70','white')
837           bx  <-     boxplot(x=resd,add=TRUE,ylim=c(-2,2),xlim=c(0,nSoil+1)
                  ,at=ii,col=colr,axes=FALSE)
838           if  (!is.na(bx$stats[1,1])) {
839                 if  (bx$stats[5,1]<=-2) {arrows(x0=ii,y0=-1,y1=-1.75,length
                        =0.1)}
840                 if  (bx$stats[1,1]>=2) {arrows(x0=ii,y0=1,y1=1.75,length=0.1)
                        }
841                 text(x=ii,y=2,labels=bx$n,cex=0.5)
842           }
843       }
844       axis(2,at=c(-1,-0.5,0,0.5,1),las=2)
845       mtext(side=2,at=(yFigs[jj+1]+yFigs[jj])/2,line=-2,outer=T,text=mc_
              list[jj])
846 }
847 axis(1,at=seq(1,nSoil,1),labels=soil_order,las=2)
848 mtext(side=2,at=0.525,line=-1,text='log (obs / mod)',outer=T)
849 #mtext(side=2,at=0.525,line=-1,text='obs - mod',outer=T)
850 dev.off()
```

D.1.1 Lognormal distribution of particle sizes

```
1  dat_path      <-  '../data/'
2  out_path      <-  '../output/'
3  fig_path      <-  '../figs/'
4
5  prop.raw      <-  read.table(file=paste(dat_path,'soil_properties.csv',sep
       ='')),header=TRUE,stringsAsFactors=FALSE,sep=',',as.is=TRUE)
6
7  rho.clay=1.20 #g/cm3 =
8  rho.silt=1.28 #g/cm3
9  rho.sand=1.44 #g/cm3
10
11 mu=1.002e-3 #kg/m3
12 g=9.8        #m/s2
13 rho.f=1000   #kg/m3
14
15 R.p=function(rho.p,rho.f,g,mu,t,x) {
16       Rsq=(mu*9*x)/(g*2*t*(rho.p-rho.f))
17       R.p=sqrt(Rsq)
18       return(R.p)
```

```
}

erf <- function(x) 2 * pnorm(x * sqrt(2)) - 1

sigma=1
mu.x=1
x=1

ln.fit  <-  function(params,psize,obs) {
    mu.x=params[1]
    sigma=params[2]

    x1=psize[1]
    x2=psize[2]

    f1.obs=obs[1]
    f2.obs=obs[2]
    f3.obs=obs[3]

    f1=0.5*(1+erf((log(x1)-mu.x)/(sigma*sqrt(2))))
    f2=0.5*(1+erf((log(x2)-mu.x)/(sigma*sqrt(2))))-f1
    f3=1-0.5*(1+erf((log(x2)-mu.x)/(sigma*sqrt(2))))

    #f3=f3.obs

    ssq=(log10(f1/f1.obs))^2+(log10(f2/f2.obs))^2+(log10(f3/f3.obs))^2
    return(ssq)
}

pl.fit  <-  function(params,psize,obs) {
    mu.x=params[1]
    sigma=params[2]

    x1=psize[1]
    x2=psize[2]

    f1.obs=obs[1]
    f2.obs=obs[2]
    f3.obs=obs[3]

    f1=plnorm(x1, meanlog = mu.x, sdlog = sigma, lower.tail = TRUE, log.
        p = FALSE)
    f2=plnorm(x2, meanlog = mu.x, sdlog = sigma, lower.tail = TRUE, log.
        p = FALSE)-f1
    f3=plnorm(x2, meanlog = mu.x, sdlog = sigma, lower.tail = FALSE, log
        .p = FALSE)

    #f3=f3.obs

    ssq=(log10(f1/f1.obs))^2+(log10(f2/f2.obs))^2+(log10(f3/f3.obs))^2

```

```
67      return(ssq)
68  }
69
70
71  params=c(1,1)
72  lnorm.out    <-  matrix(NA,nrow=40,ncol=5)
73  for (ii in 1:dim(prop.raw)[1]) {
74      soil     <-  prop.raw[ii,'SoilCode']
75
76      # Fit lognorm probability with homebrew code
77      opt.fit=optim(par=params,fn=ln.fit,psize=c(4.47,88.7)),obs=c(prop.
            raw[ii,'Clay'],prop.raw[ii,'Silt'],prop.raw[ii,'Sand'])/100,
            method='L-BFGS-B',hessian=FALSE,control=list(maxit=300))
78
79      # Fit lognorm probability with r plnorm function
80      opt.fit2=optim(par=params,fn=pl.fit,psize=c(4.47,88.7),obs=c(prop.
            raw[ii,'Clay'],prop.raw[ii,'Silt'],prop.raw[ii,'Sand'])/100,
            method='L-BFGS-B',hessian=FALSE,control=list(maxit=300))
81
82      mu  <-  opt.fit2$par[1]
83      sig <-  opt.fit2$par[2]
84      mu.df   <-  opt.fit2$par[1]-opt.fit$par[1]
85      sig.df  <-  opt.fit2$par[2]-opt.fit$par[2]
86
87      lnorm.out[ii,1] <-  match(soil,prop.raw[order(prop.raw$TOC),1])
88      lnorm.out[ii,2] <-  mu
89      lnorm.out[ii,3] <-  sig
90      lnorm.out[ii,4] <-  mu.df
91      lnorm.out[ii,5] <-  sig.df
92  }
93
94  colnames(lnorm.out) <-  c('SOILORDERNUM','MU','SIGMA','deltaMU','
        deltaSIGMA')
95  write.table(x=lnorm.out[order(lnorm.out[,1]),],file=paste(out_path,'
        lnorm_fit.csv',sep=''),sep=',',quote=FALSE,row.names=FALSE,col.names
        =FALSE)
96  prop.raw    <-  prop.raw[prop.raw$Set != 'D' & prop.raw$SoilCode !='GAS'
         & prop.raw$SoilCode !='ELL' & prop.raw$SoilCode !='BU' & prop.raw$
        SoilCode !='CM' ,]
97  write.table(x=prop.raw[order(prop.raw$TOC),1],file=paste(out_path,'
        unique_soils_v3.csv',sep=''),sep=',',quote=FALSE,row.names=FALSE,col
        .names=FALSE)
```

D.2 n-layer model

```
1
2   graphics.off()
3   rm(list=ls(all=TRUE))
4
5   name    <-  'nParticle'
6   vrs     <-  'v1'
7
```

```
8  dat_path    <-  '../data/'
9  out_path    <-  '../output/'
10 fig_path    <-  '../figs/'
11 txt_path    <-  '../text/'
12
13 ## ## functions ## ##
14
15 # Steps:    1)  determine eigenvectors (evec) and eigenvalues (evl)
16 #           2)  form fundamental matrix solution (evec * diag(exp(evl*t
       =0))) for initial state
17 #           3)  find inverse of eigenvalues (solve(evl))
18 #           4)  matrix exponential is evec*diag(exp(evl))*solve(evl)
19 #               i.e. V*D*inv(V)
20 #           5)  solve the matrix subject to C0 = c(1,0)
21 #           6)  reform V*D*inv(V) where D is evaluated at t
22 #           7)  Solution*c(t=0) yields the answer at t
23
24 mat_exp_solve <- function(eig,a,t,tzero,ct1) {
25
26     evec    <-  eig$vectors
27     evl     <-  eig$values
28     ptm <-  proc.time()
29     i_evec  <-  solve(evec)
30     d       <-  diag(exp(evl*0))
31     exptmp  <-  evec%*%d%*%i_evec
32
33     crat    <-  solve(exptmp,c(ct1,rep(0,dim(d)[1]-1)))
34
35     #ptm<-proc.time()
36     exp_at  <-  matrix(NA,nc=(dim(a)[1]+1),nr=length(t))
37     for (ii in 1:length(t)) {
38         d               <-  diag(exp(evl*(t[ii]-tzero)))
39         exptmp          <-  evec%*%d%*%i_evec
40         exp_at[ii,1]    <-  ifelse(t[ii]<=tzero,0,t[ii])
41         for (jj in 2:(dim(a)[2]+1)) {
42             exp_at[ii,jj] <-  ifelse(t[ii]<=tzero,c(0,0),c(exptmp%*%crat
                  )[jj-1])
43         }
44     }
45     #print(proc.time()-ptm)
46     return(exp_at)
47 }
48
49 nPart_full  <-  function(mx,tZero,dt1=0.1,doplot=FALSE) {
50     eig     <-  eigen(mx)
51
52     # Generates full series for plotting etc
53     c_EXPM          <-  mat_exp_solve(eig,mx,seq(0,730,dt1),-1,1)
54     cOut.series     <-  matrix(NA,nc=5,nr=length(seq(0,730,dt1)))
55     cOut.series[,1] <-  seq(0,730,dt1)
56
```

```
57      for (ii in 1:4) {
58          # First superposition(D1)
59          ct.0            <-  c_EXPM
60          cd.A            <-  ct.0[match(tZero[ii,1],ct.0[,1]),2]
61          cs.A            <-  mat_exp_solve(eig,mx,seq(0,730,dt1),tZero[ii
                ,1],-cd.A)
62          ct.A            <-  matrix(c(ct.0[,1],ct.0[,2]+cs.A[,2]),nc=2)
63
64          # Second Superposition(d2)
65          cd.1            <-  ct.A[match(tZero[ii,2],ct.A[,1]),2]
66          cs.1            <-  mat_exp_solve(eig,mx,seq(0,730,dt1),tZero[ii
                ,2],-cd.1)
67          ct.1            <-  matrix(c(ct.A[,1],ct.A[,2]+cs.1[,2]),nc=2)
68
69          # Third superposition(D3)
70          cd.2            <-  ct.1[match(tZero[ii,3],ct.1[,1]),2]
71          cs.2            <-  mat_exp_solve(eig,mx,seq(0,730,dt1),tZero[ii
                ,3],-cd.2)
72          ct.2            <-  matrix(c(ct.1[,1],ct.1[,2]+cs.2[,2]),nc=2)
73
74          # Fourth superposition(D4)
75          cd.3            <-  ct.2[match(tZero[ii,4],ct.2[,1]),2]
76          cs.3            <-  mat_exp_solve(eig,mx,seq(0,730,dt1),tZero[ii
                ,4],-cd.3)
77          ct.3            <-  matrix(c(ct.2[,1],ct.2[,2]+cs.3[,2]),nc=2)
78
79          cOut.series[,ii+1]  <-  ct.3[,2]
80      }
81      return(cOut.series)
82  }
83
84  ssq_calc_v1 <-  function(mod,obs,linear=FALSE,onlyads,hybrid=TRUE,weight
        =5) {
85
86      log.mod         <-  log10(mod)
87      log.obs         <-  log10(obs)
88
89      is.na(log.mod)  <-  !is.finite(log.mod)
90      is.na(log.obs)  <-  !is.finite(log.obs)
91
92      if (onlyads) {
93          print('ads')
94          log.ssq         <-  sum((log.obs[,1]-log.mod[,1])^2,na.rm=T)
95          lin.ssq         <-  sum((obs[,1]-mod[,1])^2,na.rm=T)
96      } else {
97          if (hybrid) {
98              print('hybrid')
99              log.ssq <-  sum((obs[,1]-mod[,1])^2,na.rm=T) + sum((log.obs-
                    log.mod)^2,na.rm=T)
100         } else {
101             print('normal')
```

```
102                 log.ssq          <-  sum((log.obs-log.mod)^2,na.rm=T)
103                 lin.ssq          <-  sum((obs-mod)^2,na.rm=T)
104             }
105         }
106
107         logads  <-  weight*sum((log.obs[,1]-log.mod[,1])^2,na.rm=T)
108         logdes  <-  sum((log.obs[,2:dim(log.obs)[1]]-log.mod[,2:dim(log.mod)
                [1]])^2,na.rm=T)
109
110         #ssq             <-  ifelse(linear,lin.ssq,log.ssq)
111         ssq     <-  sum(logads,logdes,na.rm=T)
112         return(ssq)
113     }
114
115     ssq_calc_v2 <-  function(mod,obs,weight=5) {
116
117         log.mod         <-  log10(mod)
118         log.obs         <-  log10(obs)
119
120         is.na(log.mod)  <-  !is.finite(log.mod)
121         is.na(log.obs)  <-  !is.finite(log.obs)
122
123         logads  <-  weight*sum((log.obs[,1]-log.mod[,1])^2,na.rm=T)
124         logdes  <-  sum((log.obs[,2:dim(log.obs)[2]]-log.mod[,2:dim(log.mod)
                [2]])^2,na.rm=T)
125
126         ssq     <-  sum(logads,logdes,na.rm=T)
127         return(ssq)
128     }
129
130     # n-Particle model
131     # To simplify, Q = D*A/l for that interface, allows for varying D/A/L
            based on particle fraction
132     mc.soil_fit <-  function(V,Q,pars,nP,obs.caq=c(),doplot=FALSE) {
133         mKp <-  10^pars
134         fd  <-  rep(1/(1+mKp),nP)
135
136
137         # Construct matrix
138         mx  <-  matrix(0,nc=(nP+1),nr=(nP+1))
139         # ii is rows
140         for (ii in 1:(nP+1)) {
141             # jj is columns
142             for (jj in 2:(nP+1)) {
143                 if (ii == 1) {
144                     mx[ii,jj]   <-  Q[jj-1]*fd[jj-1]*V[jj]/V[ii]
145                     mx[ii,1]    <-  mx[ii,1]-Q[jj-1]*V[jj]/V[ii]
146                 } else if (ii == jj) {
147                     mx[ii,jj]   <-  -Q[jj-1]*fd[jj-1]*V[jj]/V[ii]
148                     mx[ii,1]    <-  mx[ii,1]+Q[jj-1]*V[jj]/V[ii]
149                 } else {
```

```
150                     mx[ii,jj]=0
151                 }
152             }
153         }
154         ## Need to include particle specific fd term
155         #mx=mx*vd*fd
156 
157         # Times to zero the aqueous bulk concentration
158         t.0      <-  matrix(c
                (2,48,240,720,3,49,241,721,4,50,242,722,5,51,243,723,6,52,244,724)
                ,nr=4)
159         mod.caq <-  matrix(NA,nc=5,nr=20)
160 
161         #ptm=proc.time()
162         tmp=nPart_full(mx,t.0,doplot=doplot)
163         #rtime    <-  proc.time()-ptm
164         #print(rtime)
165 
166         for (ii in 1:4) {
167             mod.caq[(1+5*(ii-1)):(5*ii),]  <-  matrix(rep(c(tmp[match(t.0[ii
                    ,],tmp[,1]),ii+1]),5),byrow=T,ncol=5)
168         }
169 
170         if (doplot) {
171             par(mfrow=c(2,2),mar=c(0,0,0,0),oma=c(4,4,1,1))
172             for (ii in 1:4) {
173                 plot(1,type='n',xlim=c(t.0[ii,1]-2,t.0[ii,5]+2),ylim=c(0,1),
                        xlab='',ylab='',axes=F)
174                 lines(x=tmp[,1],y=tmp[,ii+1])
175                 if (length(obs.caq!=0)){
176                     points(x=matrix(rep(t.0[ii,],5),nc=5,byrow=T),y=c(obs.
                            caq[(1+5*(ii-1)):(5*ii),]),pch=21)
177                 }
178                 if (ii > 2) {
179                     axis(1,las=2)
180                 }
181                 if (ii == 1 || ii == 3) {
182                     axis(2,las=2)
183                 }
184             }
185         }
186 
187 
188         if (length(obs.caq)!=0) {
189             ssq =   ssq_calc_v2(mod.caq,obs.caq)
190             return(ssq)
191         } else {
192             return(mod.caq)
193         }
194     }
195 
```

```
196 soil_fit     <-  function(V,Q,fd,nP,obs.caq=c()) {
197     ## BUILD THIS ONE!
198 }
199
200 ## ##      end    ## ##
201
202 ## Data Fitting ##
203
204 # Read data
205 hplc.raw     <-  read.table(paste(dat_path,'hplc_data.csv', sep=''),
        header=TRUE, stringsAsFactor=FALSE,sep=',',as.is=TRUE)
206 prop.raw     <-  read.table(file=paste(dat_path,'soil_properties.csv',sep
        ='')),header=TRUE,stringsAsFactors=FALSE,sep=',',as.is=TRUE)
207 mbal.yesno  <-  read.table(file=paste(dat_path,'MB_yesno_v1.csv',sep='')
        ,sep=',',as.is=TRUE,stringsAsFactors=FALSE)
208 psize    <-  read.table(file=paste(dat_path,'lnorm_fit.csv',sep='')),sep='
        ,',as.is=TRUE,stringsAsFactors=FALSE)
209     colnames(psize) <-  c('SOIL','MU','SIGMA','deltaMU','deltaSIGMA')
210
211 soil_order  <-  prop.raw[prop.raw[,1] %in% unique(hplc.raw[,2]),]
212 soil_order  <-  soil_order[order(soil_order$TOC),]
213 nSoil       <-  length(soil_order$SoilCode)
214 mc_order    <-  c('HMX','RDX','NG','TNT','DNT')
215 nMC         <-  length(mc_order)
216
217 vList   <-  matrix(c(1, 6, 11, 16, 2, 7, 12, 17, 3, 8, 13, 18, 4, 9, 14,
        19, 5, 10, 15, 20),ncol=4,byrow=T)
218
219 # Get normalization constants
220 hplc.raw$MTOT   <-  hplc.raw$A.C*hplc.raw$V.A+
221                     hplc.raw$D1.C*hplc.raw$V.D1+
222                     hplc.raw$D2.C*hplc.raw$V.D2+
223                     hplc.raw$D3.C*hplc.raw$V.D3+
224                     hplc.raw$D4.C*hplc.raw$V.D4+
225                     hplc.raw$E1.C*hplc.raw$V.E1+
226                     hplc.raw$E2.C*hplc.raw$V.E2+
227                     hplc.raw$E3.C*hplc.raw$V.E3
228
229 hplc.raw$M.EXT  <-  hplc.raw$E1.C*hplc.raw$V.E1+
230                     hplc.raw$E2.C*hplc.raw$V.E2+
231                     hplc.raw$E3.C*hplc.raw$V.E3
232
233 ## First iteration is fitting soil/MC pairs
234 # Matrix output is nP+4 (MC,Soil,runtime,ssq,K[i])
235
236 nP = 5
237 fit.out <-  matrix(NA,nc=5,nr=nMC*nSoil)
238 for (ii in 1:nMC) {
239     for (jj in 1:nSoil) {
240         print(paste('mc - ',ii,' - soil - ',jj,sep=''))
```

```
241         sub.obs      <-  hplc.raw[hplc.raw$SOILCODE==soil_order$SoilCode[
                jj] & hplc.raw$MC==mc_order[ii],]
242
243         norm.obs     <-  matrix(c(sub.obs[,'MC'],sub.obs[,'VIAL'],
244                                   sub.obs$A.C*sub.obs$V.A/sub.obs$MTOT,
245                                   sub.obs$D1.C*sub.obs$V.D1/sub.obs$MTOT,
246                                   sub.obs$D2.C*sub.obs$V.D2/sub.obs$MTOT,
247                                   sub.obs$D3.C*sub.obs$V.D3/sub.obs$MTOT,
248                                   sub.obs$D4.C*sub.obs$V.D4/sub.obs$MTOT,
249                                   sub.obs$M.EXT/sub.obs$MTOT),ncol=8)
250
251         # # TEST CASE - KA/HMX - Backderived variables!
252         # h1  =   0.860063
253         # h2  =   0.139937
254         # V   =   c(h1,h2)
255         # A   =   c(1,1)
256         # fd  =   rep(1/(1+0.4118911),2)
257         # vd  =   0.03325975
258         # Q   =   vd*A
259         # ## Split into nP particle sizes
260         # nP = 5
261         ## Determine l. l is average? diffusive length for that particle
                class?
262             #   determine l from fractions of norm distribution!
263             mu       <-  psize[psize[,1]==soil_order$SoilCode[jj],'MU']
264             sigma    <-  psize[psize[,1]==soil_order$SoilCode[jj],'SIGMA'
                    ]
265
266             breaks   =   seq(0,1,length.out=nP+2)
267             breaks   =   breaks[2:(length(breaks)-1)]
268
269             l.part   <-  qlnorm(breaks,mu,sigma)/2e4          #   cm
270         ## A is surface area for single particle * f_particle_class * n_
                total particles
271             # A = 4 pi r^2
272             A.part   <-  4*pi*l.part^2                        #   cm^2
273         ## Calculate V's for each particle size
274             # V = 4/3 pi r^3
275             V.part   <-  A.part*l.part/3                      #   cm^3
276             AonV     <-  A.part/V.part                        #   cm^2/cm
                    ^3
277             V.aq     <-  5                                    #   mL =
                    cm^3
278             V.p      <-  breaks*5/2.6                         #   fraction
                    of total particulate volume in each size bin *** BIG
                    ASSUMPTION - Density is constant in all size fracs...
279             V        <-  c(V.aq,V.p)
280         # D is a set constant (second iteration should allow model to
                fit this...)
281             D    =   1                                       #   cm^2/d
282             D    =   D/24                                    #   cm^2/hr
```

```
283             ## Determine 'Q' for each particle size
284                 # Q = D*A/l
285                 Q    =    D*AonV/l.part                                    #    cm^3/hr
286             ## submit fit to optim
287             theta = 0.5
288
289             obs.num <-   matrix(as.numeric(norm.obs[,3:7]),nr=20)
290
291             # Not sure yet... but extremely slow get timing
292             ptm <- proc.time()
293             opt.fit <-   optim(par=theta,fn=mc.soil_fit,V=V,Q=Q,nP=nP,doplot=
                    FALSE,obs.caq=obs.num,control=list(maxit=100),method='Brent'
                    ,lower=-9,upper=2)
294             mc.soil_fit(V,Q,opt.fit$par,nP,obs.num,TRUE)
295             rtime    <-   proc.time() - ptm
296
297             fit.out[nSoil*(ii-1)+jj,]    <-   c(soil_order$SoilCode[jj],mc_
                    order[ii],rtime[3],opt.fit$value,opt.fit$par)
298         }
299     }
300
301     write.table(x=fit.out,file=paste(dat_path,'nParticle_v1.csv',sep='')),sep
        =',')
```

Appendix E

DATA TABLES

E.1 Column experiment

Data was analyzed at the University of Delaware. Data consists of chloride, RDX and TNT aqueous concentrations for 48 hrs. Following this are extractions of the column every 2 cm.

Column Name	*Description*	*Units*
Depth	Column depth	[cm]
M_{RDX}	Mass of RDX in Extraction	[μg]
M_{TNT}	Mass of TNT in Extraction	[μg]
t	Experimental time	[h]
C_{Cl}	Chloride concentration	$[mg/L]$
C_{RDX}	RDX concentration	$[mg/L]$
C_{TNT}	TNT concentration	$[mg/L]$

Table E.1: Column experiment concentrations

t	C_{Cl}	C_{RDX}	C_{TNT}
0.0	0.000	0.000	0.000
0.5	0.000	0.000	0.000
1.0	0.000		
2.0	0.985	0.865	0.000
3.0	9.205		
4.0	10.413	2.253	0.000
5.0	12.033		
6.0	10.025	4.663	1.250
8.0		5.361	2.406
10.0		5.498	3.227
12.0	10.049	5.572	3.763
14.0		5.606	4.189
16.0		5.655	4.518
18.0	10.203	5.729	4.855
20.0		5.675	5.046
22.0		5.683	5.142
24.0	10.288	5.717	5.252
25.0	10.537		
26.0	10.117	5.704	5.521
27.0	6.480		
28.0	1.698	4.295	5.539
29.0	1.114		
30.0	0.000	1.681	4.781
32.0	0.000	0.971	3.871
34.0		0.601	3.214
36.0	0.000	0.404	2.827
38.0		0.304	2.507
40.0		0.266	2.100
42.0	0.000	0.230	2.077
44.0		0.214	1.911
46.0		0.203	1.801
48.0	0.000	0.194	1.657

Table E.2: Extracted concentrations by depth

Depth	M_{RDX}	M_{TNT}
0-2	10.006	29.067
0-2	9.899	28.981
2-4	8.202	35.684
2-4	8.168	35.860
4-6	9.393	28.350
4-6	9.573	27.971
6-8	*	*
6-8	*	*
8-10	27.012	30.412
8-10	26.931	30.526

E.2 Batch experiment

E.2.1 Soils used

Soils used in the 25 Soil Sequential Desorption experiment.

Soil Code	*Soil Name*
AM	Anne Messex
B	Massachusetts Military Reservation B
BA	Aberdeen BA
BOX	Boxtel
BT	Aberdeen Bti
BU	Boontown Union
CM	Chile Muestra
ELL	Elliot IE
FT	Ft. McClellen
GUA	Guadalajara
H	Houthalien
J	Joplin
KA	Kaolinite
LCL	Lewis Clean
LCO	Lewis Core
M	Matapeake
N	Nevada
P	Pahokee Peat
PO	Pokomoke
R	Rhydtalog
SOU	Souli
SSL1	Sassafras 1
SSL2	Sassafras 2
SSL3	Sassafras 3
ST	Scitico
W	Whippany
W1	Washington 1
W2	Washington 2
Z	Zegveld

E.2.2 General soil properties

Properties for studied soils. Analysis performed by Plant and Soil Science Department at University of Delaware except where noted.

Column Name	*Description*	*Units*
Soil	Soil Code - See list of soils	[–]
pH	Measured pH	[–]
Buffer	Buffer solution pH	[–]
CEC	Cation Exchange Capacity at pH 7.0	$[^{meq}/_{100g}]$
CaEx	Exchangable Ca	$[^{meq}/_{100g}]$
KEx	Exchangable K	$[^{meq}/_{100g}]$
MgEx	Exchangable Mg	$[^{meq}/_{100g}]$
NaEx	Exchangable Na	$[^{meq}/_{100g}]$
Sand	Fraction sand	[%]
Silt	Fraction silt	[%]
Clay	Fraction clay	[%]
TN	Total Nitrogen	[%]
TC	Total Carbon	[%]
TOC	Total organic carbon	[%]
Cs	Cesium sites* (* Performed by R. Gonzalez)	$[^{mg}/_{kg}]$
FeOx	Oxalate extractable iron* (* Performed by R. Gonzalez)	$[^{mg}/_{kg}]$
Class	Textural class: S - Sand L - Loam C - Clay T - Silt	

Table E.3: Soil properties

Soil	pH	Buffer	CEC	CaEx	Kex	MgEx	NaEx	Sand	Silt	Clay	TN	TC	TOC	Cs	FeOx	Class
AM	6.30	7.74	13.20	5.74	0.72	2.13	0.10	47.40	40.40	12.10	0.229	2.660	2.300	7.400		L
B	4.30	7.68	2.50	0.06	0.03	0.04	0.08	53.50	30.30	16.20	0.015	0.290	0.240	3.188	1.471E+03	SL
BA	5.50	7.85	3.80	1.28	0.07	0.82	0.15	69.60	14.20	16.20	0.013	0.160	0.160	3.313	2.209E+03	SL
BOX	5.40	7.76	11.00	6.58	0.38	1.40	0.19	71.50	18.30	10.20	0.245	2.570	2.320	6.593	5.001E+03	SL
BT	4.80	7.89	1.90	0.58	0.06	0.40	0.13	83.80	7.10	9.10	0.005	0.070	0.070	1.967	1.314E+03	SL
BU	4.70	7.13	20.80	1.58	1.69	0.49	1.90	53.30	34.50	12.20	0.396	6.060	6.000			SL
CM	6.60	7.81	21.00	16.40	0.38	2.02	0.26	55.10	30.60	14.30	0.119	1.280	1.200	8.556	7.083E+03	SL
ELL	6.30	7.62	20.40	12.73	0.52	4.49	0.14	9.60	53.40	37.00	0.281	3.170	2.860	12.624		LCT
FT	3.80	7.03	11.00	0.15	0.07	0.08	0.13	37.00	24.40	38.60	0.022	0.380	0.310	3.503	1.044E+02	LC
GUA	8.00	8.00	11.60	27.94	0.34	1.08	0.14	51.50	30.30	18.20	0.086	3.380	2.330	8.467		L
H	3.90	7.52	2.90	0.14	0.04	0.05	0.11	85.90	10.10	4.00	0.095	2.460	2.310	2.986	5.017E+02	SL
J	6.50	7.81	43.80	28.10	0.51	2.74	0.14	29.50	51.80	18.70	0.522	10.990	10.120	17.486	3.436E+03	LT
KA								4.00	26.00	70.00	0.012	0.040	0.040			LCT
LCL	5.10	7.08	31.40	2.20	0.11	0.23	0.23	64.70	27.00	8.30	0.409	6.670	6.360	10.526	6.130E+03	SL
LCO	5.60	7.03	37.20	5.54	0.06	0.75	0.27	59.90	33.80	6.30	0.484	7.980	7.590	13.483	7.269E+03	SL
M	5.70	7.76	9.90	4.53	0.58	1.74	0.66	20.90	56.80	22.30	0.155	1.780	1.540	6.742	2.304E+03	LT
N	3.40	4.23	11.20	69.33	0.01	7.53	0.16	45.50	33.50	20.90	0.034	0.210	0.200	7.204	1.887E+03	L
P								80.00	9.00	11.00	3.420	47.430	28.130			SL
PO	4.50	7.42	13.10	1.64	0.24	0.43	0.14	71.80	17.10	11.10	0.231	3.910	3.500			SL
R	5.00	7.21	35.90	7.51	0.39	1.43	0.58	43.80	43.70	12.50	0.562	13.350	12.830	9.974	1.526E+03	L
SOU	6.90	7.79	16.10	12.93	0.44	1.57	0.09	42.40	14.40	43.20	0.074	0.740	0.610	9.307	1.596E+03	C
SSL1	4.40	7.52	8.50	1.39	0.26	0.57	0.06	52.90	30.70	16.40	0.230	1.820	1.630	4.447	1.120E+03	SL
SSL2	4.50	7.46	8.80	1.37	0.25	0.57	0.08	49.70	32.20	18.10	0.153	1.450	1.350	4.364		L
SSL3	4.40	7.65	5.00	1.44	0.29	0.48	0.09	53.40	28.30	18.20	0.099	0.980	0.970	4.305	1.364E+03	SL
ST	5.40	7.55	10.20	5.62	0.11	2.79	0.27	20.60	44.80	34.60	0.134	1.920	1.770			LC
W	5.90	7.76	15.50	8.08	0.07	2.56	0.21	14.80	62.90	22.30	0.144	2.060	1.750	6.220	2.496E+03	LT
W1	6.90	7.87	17.80	11.11	0.31	5.00	0.17	8.30	67.30	24.50	0.088	0.770	0.630	6.753		LT
W2	6.90	7.93	20.30	11.37	0.36	4.68	0.15	11.10	64.60	24.20	0.071	0.600	0.680	6.671		LT
Z	4.80	6.80	54.80	21.31	1.25	3.33	0.39	45.80	32.50	21.70	2.148	20.350	18.230	28.232	1.195E+04	L

E.2.3 Trace metal analysis using USEPA 3051

Properties for studied soils. Analysis performed by Plant and Soil Science Department at University of Delaware using EPA method 3051 for microwave digestion.

Column Name	*Description*	*Units*
Soil	Soil Code - See list of soils	[–]
Al	Al content determined by microwave digestion	$[^{mg}/_{kg}]$
Ca	Ca content determined by microwave digestion	$[^{mg}/_{kg}]$
Fe	Fe content determined by microwave digestion	$[^{mg}/_{kg}]$
K	K content determined by microwave digestion	$[^{mg}/_{kg}]$
Mg	Mg content determined by microwave digestion	$[^{mg}/_{kg}]$
Mn	Mn content determined by microwave digestion	$[^{mg}/_{kg}]$
Na	Na content determined by microwave digestion	$[^{mg}/_{kg}]$

Table E.4: Trace metal analysis

Soil	Al	Ca	Fe	K	Mg	Mn	Na
AM	9.14E+03	1.37E+03	1.19E+04	906	886	304	15.4
B	1.03E+04	66.5	9.51E+03	320	1.17E+03	85.8	15.1
BA	7.27E+03	379	1.28E+04	604	1.2E+03	88.9	41.6
BOX	5.76E+03	2.1E+03	1.16E+04	582	937	269	57.1
BT	7.59E+03	158	9.39E+03	684	1.04E+03	59.2	15.2
BU	1.55E+04	966	1.42E+04	1.12E+03	1.43E+03	1.29E+03	334
C	4.22E+03	82.3	4.79E+03	159	180	16.4	15.2
CM	1.41E+04	5.98E+03	2.52E+04	1.36E+03	6.14E+03	652	310
D	1.12E+04	916	1.49E+04	578	2.92E+03	328	29.1
ELL	1.04E+04	3.73E+03	1.92E+04	1.7E+03	2.75E+03	811	29.7
FT	1.41E+04	34.2	3.99E+04	2.21E+03	469	30.7	9.23
GAS	4.28E+03	1.37E+04	5.16E+03	131	3.01E+03	66.7	1.36E+03
GUA	1.06E+04	7.81E+04	1.1E+04	1.9E+03	3.1E+03	152	50
H	711	41.5	1.62E+03	35.7	25.7	3.32	1.17
J	1.03E+04	1.26E+04	2.15E+04	958	1.62E+03	484	56
K	5.06E+03	1.41E+03	6.72E+03	253	589	99.8	38.6
KA							
LCL	2.75E+04	2.78E+03	1.94E+04	495	4.53E+03	575	97.2
LCO	2.76E+04	3.7E+03	2.23E+04	393	3.47E+03	591	134
M	1.81E+04	1.4E+03	1.8E+04	1.08E+03	2.02E+03	373	136
MT	6.49E+03	1.42E+03	2.81E+04	2.64E+03	2.31E+03	327	361
MW	6.93E+03	974	6.25E+03	516	745	149	17.6
N	6.44E+03	1.41E+04	3.41E+04	2.22E+03	1.83E+03	220	116
NOT	4.21E+03	481	9.79E+03	728	1.21E+03	101	27.4
P							
PAX	1.47E+04	1.58E+03	1.67E+04	727	2.43E+03	317	59.1
PO	5.04E+03	469	794	250	151	16.3	20.6
R	2.28E+03	2.37E+03	2.79E+03	369	264	113	30.2
SOU	1.48E+04	3.03E+03	3E+04	1.3E+03	915	910	46.6
SSL1	1.05E+04	373	1.35E+04	634	1.14E+03	83	16.2
SSL2	9.12E+03	340	1.29E+04	519	1.06E+03	73.7	11.4
SSL3	8.92E+03	413	1.26E+04	401	774	716	6.87
ST	2.04E+04	2.42E+03	2.95E+04	2.79E+03	7.57E+03	668	162
T	1.59E+04	1E+04	2.48E+04	1.61E+03	7.01E+03	830	471
W	1.07E+04	2.07E+03	1.18E+04	211	1.98E+03	108	132
W1	1.43E+04	3.82E+03	2.08E+04	1.48E+03	4.73E+03	552	93.2
W2	1.36E+04	3.15E+03	1.89E+04	1.5E+03	4.18E+03	432	84.4
Z	2.14E+04	1.14E+04	1.97E+04	3.25E+03	3.47E+03	389	180

E.2.4 25 soil sequential desorption experiment

This experiment consisted of 4 adsorption times followed by 4 sequential desorptions. Desorptions were performed at intervals of 1, 12, 24, 72 or 720 hrs. Extractions were not performed so sorbed concentrations, q_i, are reported by difference.

Column Name	*Description*	*Units*
MC	Munition Constituent	[–]
S	Sorbent - See list of soils	[–]
t_{Ads}	Length of adsorption time	[hrs]
t_{Des}	Length of desorption time	[hrs]
C_{CTRL}	Aqueous concentration of control	$[^{mg}/_{L}]$
C_A	Aqueous concentration after adsorption	$[^{mg}/_{L}]$
C_{D1}	Aqueous concentration after desorption 1	$[^{mg}/_{L}]$
C_{D2}	Aqueous concentration after desorption 2	$[^{mg}/_{L}]$
C_{D3}	Aqueous concentration after desorption 3	$[^{mg}/_{L}]$
C_{D4}	Aqueous concentration after desorption 4	$[^{mg}/_{L}]$
q_A	Soil concentration after adsorption	$[^{mg}/_{kg}]$
q_{D1}	Soil concentration after desorption 1	$[^{mg}/_{kg}]$
q_{D2}	Soil concentration after desorption 2	$[^{mg}/_{kg}]$
q_{D3}	Soil concentration after desorption 3	$[^{mg}/_{kg}]$
q_{D4}	Soil concentration after desorption 4	$[^{mg}/_{kg}]$
M_{CTRL}	Mass of MC in the control sample	$[\mu g]$
M_{CA}	Dissolved mass after adsorption	$[\mu g]$
M_{D1}	Dissolved mass after desorption 1	$[\mu g]$
M_{D2}	Dissolved mass after desorption 2	$[\mu g]$
M_{D3}	Dissolved mass after desorption 3	$[\mu g]$
M_{D4}	Dissolved mass after desorption 4	$[\mu g]$
M_{QA}	Sorbed mass after adsorption (by difference)	$[\mu g]$
M_{Q1}	Sorbed mass after desorption 1 (by difference)	$[\mu g]$
M_{Q2}	Sorbed mass after desorption 2 (by difference)	$[\mu g]$
M_{Q3}	Sorbed mass after desorption 3 (by difference)	$[\mu g]$
M_{Q4}	Sorbed mass after desorption 4 (by difference)	$[\mu g]$
K_P	Partition coefficient	$[^{L}/_{kg}]$

Table E.5: **Concentration data for 25 soil experiment**

MC	S	t_{Ads}	C_{CTRL}	C_A	C_{D1}	C_{D2}	C_{D3}	C_{D4}	q_A	q_{D1}	q_{D2}	q_{D3}	q_{D4}
D	AM	2	1.07e+01	2.64e+00	1.52e+00	1.15e+00	9.25e-01	7.42e-01	1.21e+01	1.04e+01	9.15e+00	8.14e+00	7.36e+00
D	AM	2	1.08e+01	2.43e+00	1.38e+00	1.06e+00	8.59e-01	7.22e-01	1.22e+01	1.07e+01	9.58e+00	8.64e+00	7.88e+00
D	AM	2	2.05e+01	5.98e+00	3.49e+00	2.49e+00	1.94e+00	1.59e+00	2.34e+01	1.96e+01	1.70e+01	1.49e+01	1.33e+01
D	AM	2	1.87e+01	5.09e+00	2.90e+00	2.15e+00	NA	1.36e+00	NA	NA	NA	1.31e+01	1.17e+01
D	AM	2	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
D	AM	48	1.07e+01	2.13e+00	1.51e+00	1.21e+00	0.00e+00	7.72e-01	1.29e+01	1.13e+01	1.00e+01	1.00e+01	9.23e+00
D	AM	48	1.08e+01	2.10e+00	1.51e+00	1.24e+00	1.58e+00	7.86e-01	1.43e+01	1.27e+01	1.14e+01	9.72e+00	8.91e+00
D	AM	48	2.05e+01	4.41e+00	3.09e+00	2.39e+00	1.85e+00	1.52e+00	2.78e+01	2.45e+01	2.19e+01	2.00e+01	1.85e+01
D	AM	48	1.85e+01	3.69e+00	2.69e+00	2.08e+00	NA	1.31e+00	NA	NA	NA	1.41e+01	1.28e+01
D	AM	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	NA	0.00e+00	NA	NA	NA	0.00e+00	0.00e+00
D	AM	240	1.07e+01	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	8.95e-02	8.95e-02	8.95e-02	8.95e-02	8.95e-02
D	AM	240	1.07e+01	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
D	AM	240	2.00e+01	3.40e-01	3.49e-01	3.07e-01	0.00e+00	2.24e-01	2.70e+00	2.34e+00	2.02e+00	2.02e+00	1.78e+00
D	AM	240	1.84e+01	0.00e+00	1.05e-01	NA	0.00e+00	0.00e+00	NA	NA	2.77e-01	2.77e-01	2.77e-01
D	AM	240	0.00e+00	NA	0.00e+00	0.00e+00	NA	NA	NA	NA	NA	NA	0.00e+00
D	AM	720	1.07e+01	1.71e+00	1.21e+00	1.00e+00	8.19e-01	6.46e-01	1.08e+01	9.44e+00	8.40e+00	7.50e+00	6.80e+00
D	AM	720	1.06e+01	1.68e+00	1.21e+00	9.86e-01	8.15e-01	6.62e-01	1.15e+01	1.01e+01	9.11e+00	8.21e+00	7.50e+00
D	AM	720	2.04e+01	4.03e+00	2.88e+00	2.23e+00	1.82e+00	1.44e+00	2.11e+01	1.80e+01	1.57e+01	1.37e+01	1.22e+01
D	AM	720	1.85e+01	2.82e+00	1.98e+00	1.16e-01	1.05e-01	1.00e+00	6.12e+00	3.96e+00	3.84e+00	3.72e+00	2.66e+00
D	AM	720	0.00e+00	0.00e+00	0.00e+00	NA	NA	0.00e+00	NA	NA	NA	0.00e+00	0.00e+00
D	B	2	1.13e+01	8.43e+00	2.74e+00	NA	NA	NA	NA	NA	NA	NA	0.00e+00
D	B	2	1.16e+01	8.53e+00	2.76e+00	NA	NA	NA	NA	NA	NA	NA	0.00e+00
D	B	2	2.19e+01	1.61e+01	5.72e+00	NA	NA	NA	NA	NA	NA	NA	0.00e+00
D	B	2	2.01e+01	1.49e+01	4.86e+00	NA	NA	NA	NA	NA	NA	NA	0.00e+00
D	B	2	0.00e+00	0.00e+00	0.00e+00	NA	NA	NA	NA	NA	NA	NA	0.00e+00
D	B	48	1.14e+01	9.85e+00	2.69e+00	1.08e+00	5.33e-01	3.04e-01	5.21e+00	2.44e+00	1.31e+00	7.61e-01	4.40e-01
D	B	48	1.15e+01	8.10e+00	2.72e+00	1.05e+00	5.29e-01	3.09e-01	5.78e+00	2.95e+00	1.85e+00	1.31e+00	9.80e-01
D	B	48	1.91e+01	1.42e+01	5.45e+00	2.16e+00	1.06e+00	6.19e-01	1.13e+01	5.55e+00	3.26e+00	2.20e+00	1.53e+00
D	B	48	1.93e+01	1.20e+01	3.95e+00	1.21e+00	7.67e-01	5.56e-01	7.31e+00	3.30e+00	2.03e+00	1.26e+00	6.67e-01
D	B	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
D	B	240	1.15e+01	7.51e+00	2.76e+00	1.13e+00	6.36e-01	2.70e-01	6.72e+00	3.40e+00	1.98e+00	1.30e+00	1.02e+00
D	B	240	1.12e+01	7.40e+00	2.84e+00	1.12e+00	5.82e-01	2.90e-01	6.72e+00	3.41e+00	1.99e+00	1.37e+00	1.06e+00
D	B	240	2.25e+01	1.49e+01	5.51e+00	2.23e+00	1.22e+00	5.46e-01	1.33e+01	6.83e+00	4.02e+00	2.70e+00	2.12e+00
D	B	240	1.93e+01	1.14e+01	4.25e+00	1.88e+00	0.00e+00	2.86e-01	7.53e+00	2.51e+00	3.07e-01	3.07e-01	0.00e+00
D	B	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	NA	0.00e+00	NA	NA	NA	1.28e+00	1.28e+00
D	B	720	1.18e+01	6.81e+00	2.99e+00	1.35e+00	3.98e-01	1.41e-01	5.72e+00	2.59e+00	1.13e+00	7.19e-01	5.61e-01
D	B	720	1.18e+01	7.26e+00	3.12e+00	1.34e+00	3.49e-01	1.07e-01	5.56e+00	2.41e+00	9.50e-01	5.90e-01	4.74e-01
D	B	720	2.29e+01	1.59e+01	5.91e+00	2.35e+00	5.01e-01	1.84e-01	1.01e+01	3.97e+00	1.45e+00	9.21e-01	7.20e-01
D	B	720	2.05e+01	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
D	B	720	0.00e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00

Table E.5 – continued from previous page

MC	S	t_{Ads}	C_{CTRL}	C_A	C_{D1}	C_{D2}	C_{D3}	C_{D4}	q_A	q_{D1}	q_{D2}	q_{D3}	q_{D4}
D	BA	2	1.18e+01	8.77e+00	2.97e+00	1.14e+00	5.10e-01	3.22e-01	5.74e+00	2.68e+00	1.46e+00	9.23e-01	6.01e-01
D	BA	2	1.18e+01	8.78e+00	2.97e+00	1.14e+00	5.17e-01	3.29e-01	5.66e+00	2.64e+00	1.41e+00	8.67e-01	5.49e-01
D	BA	2	2.26e+01	1.70e+01	5.65e+00	2.14e+00	9.62e-01	5.75e-01	1.05e+01	4.76e+00	2.47e+00	1.46e+00	8.72e-01
D	BA	2	2.04e+01	1.56e+01	5.14e+00	1.99e+00	8.69e-01	5.38e-01	9.81e+00	4.55e+00	2.41e+00	1.48e+00	9.29e-01
D	BA	2	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
D	BA	48	1.19e+01	8.00e+00	3.13e+00	1.36e+00	6.19e-01	3.90e-01	6.45e+00	3.25e+00	1.83e+00	1.17e+00	7.60e-01
D	BA	48	1.19e+01	7.74e+00	3.14e+00	1.35e+00	6.23e-01	3.90e-01	6.04e+00	2.78e+00	1.36e+00	7.02e-01	2.94e-01
D	BA	48	2.30e+01	1.57e+01	5.98e+00	2.48e+00	1.09e+00	6.72e-01	1.20e+01	5.87e+00	3.23e+00	2.08e+00	1.37e+00
D	BA	48	2.03e+01	1.46e+01	5.42e+00	2.32e+00	1.03e+00	6.34e-01	1.10e+01	5.37e+00	2.94e+00	1.86e+00	1.20e+00
D	BA	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
D	BA	240	1.19e+01	7.41e+00	2.97e+00	NA	6.82e-01	3.17e-01	NA	NA	2.12e+00	1.43e+00	1.09e+00
D	BA	240	1.19e+01	7.23e+00	3.00e+00	1.49e+00	7.18e-01	3.48e-01	7.04e+00	3.97e+00	2.39e+00	1.65e+00	1.28e+00
D	BA	240	2.28e+01	1.51e+01	5.88e+00	2.72e+00	1.26e+00	6.00e-01	1.16e+01	5.46e+00	2.57e+00	1.27e+00	6.26e-01
D	BA	240	2.04e+01	1.32e+01	5.28e+00	2.50e+00	1.20e+00	5.89e-01	1.25e+01	7.08e+00	4.42e+00	3.21e+00	2.57e+00
D	BA	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
D	BA	720	1.15e+01	7.60e+00	3.03e+00	1.36e+00	6.16e-01	3.01e-01	6.24e+00	3.05e+00	1.61e+00	9.36e-01	6.19e-01
D	BA	720	1.15e+01	7.85e+00	3.08e+00	1.35e+00	6.23e-01	2.97e-01	6.53e+00	3.31e+00	1.86e+00	1.18e+00	8.67e-01
D	BA	720	2.19e+01	1.56e+01	5.97e+00	2.71e+00	1.14e+00	5.64e-01	1.25e+01	6.05e+00	3.35e+00	2.12e+00	1.52e+00
D	BA	720	1.99e+01	1.40e+01	5.39e+00	2.24e+00	1.04e+00	5.16e-01	1.10e+01	5.11e+00	2.77e+00	1.64e+00	1.09e+00
D	BA	720	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
D	BOX	2	1.03e+01	3.33e+00	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
D	BOX	2	1.06e+01	3.13e+00	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
D	BOX	2	2.02e+01	6.72e+00	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
D	BOX	2	1.83e+01	5.87e+00	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
D	BOX	2	0.00e+00	0.00e+00	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
D	BOX	48	1.04e+01	NA	1.43e+00	1.13e+00	9.14e-01	7.56e-01	8.82e+00	7.30e+00	6.09e+00	5.11e+00	4.31e+00
D	BOX	48	1.04e+01	2.34e+00	1.52e+00	1.13e+00	9.11e-01	7.45e-01	9.03e+00	7.42e+00	6.22e+00	5.24e+00	4.45e+00
D	BOX	48	1.76e+01	4.45e+00	3.22e+00	2.43e+00	1.85e+00	0.00e+00	1.60e+01	1.27e+01	1.01e+01	8.17e+00	8.17e+00
D	BOX	48	1.73e+01	4.70e+00	2.01e+00	1.86e+00	7.78e-01	9.60e-01	1.18e+01	9.74e+00	7.76e+00	6.95e+00	5.93e+00
D	BOX	48	0.00e+00	NA	0.00e+00	0.00e+00	0.00e+00	NA	NA	NA	NA	NA	0.00e+00
D	BOX	240	1.05e+01	2.48e+00	1.77e+00	2.22e+00	9.63e-01	7.61e-01	1.22e+01	1.00e+01	7.06e+00	6.05e+00	5.24e+00
D	BOX	240	1.04e+01	2.60e+00	1.74e+00	0.00e+00	1.01e+00	7.56e-01	9.38e+00	7.22e+00	7.22e+00	6.17e+00	5.35e+00
D	BOX	240	2.04e+01	5.22e+00	3.54e+00	2.56e+00	1.95e+00	1.52e+00	2.09e+01	1.65e+01	1.31e+01	1.11e+01	9.44e+00
D	BOX	240	1.72e+01	3.98e+00	2.57e+00	NA	1.25e+00	8.75e-01	NA	NA	1.06e+01	9.34e+00	8.40e+00
D	BOX	240	0.00e+00	0.00e+00	0.00e+00	NA	0.00e+00	0.00e+00	NA	NA	0.00e+00	0.00e+00	0.00e+00
D	BOX	720	1.07e+01	2.33e+00	1.75e+00	1.35e+00	5.79e-01	3.56e-01	7.94e+00	6.10e+00	4.64e+00	4.05e+00	3.66e+00
D	BOX	720	1.07e+01	2.32e+00	1.74e+00	1.38e+00	5.65e-01	3.85e-01	8.16e+00	6.35e+00	4.85e+00	4.27e+00	3.85e+00
D	BOX	720	2.04e+01	4.84e+00	3.60e+00	2.69e+00	1.48e+00	1.01e+00	1.64e+01	1.27e+01	9.76e+00	8.24e+00	7.13e+00
D	BOX	720	1.83e+01	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
D	BOX	720	0.00e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00

Table E.5 – continued from previous page

MC	S	t_{Ads}	C_{CTRL}	C_A	C_{D1}	C_{D2}	C_{D3}	C_{D4}	q_A	q_{D1}	q_{D2}	q_{D3}	q_{D4}
D	BT	2	1.18e+01	9.18e+00	2.85e+00	9.98e-01	4.27e-01	2.62e-01	5.12e+00	2.09e+00	1.03e+00	5.74e-01	3.03e-01
D	BT	2	1.18e+01	9.23e+00	2.91e+00	1.03e+00	4.44e-01	2.73e-01	5.34e+00	2.29e+00	1.20e+00	7.20e-01	4.38e-01
D	BT	2	2.28e+01	1.77e+01	5.46e+00	1.88e+00	7.72e-01	4.50e-01	9.56e+00	3.89e+00	1.90e+00	1.09e+00	6.23e-01
D	BT	2	2.06e+01	1.61e+01	5.21e+00	1.85e+00	7.84e-01	4.59e-01	9.33e+00	3.93e+00	1.98e+00	1.15e+00	6.66e-01
D	BT	2	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
D	BT	48	1.18e+01	8.31e+00	2.91e+00	1.17e+00	4.87e-01	3.17e-01	5.55e+00	2.59e+00	1.37e+00	8.67e-01	5.29e-01
D	BT	48	1.18e+01	8.80e+00	2.93e+00	1.18e+00	4.88e-01	3.10e-01	6.48e+00	3.55e+00	2.33e+00	1.82e+00	1.50e+00
D	BT	48	2.27e+01	1.70e+01	5.56e+00	2.21e+00	8.94e-01	5.30e-01	1.01e+01	4.56e+00	2.24e+00	1.30e+00	7.52e-01
D	BT	48	2.04e+01	1.52e+01	4.97e+00	2.04e+00	8.87e-01	5.35e-01	9.23e+00	4.28e+00	2.20e+00	1.27e+00	7.17e-01
D	BT	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	NA	NA	NA	NA	NA	0.00e+00
D	BT	240	1.20e+01	7.86e+00	2.77e+00	1.24e+00	5.04e-01	2.21e-01	5.59e+00	2.74e+00	1.42e+00	8.96e-01	6.68e-01
D	BT	240	1.20e+01	7.93e+00	2.77e+00	1.24e+00	5.15e-01	2.26e-01	5.65e+00	2.79e+00	1.48e+00	9.71e-01	7.33e-01
D	BT	240	2.30e+01	1.63e+01	5.26e+00	2.19e+00	8.66e-01	3.77e-01	1.01e+01	4.74e+00	2.43e+00	1.56e+00	1.16e+00
D	BT	240	2.07e+01	1.45e+01	4.92e+00	2.14e+00	8.64e-01	3.92e-01	1.01e+01	4.95e+00	2.62e+00	1.76e+00	1.35e+00
D	BT	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
D	BT	720	1.15e+01	8.04e+00	2.80e+00	1.09e+00	4.63e-01	2.03e-01	5.21e+00	2.24e+00	1.17e+00	6.49e-01	4.39e-01
D	BT	720	1.14e+01	8.27e+00	2.84e+00	1.17e+00	4.93e-01	NA	NA	NA	NA	NA	3.11e-01
D	BT	720	2.20e+01	1.62e+01	5.48e+00	2.17e+00	9.03e-01	3.99e-01	1.01e+01	4.73e+00	2.48e+00	1.50e+00	1.09e+00
D	BT	720	1.98e+01	1.44e+01	4.90e+00	1.90e+00	7.79e-01	3.68e-01	8.80e+00	3.90e+00	2.03e+00	1.19e+00	8.02e-01
D	BT	720	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
D	BU	2	1.08e+01	1.21e+00	3.75e-01	NA	NA	NA	NA	NA	NA	NA	0.00e+00
D	BU	2	1.12e+01	1.05e+00	3.51e-01	NA	NA	NA	NA	NA	NA	NA	0.00e+00
D	BU	2	2.13e+01	2.45e+00	8.91e-01	NA	NA	NA	NA	NA	NA	NA	0.00e+00
D	BU	2	1.95e+01	1.92e+00	7.18e-01	NA	NA	NA	NA	NA	NA	NA	0.00e+00
D	BU	2	0.00e+00	0.00e+00	0.00e+00	NA	NA	NA	NA	NA	NA	NA	0.00e+00
D	BU	48	9.40e+00	4.58e-01	7.85e-02	9.96e-02	1.14e-01	1.56e-01	1.03e+01	1.02e+01	1.01e+01	9.98e+00	9.82e+00
D	BU	48	9.48e+00	3.90e-01	1.88e-01	7.87e-02	8.80e-02	1.26e-01	1.06e+01	1.04e+01	1.03e+01	1.02e+01	1.01e+01
D	BU	48	1.91e+01	9.59e-01	3.33e-01	2.96e-01	3.12e-01	3.63e-01	2.06e+01	2.02e+01	1.99e+01	1.96e+01	1.92e+01
D	BU	48	1.83e+01	5.85e-01	0.00e+00	0.00e+00	0.00e+00	0.00e+00	1.87e+01	1.87e+01	1.87e+01	1.87e+01	1.87e+01
D	BU	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
D	BU	240	1.11e+01	2.11e-01	1.94e-01	1.84e-01	1.83e-01	1.50e-01	1.20e+01	1.17e+01	1.15e+01	1.13e+01	1.11e+01
D	BU	240	1.11e+01	2.27e-01	2.02e-01	1.83e-01	1.67e-01	1.54e-01	1.21e+01	1.19e+01	1.17e+01	1.15e+01	1.13e+01
D	BU	240	2.15e+01	5.84e-01	4.89e-01	4.76e-01	0.00e+00	3.82e-01	2.21e+01	2.15e+01	2.10e+01	2.10e+01	2.06e+01
D	BU	240	1.88e+01	3.62e-01	3.35e-01	2.73e-01	2.04e-01	1.81e-01	1.73e+01	1.68e+01	1.66e+01	1.64e+01	1.62e+01
D	BU	240	0.00e+00	0.00e+00	NA	0.00e+00	0.00e+00	0.00e+00	NA	0.00e+00	0.00e+00	0.00e+00	0.00e+00
D	BU	720	1.11e+01	1.16e-01	1.13e-01	NA	0.00e+00	0.00e+00	NA	NA	7.68e+00	7.68e+00	7.68e+00
D	BU	720	1.11e+01	1.08e-01	1.13e-01	NA	0.00e+00	0.00e+00	NA	NA	7.49e+00	7.49e+00	7.49e+00
D	BU	720	2.15e+01	3.29e-01	2.79e-01	NA	1.18e-01	1.09e-01	NA	NA	1.59e+01	1.58e+01	1.57e+01
D	BU	720	1.93e+01	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
D	BU	720	0.00e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00

Table E.5 – continued from previous page

MC	S	t_{Ads}	C_{CTRL}	C_A	C_{D1}	C_{D2}	C_{D3}	C_{D4}	q_A	q_{D1}	q_{D2}	q_{D3}	q_{D4}
D	CM	2	1.00e+01	4.03e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA
D	CM	2	1.01e+01	3.82e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA
D	CM	2	1.90e+01	8.19e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA
D	CM	2	1.74e+01	7.11e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA
D	CM	2	0.00e+00	0.00e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA
D	CM	48	1.01e+01	2.16e+00	1.53e+00	1.05e+00	7.90e-01	6.67e-01	NA	NA	NA	NA	NA
D	CM	48	1.02e+01	2.14e+00	1.46e+00	1.07e+00	7.88e-01	6.44e-01	NA	NA	NA	NA	NA
D	CM	48	1.97e+01	5.06e+00	3.18e+00	2.22e+00	1.69e+00	1.40e+00	NA	NA	NA	NA	NA
D	CM	48	1.70e+01	4.61e+00	2.29e+00	1.28e+00	7.12e-01	8.64e-01	NA	NA	NA	NA	NA
D	CM	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	NA	NA	NA	NA	NA
D	CM	240	9.97e+00	2.81e+00	1.72e+00	1.31e+00	9.57e-01	7.27e-01	NA	NA	NA	NA	NA
D	CM	240	1.03e+01	2.82e+00	1.76e+00	1.31e+00	9.50e-01	7.26e-01	NA	NA	NA	NA	NA
D	CM	240	2.00e+01	6.26e+00	3.79e+00	2.75e+00	1.94e+00	1.43e+00	NA	NA	NA	NA	NA
D	CM	240	1.71e+01	4.72e+00	2.74e+00	1.91e+00	1.26e+00	8.68e-01	NA	NA	NA	NA	NA
D	CM	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	NA	NA	NA	NA	NA
D	CM	720	1.03e+01	2.28e+00	1.66e+00	4.06e-01	3.84e-01	2.88e-01	NA	NA	NA	NA	NA
D	CM	720	1.03e+01	2.40e+00	1.69e+00	4.20e-01	4.34e-01	3.08e-01	NA	NA	NA	NA	NA
D	CM	720	1.98e+01	5.38e+00	3.62e+00	9.36e-01	1.21e+00	8.76e-01	NA	NA	NA	NA	NA
D	CM	720	1.65e+01	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
D	CM	720	0.00e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
D	ELL	2	1.08e+01	2.18e+00	1.17e+00	9.18e-01	7.43e-01	6.17e-01	1.09e+01	9.67e+00	8.72e+00	7.91e+00	7.26e+00
D	ELL	2	1.08e+01	2.19e+00	1.23e+00	9.24e-01	7.76e-01	6.50e-01	1.11e+01	9.72e+00	8.79e+00	7.93e+00	7.25e+00
D	ELL	2	2.07e+01	5.03e+00	2.78e+00	2.03e+00	1.67e+00	1.32e+00	2.11e+01	1.80e+01	1.59e+01	1.41e+01	1.27e+01
D	ELL	2	1.88e+01	4.24e+00	2.35e+00	1.80e+00	1.42e+00	1.17e+00	1.93e+01	1.67e+01	1.49e+01	1.33e+01	1.21e+01
D	ELL	2	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
D	ELL	48	1.08e+01	1.43e+00	1.06e+00	8.70e-01	7.12e-01	6.00e-01	1.19e+01	1.09e+01	9.97e+00	9.17e+00	8.54e+00
D	ELL	48	1.08e+01	1.42e+00	1.13e+00	9.08e-01	7.56e-01	6.27e-01	1.24e+01	1.12e+01	1.03e+01	9.43e+00	8.78e+00
D	ELL	48	2.06e+01	3.41e+00	2.62e+00	1.90e+00	1.67e+00	1.40e+00	2.27e+01	2.00e+01	1.80e+01	1.62e+01	1.47e+01
D	ELL	48	1.86e+01	2.76e+00	2.09e+00	1.61e+00	1.32e+00	1.09e+00	1.91e+01	1.69e+01	1.52e+01	1.37e+01	1.26e+01
D	ELL	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
D	ELL	240	1.12e+01	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	1.15e+00	1.15e+00	1.15e+00	1.15e+00	1.15e+00
D	ELL	240	1.10e+01	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	1.03e+00	1.03e+00	1.03e+00	1.03e+00	1.03e+00
D	ELL	240	2.11e+01	6.82e-02	1.62e-01	1.57e-02	1.15e-02	0.00e+00	2.34e+00	2.17e+00	2.15e+00	2.14e+00	2.14e+00
D	ELL	240	1.90e+01	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	5.19e-01	5.19e-01	5.19e-01	5.19e-01	5.19e-01
D	ELL	240	0.00e+00	NA	NA	0.00e+00	NA	NA	NA	NA	NA	NA	0.00e+00
D	ELL	720	1.07e+01	1.12e+00	8.01e-01	6.69e-01	5.63e-01	4.81e-01	1.00e+01	9.16e+00	8.43e+00	7.84e+00	7.32e+00
D	ELL	720	1.06e+01	1.14e+00	8.01e-01	6.68e-01	5.78e-01	4.42e-01	9.26e+00	8.43e+00	7.69e+00	7.08e+00	6.60e+00
D	ELL	720	2.02e+01	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
D	ELL	720	1.82e+01	9.37e-02	1.51e+00	1.21e+00	0.00e+00	7.59e-01	1.15e+01	9.89e+00	8.58e+00	8.58e+00	7.74e+00
D	ELL	720	0.00e+00	NA	NA	NA	NA	0.00e+00	NA	NA	NA	0.00e+00	0.00e+00

Table E.5 – continued from previous page

MC	S	t_{Ads}	C_{CTRL}	C_A	C_{D1}	C_{D2}	C_{D3}	C_{D4}	q_A	q_{D1}	q_{D2}	q_{D3}	q_{D4}
D	FT	2	1.07e+01	7.90e+00	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
D	FT	2	1.07e+01	7.94e+00	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
D	FT	2	2.07e+01	1.53e+01	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
D	FT	2	1.90e+01	1.39e+01	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
D	FT	2	0.00e+00	0.00e+00	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
D	FT	48	9.06e+00	6.17e+00	2.96e+00	1.35e+00	8.10e-01	3.66e-01	6.35e+00	3.22e+00	1.80e+00	9.70e-01	5.78e-01
D	FT	48	9.22e+00	6.16e+00	2.91e+00	1.36e+00	8.04e-01	4.00e-01	6.18e+00	3.17e+00	1.71e+00	8.73e-01	4.29e-01
D	FT	48	1.84e+01	1.32e+01	5.96e+00	2.69e+00	1.29e+00	0.00e+00	1.20e+01	5.83e+00	2.96e+00	1.65e+00	1.65e+00
D	FT	48	1.75e+01	1.16e+01	4.55e+00	1.65e+00	9.09e-01	3.22e-01	9.00e+00	4.39e+00	2.63e+00	1.69e+00	1.33e+00
D	FT	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
D	FT	240	1.05e+01	7.39e+00	3.16e+00	1.31e+00	7.12e-01	3.30e-01	7.79e+00	3.96e+00	2.18e+00	1.43e+00	1.08e+00
D	FT	240	1.06e+01	7.27e+00	3.13e+00	1.34e+00	7.36e-01	3.27e-01	7.74e+00	3.96e+00	2.14e+00	1.36e+00	1.01e+00
D	FT	240	2.07e+01	1.46e+01	6.26e+00	2.66e+00	1.43e+00	6.62e-01	1.49e+01	7.48e+00	3.85e+00	2.34e+00	1.64e+00
D	FT	240	1.75e+01	1.25e+01	4.81e+00	1.91e+00	8.40e-01	4.57e-01	1.05e+01	4.75e+00	2.20e+00	1.30e+00	8.01e-01
D	FT	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
D	FT	720	1.08e+01	7.19e+00	3.23e+00	1.58e+00	4.11e-01	1.91e-01	6.00e+00	2.63e+00	9.16e-01	4.68e-01	2.66e-01
D	FT	720	1.08e+01	7.20e+00	3.31e+00	1.36e+00	3.96e-01	1.89e-01	5.73e+00	2.31e+00	8.51e-01	4.19e-01	2.20e-01
D	FT	720	2.08e+01	1.48e+01	6.34e+00	2.55e+00	9.93e-01	3.44e-01	1.14e+01	4.74e+00	1.97e+00	8.89e-01	5.25e-01
D	FT	720	1.89e+01	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
D	FT	720	0.00e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
D	GAS	2	1.04e+01	1.88e-01	2.91e-02	NA	NA	NA	NA	NA	NA	NA	0.00e+00
D	GAS	2	1.04e+01	1.04e-01	1.89e-02	NA	NA	NA	NA	NA	NA	NA	0.00e+00
D	GAS	2	2.01e+01	1.69e-01	9.22e-02	NA	NA	NA	NA	NA	NA	NA	0.00e+00
D	GAS	2	1.82e+01	2.02e-01	7.99e-02	NA	NA	NA	NA	NA	NA	NA	0.00e+00
D	GAS	2	0.00e+00	0.00e+00	0.00e+00	NA	NA	NA	NA	NA	NA	NA	0.00e+00
D	GAS	48	1.05e+01	2.50e-02	0.00e+00	0.00e+00	0.00e+00	1.64e-02	9.48e+00	9.48e+00	9.48e+00	9.48e+00	9.46e+00
D	GAS	48	1.04e+01	1.43e-02	0.00e+00	0.00e+00	0.00e+00	1.44e-02	8.98e+00	8.98e+00	8.98e+00	8.98e+00	8.97e+00
D	GAS	48	2.00e+01	5.94e-02	3.41e-02	3.59e-02	3.84e-02	4.27e-02	1.77e+01	1.77e+01	1.77e+01	1.76e+01	1.76e+01
D	GAS	48	1.70e+01	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	1.61e+01	1.61e+01	1.61e+01	1.61e+01	1.61e+01
D	GAS	48	0.00e+00	0.00e+00	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
D	GAS	240	1.03e+01	3.79e-02	3.11e-02	3.10e-02	4.01e-02	3.58e-02	9.64e+00	9.61e+00	9.57e+00	9.53e+00	9.49e+00
D	GAS	240	1.03e+01	3.27e-02	2.82e-02	2.38e-02	2.44e-02	2.84e-02	9.01e+00	8.98e+00	8.95e+00	8.93e+00	8.90e+00
D	GAS	240	1.98e+01	1.01e-01	7.03e-02	7.16e-02	5.72e-02	6.31e-02	1.77e+01	1.77e+01	1.76e+01	1.75e+01	1.74e+01
D	GAS	240	1.73e+01	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	1.52e+01	1.52e+01	1.52e+01	1.52e+01	1.52e+01
D	GAS	240	0.00e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
D	GAS	720	1.06e+01	0.00e+00	0.00e+00	1.23e+00	1.59e-02	0.00e+00	7.39e+00	7.39e+00	6.04e+00	6.03e+00	6.03e+00
D	GAS	720	1.06e+01	0.00e+00	0.00e+00	1.19e+00	1.84e-02	0.00e+00	6.80e+00	6.80e+00	5.50e+00	5.48e+00	5.48e+00
D	GAS	720	2.07e+01	0.00e+00	2.93e-02	2.62e+00	3.68e-02	0.00e+00	1.58e+01	1.57e+01	1.29e+01	1.28e+01	1.28e+01
D	GAS	720	1.85e+01	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
D	GAS	720	0.00e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00

Table E.5 – continued from previous page

MC	S	t_{Ads}	C_{CTRL}	C_A	C_{D1}	C_{D2}	C_{D3}	C_{D4}	q_A	q_{D1}	q_{D2}	q_{D3}	q_{D4}
D	GUA	2	1.11e+01	6.74e+00	2.91e+00	1.48e+00	8.35e-01	4.75e-01	6.78e+00	3.75e+00	2.25e+00	1.35e+00	8.75e-01
D	GUA	2	1.11e+01	6.84e+00	2.72e+00	1.49e+00	8.33e-01	4.88e-01	6.71e+00	3.87e+00	2.37e+00	1.48e+00	1.03e+00
D	GUA	2	2.15e+01	1.34e+01	5.68e+00	2.82e+00	1.52e+00	8.60e-01	1.28e+01	6.73e+00	3.86e+00	2.28e+00	1.46e+00
D	GUA	2	1.92e+01	1.14e+01	4.82e+00	2.49e+00	1.37e+00	7.64e-01	1.12e+01	6.04e+00	3.51e+00	2.05e+00	1.39e+00
D	GUA	2	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
D	GUA	48	1.06e+01	5.22e+00	2.86e+00	1.63e+00	8.54e-01	4.95e-01	7.64e+00	4.86e+00	3.13e+00	2.22e+00	1.70e+00
D	GUA	48	1.06e+01	6.14e+00	3.11e+00	NA	7.76e-01	4.79e-01	NA	NA	2.60e+00	1.78e+00	1.27e+00
D	GUA	48	2.04e+01	7.03e+00	5.61e+00	2.85e+00	1.52e+00	8.83e-01	1.34e+01	7.47e+00	4.45e+00	2.82e+00	1.89e+00
D	GUA	48	1.95e+01	1.14e+01	5.25e+00	2.61e+00	1.41e+00	9.57e-01	1.29e+01	7.09e+00	4.37e+00	2.87e+00	1.87e+00
D	GUA	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
D	GUA	240	1.05e+01	4.75e+00	2.60e+00	1.37e+00	7.74e-01	5.22e-01	6.94e+00	4.26e+00	2.84e+00	2.01e+00	1.45e+00
D	GUA	240	1.06e+01	5.23e+00	3.00e+00	1.46e+00	8.04e-01	5.75e-01	7.61e+00	4.53e+00	3.00e+00	2.15e+00	1.54e+00
D	GUA	240	2.02e+01	1.24e+01	6.42e+00	3.28e+00	1.83e+00	1.21e+00	1.63e+01	9.67e+00	6.27e+00	4.34e+00	3.03e+00
D	GUA	240	1.91e+01	9.00e+00	4.43e+00	2.44e+00	1.26e+00	1.89e-01	9.79e+00	5.25e+00	2.66e+00	1.33e+00	1.13e+00
D	GUA	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	NA	NA	NA	NA	NA	0.00e+00
D	GUA	720	1.06e+01	9.45e-02	3.58e-02	0.00e+00	0.00e+00	0.00e+00	2.34e-01	1.97e-01	1.97e-01	1.97e-01	1.97e-01
D	GUA	720	1.06e+01	4.01e-02	2.97e-02	0.00e+00	0.00e+00	0.00e+00	1.93e-01	1.62e-01	1.62e-01	1.62e-01	1.62e-01
D	GUA	720	2.03e+01	7.84e-01	3.82e-01	0.00e+00	0.00e+00	5.11e-02	7.90e-01	3.91e-01	3.91e-01	3.91e-01	3.36e-01
D	GUA	720	1.92e+01	7.93e-01	4.27e-01	1.39e-01	0.00e+00	4.41e-02	9.98e-01	5.71e-01	4.20e-01	4.20e-01	3.74e-01
D	GUA	720	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
D	H	2	1.21e+01	3.32e+00	2.01e+00	1.42e+00	1.09e+00	7.65e-01	9.66e+00	7.55e+00	6.08e+00	4.93e+00	4.12e+00
D	H	2	1.21e+01	3.35e+00	1.98e+00	1.43e+00	1.09e+00	7.97e-01	9.48e+00	7.39e+00	5.90e+00	4.75e+00	3.91e+00
D	H	2	2.33e+01	6.43e+00	3.93e+00	2.73e+00	2.06e+00	1.51e+00	1.79e+01	1.36e+01	1.07e+01	8.55e+00	6.99e+00
D	H	2	2.09e+01	3.24e-01	3.21e+00	2.39e+00	1.81e+00	1.35e+00	1.59e+01	1.25e+01	1.00e+01	8.11e+00	6.69e+00
D	H	2	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
D	H	48	1.14e+01	2.07e+00	1.60e+00	1.21e+00	8.65e-01	7.61e-01	9.12e+00	7.46e+00	6.20e+00	5.31e+00	4.53e+00
D	H	48	1.14e+01	2.17e+00	1.70e+00	1.20e+00	8.80e-01	7.42e-01	8.95e+00	7.15e+00	5.90e+00	4.97e+00	4.22e+00
D	H	48	2.20e+01	4.27e+00	3.29e+00	2.34e+00	1.81e+00	1.49e+00	1.70e+01	1.35e+01	1.10e+01	9.12e+00	7.60e+00
D	H	48	2.10e+01	4.63e+00	3.29e+00	2.29e+00	1.75e+00	1.47e+00	1.77e+01	1.41e+01	1.17e+01	9.88e+00	8.31e+00
D	H	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	NA	0.00e+00	NA	NA	NA	0.00e+00	0.00e+00
D	H	240	1.14e+01	1.51e+00	1.25e+00	1.00e+00	8.21e-01	6.90e-01	8.44e+00	7.16e+00	6.14e+00	5.28e+00	4.55e+00
D	H	240	1.14e+01	1.59e+00	1.31e+00	1.02e+00	8.02e-01	6.88e-01	8.44e+00	7.09e+00	6.03e+00	5.20e+00	4.46e+00
D	H	240	2.19e+01	3.43e+00	2.80e+00	2.12e+00	1.70e+00	1.42e+00	1.66e+01	1.38e+01	1.15e+01	9.77e+00	8.28e+00
D	H	240	2.07e+01	3.05e+00	2.44e+00	2.05e+00	1.59e+00	1.33e+00	1.86e+01	1.61e+01	1.39e+01	1.23e+01	1.09e+01
D	H	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
D	H	720	1.14e+01	1.45e+00	1.06e+00	2.73e-01	2.35e-01	2.99e-01	8.61e+00	7.50e+00	7.22e+00	6.97e+00	6.67e+00
D	H	720	1.14e+01	1.58e+00	1.17e+00	3.07e-01	2.64e-01	2.94e-01	8.25e+00	7.03e+00	6.71e+00	6.44e+00	6.13e+00
D	H	720	2.20e+01	3.39e+00	2.34e+00	6.46e-01	9.12e-01	5.64e-01	1.57e+01	1.32e+01	1.25e+01	1.16e+01	1.10e+01
D	H	720	2.07e+01	3.14e+00	2.42e+00	8.22e-01	5.81e-01	5.27e-01	1.45e+01	1.20e+01	1.11e+01	1.05e+01	9.97e+00
D	H	720	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00

Table E.5 – continued from previous page

MC	S	t_{Ads}	C_{CTRL}	C_A	C_{D1}	C_{D2}	C_{D3}	C_{D4}	q_A	q_{D1}	q_{D2}	q_{D3}	q_{D4}
D	J	2	1.11e+01	7.02e-01	3.28e-01	2.02e-01	1.45e-01	1.15e-01	1.84e+01	1.78e+01	1.75e+01	1.72e+01	1.70e+01
D	J	2	1.12e+01	5.89e-01	2.04e-01	1.52e-01	1.15e-01	8.11e-02	1.62e+01	1.58e+01	1.55e+01	1.53e+01	1.52e+01
D	J	2	2.09e+01	1.74e+00	6.10e-01	4.91e-01	3.89e-01	3.19e-01	3.30e+01	3.19e+01	3.10e+01	3.03e+01	2.98e+01
D	J	2	1.91e+01	1.20e+00	4.79e-01	3.65e-01	3.02e-01	2.68e-01	2.72e+01	2.63e+01	2.57e+01	2.52e+01	2.47e+01
D	J	2	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
D	J	48	1.06e+01	1.66e-01	1.41e-01	1.33e-01	1.21e-01	1.11e-01	1.69e+01	1.67e+01	1.64e+01	1.62e+01	1.60e+01
D	J	48	1.06e+01	1.68e-01	1.48e-01	1.38e-01	1.15e-01	1.11e-01	1.40e+01	1.37e+01	1.35e+01	1.33e+01	1.31e+01
D	J	48	2.04e+01	4.61e-01	3.78e-01	3.73e-01	3.06e-01	3.05e-01	3.31e+01	3.24e+01	3.18e+01	3.12e+01	3.07e+01
D	J	48	1.96e+01	4.65e-01	3.79e-01	3.32e-01	2.87e-01	2.71e-01	3.13e+01	3.06e+01	3.00e+01	2.95e+01	2.91e+01
D	J	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
D	J	240	1.06e+01	1.03e-01	9.26e-02	7.59e-02	7.30e-02	6.86e-02	1.82e+01	1.80e+01	1.79e+01	1.77e+01	1.76e+01
D	J	240	1.06e+01	1.04e-01	8.21e-02	6.85e-02	6.44e-02	6.18e-02	1.83e+01	1.82e+01	1.81e+01	1.79e+01	1.78e+01
D	J	240	2.04e+01	3.42e-01	2.61e-01	2.31e-01	2.03e-01	2.07e-01	3.76e+01	3.71e+01	3.67e+01	3.64e+01	3.60e+01
D	J	240	1.92e+01	2.33e-01	1.98e-01	1.88e-01	1.62e-01	1.57e-01	3.30e+01	3.26e+01	3.23e+01	3.20e+01	3.18e+01
D	J	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
D	J	720	1.06e+01	5.73e-02	4.01e-02	0.00e+00	0.00e+00	0.00e+00	1.80e+01	1.79e+01	1.79e+01	1.79e+01	1.79e+01
D	J	720	1.06e+01	4.79e-02	3.40e-02	0.00e+00	0.00e+00	0.00e+00	1.82e+01	1.82e+01	1.82e+01	1.82e+01	1.82e+01
D	J	720	2.04e+01	1.02e-01	8.75e-02	0.00e+00	0.00e+00	0.00e+00	3.92e+01	3.91e+01	3.91e+01	3.91e+01	3.91e+01
D	J	720	1.92e+01	6.93e-02	5.68e-02	0.00e+00	0.00e+00	0.00e+00	2.77e+01	2.76e+01	2.76e+01	2.76e+01	2.76e+01
D	J	720	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
D	KA	2	1.18e+01	9.98e+00	2.98e+00	9.40e-01	2.79e-01	7.77e-02	7.73e+00	2.43e+00	7.69e-01	2.82e-01	1.42e-01
D	KA	2	1.17e+01	1.01e+01	2.90e+00	9.28e-01	2.68e-01	7.38e-02	7.48e+00	2.30e+00	6.51e-01	1.86e-01	5.39e-02
D	KA	2	2.22e+01	1.93e+01	5.71e+00	1.80e+00	5.31e-01	1.53e-01	1.46e+01	4.51e+00	1.28e+00	3.66e-01	9.09e-02
D	KA	2	2.03e+01	1.77e+01	4.95e+00	1.60e+00	4.63e-01	1.34e-01	1.27e+01	3.97e+00	1.11e+00	2.97e-01	5.69e-02
D	KA	2	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
D	KA	48	1.11e+01	9.16e+00	3.13e+00	8.53e-01	2.36e-01	7.32e-02	7.60e+00	2.05e+00	5.45e-01	1.27e-01	0.00e+00
D	KA	48	1.11e+01	9.94e+00	NA	8.68e-01	2.36e-01	7.50e-02	NA	2.09e+00	5.42e-01	1.31e-01	0.00e+00
D	KA	48	2.14e+01	1.78e+01	5.86e+00	1.78e+00	4.92e-01	1.50e-01	1.35e+01	4.28e+00	1.14e+00	2.64e-01	0.00e+00
D	KA	48	2.04e+01	1.85e+01	5.41e+00	1.58e+00	4.57e-01	1.65e-01	1.39e+01	4.19e+00	1.37e+00	5.70e-01	2.83e-01
D	KA	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
D	KA	240	1.11e+01	9.58e+00	2.90e+00	8.29e-01	2.47e-01	1.25e-01	7.26e+00	2.13e+00	6.53e-01	2.16e-01	0.00e+00
D	KA	240	1.11e+01	9.61e+00	2.92e+00	8.60e-01	2.47e-01	8.14e-02	7.17e+00	2.09e+00	5.73e-01	1.41e-01	0.00e+00
D	KA	240	2.13e+01	1.81e+01	5.69e+00	1.66e+00	4.88e-01	1.44e-01	1.40e+01	4.07e+00	1.11e+00	2.50e-01	0.00e+00
D	KA	240	2.01e+01	1.73e+01	5.22e+00	1.58e+00	3.78e-01	1.35e-01	1.28e+01	3.68e+00	9.05e-01	2.39e-01	0.00e+00
D	KA	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
D	KA	720	1.11e+01	9.39e+00	2.68e+00	6.15e-01	9.33e-02	0.00e+00	6.03e+00	1.23e+00	1.61e-01	0.00e+00	0.00e+00
D	KA	720	1.11e+01	9.63e+00	2.76e+00	6.03e-01	8.21e-02	0.00e+00	6.83e+00	1.91e+00	8.36e-01	6.94e-01	6.94e-01
D	KA	720	2.14e+01	1.80e+01	5.24e+00	1.11e+00	1.01e-01	6.48e-02	1.18e+01	2.38e+00	4.30e-01	2.55e-01	1.41e-01
D	KA	720	2.00e+01	NA	5.14e+00	1.27e+00	9.19e-02	4.52e-02	1.14e+01	2.59e+00	3.17e-01	1.51e-01	7.12e-02
D	KA	720	0.00e+00	0.00e+00	NA	0.00e+00	0.00e+00	0.00e+00	NA	0.00e+00	0.00e+00	0.00e+00	0.00e+00

Table E.5 – continued from previous page

MC	S	t_{Ads}	C_{CTRL}	C_A	C_{D1}	C_{D2}	C_{D3}	C_{D4}	q_A	q_{D1}	q_{D2}	q_{D3}	q_{D4}
D	LCL	2	9.92e+00	2.24e+00	8.73e-01	NA	NA	NA	NA	NA	NA	NA	0.00e+00
D	LCL	2	9.87e+00	2.19e+00	8.51e-01	NA	NA	NA	NA	NA	NA	NA	0.00e+00
D	LCL	2	1.92e+01	4.34e+00	1.91e+00	NA	NA	NA	NA	NA	NA	NA	0.00e+00
D	LCL	2	1.75e+01	3.83e+00	0.00e+00	NA	NA	NA	NA	NA	NA	NA	0.00e+00
D	LCL	2	0.00e+00	0.00e+00	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
D	LCL	48	8.30e+00	1.09e+00	3.34e-01	3.07e-01	3.24e-01	3.17e-01	1.00e+01	9.68e+00	9.35e+00	9.00e+00	8.66e+00
D	LCL	48	8.31e+00	1.01e+00	3.21e-01	2.80e-01	2.98e-01	2.98e-01	9.77e+00	9.43e+00	9.14e+00	8.82e+00	8.51e+00
D	LCL	48	1.68e+01	1.90e+00	1.01e+00	7.97e-01	7.71e-01	7.18e-01	1.96e+01	1.86e+01	1.77e+01	1.69e+01	1.61e+01
D	LCL	48	1.62e+01	9.28e-01	7.21e-01	4.43e-01	4.39e-01	2.80e-01	1.68e+01	1.61e+01	1.56e+01	1.52e+01	1.49e+01
D	LCL	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
D	LCL	240	9.83e+00	5.76e-01	4.61e-01	4.44e-01	3.78e-01	3.44e-01	1.08e+01	1.02e+01	9.76e+00	9.37e+00	9.00e+00
D	LCL	240	9.84e+00	5.96e-01	4.64e-01	4.45e-01	3.68e-01	3.52e-01	1.09e+01	1.03e+01	9.81e+00	9.43e+00	9.05e+00
D	LCL	240	1.91e+01	1.42e+00	1.08e+00	1.00e+00	8.19e-01	6.42e-01	2.20e+01	2.07e+01	1.97e+01	1.88e+01	1.81e+01
D	LCL	240	1.66e+01	7.95e-01	6.67e-01	4.36e-01	3.16e-01	4.47e-01	1.63e+01	1.55e+01	1.50e+01	1.47e+01	1.42e+01
D	LCL	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
D	LCL	720	1.00e+01	2.99e-01	2.74e-01	2.44e-01	0.00e+00	1.04e-01	7.07e+00	6.78e+00	6.51e+00	6.51e+00	6.40e+00
D	LCL	720	1.00e+01	3.00e-01	2.65e-01	2.37e-01	0.00e+00	NA	NA	NA	NA	NA	6.50e+00
D	LCL	720	1.92e+01	8.26e-01	7.14e-01	6.28e-01	3.44e-01	1.78e-01	1.50e+01	1.43e+01	1.36e+01	1.32e+01	1.31e+01
D	LCL	720	1.73e+01	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
D	LCL	720	0.00e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
D	LCO	2	1.09e+01	1.40e+00	3.12e-01	NA	NA	NA	NA	NA	NA	NA	0.00e+00
D	LCO	2	1.11e+01	1.77e+00	2.99e-01	NA	NA	NA	NA	NA	NA	NA	0.00e+00
D	LCO	2	2.11e+01	2.70e+00	8.53e-01	NA	NA	NA	NA	NA	NA	NA	0.00e+00
D	LCO	2	1.92e+01	1.92e+00	7.31e-01	NA	NA	NA	NA	NA	NA	NA	0.00e+00
D	LCO	2	0.00e+00	0.00e+00	0.00e+00	NA	NA	NA	NA	NA	NA	NA	0.00e+00
D	LCO	48	9.31e+00	4.09e-01	1.78e-01	6.51e-02	1.61e-01	1.05e-01	1.06e+01	1.04e+01	1.03e+01	1.01e+01	1.00e+01
D	LCO	48	9.35e+00	4.22e-01	1.06e-01	6.93e-02	1.54e-01	8.29e-02	1.05e+01	1.04e+01	1.03e+01	1.01e+01	1.00e+01
D	LCO	48	1.89e+01	9.42e-01	3.07e-01	3.12e-01	3.11e-01	3.23e-01	2.37e+01	2.34e+01	2.31e+01	2.28e+01	2.24e+01
D	LCO	48	1.80e+01	6.06e-01	0.00e+00	0.00e+00	0.00e+00	0.00e+00	1.72e+01	1.72e+01	1.72e+01	1.72e+01	1.72e+01
D	LCO	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
D	LCO	240	1.09e+01	2.52e-01	1.81e-01	1.66e-01	1.59e-01	1.38e-01	1.12e+01	1.10e+01	1.08e+01	1.06e+01	1.05e+01
D	LCO	240	1.09e+01	2.10e-01	1.74e-01	1.60e-01	1.50e-01	1.37e-01	1.12e+01	1.09e+01	1.07e+01	1.05e+01	1.04e+01
D	LCO	240	2.13e+01	5.86e-01	4.87e-01	4.45e-01	3.96e-01	3.72e-01	2.11e+01	2.05e+01	1.99e+01	1.95e+01	1.91e+01
D	LCO	240	1.80e+01	3.86e-01	2.81e-01	2.72e-01	1.76e-01	1.84e-01	1.57e+01	1.53e+01	1.50e+01	1.48e+01	1.46e+01
D	LCO	240	0.00e+00	NA	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
D	LCO	720	1.12e+01	9.66e-02	7.71e-02	7.89e-02	7.67e-02	0.00e+00	8.28e+00	8.20e+00	8.11e+00	8.03e+00	8.03e+00
D	LCO	720	1.11e+01	1.12e-01	9.88e-02	1.04e-01	8.74e-02	0.00e+00	8.70e+00	8.60e+00	8.49e+00	8.40e+00	8.40e+00
D	LCO	720	2.14e+01	2.87e-01	2.62e-01	2.47e-01	2.35e-01	8.52e-02	1.59e+01	1.56e+01	1.53e+01	1.51e+01	1.50e+01
D	LCO	720	1.93e+01	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
D	LCO	720	0.00e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00

Table E.5 – continued from previous page

MC	S	t_{Ads}	C_{CTRL}	C_A	C_{D1}	C_{D2}	C_{D3}	C_{D4}	q_A	q_{D1}	q_{D2}	q_{D3}	q_{D4}
D	M	2	1.16e+01	4.85e+00	2.29e+00	1.47e+00	9.49e-01	6.53e-01	8.28e+00	5.80e+00	4.35e+00	3.29e+00	2.60e+00
D	M	2	1.16e+01	5.03e+00	2.29e+00	1.48e+00	1.04e+00	6.84e-01	8.55e+00	6.03e+00	4.55e+00	3.40e+00	2.66e+00
D	M	2	2.23e+01	1.01e+01	4.84e+00	2.93e+00	1.97e+00	1.26e+00	1.58e+01	1.05e+01	7.58e+00	5.42e+00	4.07e+00
D	M	2	2.00e+01	8.97e+00	4.18e+00	2.64e+00	1.71e+00	1.14e+00	1.40e+01	9.51e+00	6.85e+00	4.99e+00	3.79e+00
D	M	2	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
D	M	48	1.06e+01	3.23e+00	1.97e+00	1.32e+00	8.81e-01	6.68e-01	7.96e+00	5.94e+00	4.58e+00	3.65e+00	2.98e+00
D	M	48	1.06e+01	3.25e+00	2.18e+00	1.35e+00	8.93e-01	6.68e-01	8.62e+00	6.38e+00	4.95e+00	4.00e+00	3.31e+00
D	M	48	2.04e+01	7.02e+00	4.13e+00	2.72e+00	1.77e+00	1.25e+00	1.58e+01	1.16e+01	8.72e+00	6.84e+00	5.56e+00
D	M	48	1.96e+01	7.08e+00	4.07e+00	2.64e+00	1.61e+00	1.34e+00	1.59e+01	1.14e+01	8.65e+00	6.96e+00	5.53e+00
D	M	48	0.00e+00	NA	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
D	M	240	1.06e+01	2.88e+00	1.87e+00	1.20e+00	8.06e-01	7.21e-01	8.91e+00	6.89e+00	5.63e+00	4.77e+00	4.07e+00
D	M	240	1.06e+01	2.89e+00	1.90e+00	1.22e+00	8.30e-01	7.08e-01	9.18e+00	7.10e+00	5.81e+00	4.93e+00	4.22e+00
D	M	240	2.03e+01	6.65e+00	4.17e+00	2.60e+00	1.68e+00	1.39e+00	1.71e+01	1.26e+01	9.87e+00	8.08e+00	6.69e+00
D	M	240	1.92e+01	5.46e+00	3.36e+00	2.29e+00	1.51e+00	1.03e+00	1.41e+01	1.07e+01	8.24e+00	6.66e+00	5.55e+00
D	M	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
D	M	720	1.06e+01	2.00e+00	1.16e+00	6.87e-01	2.90e-01	2.19e-01	7.59e+00	6.34e+00	5.60e+00	5.31e+00	5.08e+00
D	M	720	1.06e+01	2.17e+00	1.32e+00	NA	2.42e-01	2.58e-01	NA	NA	5.92e+00	5.68e+00	5.41e+00
D	M	720	2.04e+01	5.27e+00	3.14e+00	1.87e+00	7.72e-01	5.50e-01	1.70e+01	1.36e+01	1.16e+01	1.08e+01	1.02e+01
D	M	720	1.92e+01	3.31e-01	2.62e+00	1.73e+00	6.41e-01	NA	NA	NA	NA	NA	7.33e+00
D	M	720	0.00e+00	NA	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
D	N	2	1.16e+01	6.07e+00	2.44e+00	1.45e+00	9.16e-01	5.47e-01	6.96e+00	4.36e+00	2.86e+00	1.93e+00	1.34e+00
D	N	2	1.16e+01	6.00e+00	2.54e+00	1.45e+00	9.42e-01	5.52e-01	7.30e+00	4.60e+00	3.06e+00	2.09e+00	1.51e+00
D	N	2	2.25e+01	1.28e+01	5.20e+00	2.68e+00	1.66e+00	9.12e-01	1.32e+01	7.57e+00	4.70e+00	2.97e+00	2.02e+00
D	N	2	2.01e+01	1.11e+01	4.34e+00	2.35e+00	1.43e+00	8.12e-01	1.10e+01	6.43e+00	3.99e+00	2.52e+00	1.66e+00
D	N	2	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
D	N	48	1.09e+01	4.26e+00	2.43e+00	1.39e+00	8.40e-01	5.59e-01	8.02e+00	5.50e+00	3.98e+00	3.11e+00	2.51e+00
D	N	48	1.09e+01	4.75e+00	2.59e+00	1.42e+00	8.39e-01	5.69e-01	8.32e+00	5.63e+00	4.12e+00	3.23e+00	2.64e+00
D	N	48	2.11e+01	9.63e+00	4.99e+00	2.77e+00	1.60e+00	1.08e+00	1.51e+01	9.97e+00	6.95e+00	5.27e+00	4.13e+00
D	N	48	2.00e+01	9.39e+00	4.61e+00	2.67e+00	1.48e+00	1.14e+00	1.45e+01	9.45e+00	6.61e+00	5.07e+00	3.88e+00
D	N	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
D	N	240	1.09e+01	4.23e+00	2.42e+00	1.44e+00	8.90e-01	7.31e-01	8.86e+00	6.27e+00	4.77e+00	3.83e+00	3.04e+00
D	N	240	1.09e+01	4.09e+00	2.43e+00	1.43e+00	8.73e-01	7.31e-01	8.89e+00	6.29e+00	4.78e+00	3.86e+00	3.08e+00
D	N	240	2.10e+01	9.17e+00	5.28e+00	2.94e+00	1.79e+00	1.44e+00	1.78e+01	1.22e+01	9.04e+00	7.17e+00	5.65e+00
D	N	240	1.98e+01	6.65e+00	3.54e+00	2.32e+00	1.32e+00	8.80e-01	1.23e+01	8.64e+00	6.24e+00	4.84e+00	3.92e+00
D	N	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
D	N	720	1.10e+01	7.16e-01	4.02e-01	1.85e-01	9.80e-02	6.59e-02	1.30e+00	8.79e-01	6.82e-01	5.78e-01	5.10e-01
D	N	720	1.09e+01	0.00e+00	1.56e-01	8.09e-02	0.00e+00	0.00e+00	2.05e+00	1.89e+00	1.80e+00	1.80e+00	1.80e+00
D	N	720	2.11e+01	5.93e+00	3.17e+00	1.72e+00	6.36e-01	4.87e-01	1.39e+01	1.05e+01	8.69e+00	8.01e+00	7.51e+00
D	N	720	1.98e+01	0.00e+00	1.27e+00	8.11e-01	0.00e+00	1.97e-01	4.79e+00	3.50e+00	2.62e+00	2.62e+00	2.41e+00
D	N	720	0.00e+00	NA	0.00e+00	0.00e+00	NA	0.00e+00	NA	NA	NA	0.00e+00	0.00e+00

Table E.5 – continued from previous page

MC	S	t_{Ads}	C_{CTRL}	C_A	C_{D1}	C_{D2}	C_{D3}	C_{D4}	q_A	q_{D1}	q_{D2}	q_{D3}	q_{D4}
D	P	2	1.14e+01	2.98e-01	1.14e-01	1.04e-01	9.92e-02	7.91e-02	1.57e+01	1.55e+01	1.54e+01	1.52e+01	1.51e+01
D	P	2	1.14e+01	2.54e-01	1.01e-01	1.01e-01	8.35e-02	7.43e-02	1.65e+01	1.63e+01	1.61e+01	1.60e+01	1.59e+01
D	P	2	2.22e+01	7.94e-01	2.71e-01	2.51e-01	2.20e-01	2.10e-01	3.20e+01	3.15e+01	3.11e+01	3.07e+01	3.04e+01
D	P	2	1.98e+01	5.23e+00	1.52e-01	1.53e-01	1.24e-01	NA	NA	NA	NA	NA	0.00e+00
D	P	2	0.00e+00	0.00e+00	0.00e+00	NA	NA	NA	NA	NA	NA	NA	0.00e+00
D	P	48	1.08e+01	9.60e-02	8.69e-02	9.10e-02	8.34e-02	8.75e-02	1.60e+01	1.58e+01	1.57e+01	1.55e+01	1.54e+01
D	P	48	1.08e+01	8.15e-02	8.91e-02	7.65e-02	6.94e-02	7.64e-02	1.54e+01	1.52e+01	1.51e+01	1.50e+01	1.48e+01
D	P	48	2.07e+01	2.25e-01	2.27e-01	2.10e-01	1.91e-01	2.03e-01	2.87e+01	2.83e+01	2.79e+01	2.76e+01	2.72e+01
D	P	48	1.99e+01	1.53e-01	1.59e-01	2.41e-01	9.93e-02	1.08e-01	2.90e+01	2.87e+01	2.83e+01	2.82e+01	2.80e+01
D	P	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
D	P	240	1.07e+01	1.22e-01	9.16e-02	5.10e-02	4.74e-02	3.29e-02	1.12e+01	1.10e+01	1.09e+01	1.09e+01	1.08e+01
D	P	240	1.08e+01	6.05e-02	3.40e-02	2.88e-02	2.50e-02	3.13e-02	9.41e+00	9.36e+00	9.30e+00	9.26e+00	9.21e+00
D	P	240	2.08e+01	9.27e-02	9.21e-02	9.82e-02	8.66e-02	8.45e-02	2.36e+01	2.35e+01	2.33e+01	2.32e+01	2.30e+01
D	P	240	1.94e+01	0.00e+00	0.00e+00	0.00e+00	0.00e+00	7.26e-03	6.81e+00	6.81e+00	6.81e+00	6.81e+00	6.80e+00
D	P	240	0.00e+00	0.00e+00	0.00e+00	NA	0.00e+00	0.00e+00	NA	NA	0.00e+00	0.00e+00	0.00e+00
D	P	720	1.08e+01	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	1.51e+00	1.51e+00	1.51e+00	1.51e+00	1.51e+00
D	P	720	1.08e+01	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	2.04e+00	2.04e+00	2.04e+00	2.04e+00	2.04e+00
D	P	720	2.07e+01	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	3.70e+00	3.70e+00	3.70e+00	3.70e+00	3.70e+00
D	P	720	1.95e+01	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	9.50e-01	9.50e-01	9.50e-01	9.50e-01	9.50e-01
D	P	720	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
D	PO	2	1.05e+01	1.35e+00	5.61e-01	NA	NA	NA	NA	NA	NA	NA	0.00e+00
D	PO	2	1.05e+01	1.82e+00	8.46e-01	NA	NA	NA	NA	NA	NA	NA	0.00e+00
D	PO	2	2.02e+01	3.69e+00	1.69e+00	NA	NA	NA	NA	NA	NA	NA	0.00e+00
D	PO	2	1.84e+01	3.43e+00	1.53e+00	NA	NA	NA	NA	NA	NA	NA	0.00e+00
D	PO	2	0.00e+00	0.00e+00	0.00e+00	NA	NA	NA	NA	NA	NA	NA	0.00e+00
D	PO	48	1.05e+01	9.12e-01	4.40e-01	3.76e-01	3.58e-01	3.91e-01	1.65e+00	1.19e+00	7.90e-01	4.15e-01	0.00e+00
D	PO	48	1.04e+01	8.96e-01	4.25e-01	3.70e-01	3.57e-01	3.93e-01	1.07e+01	1.03e+01	9.90e+00	9.53e+00	9.12e+00
D	PO	48	1.76e+01	2.13e+00	1.07e+00	8.86e-01	8.55e-01	8.37e-01	2.31e+01	2.20e+01	2.11e+01	2.03e+01	1.95e+01
D	PO	48	1.72e+01	1.31e+00	9.22e-01	5.40e-01	9.44e-01	3.96e-01	1.84e+01	1.74e+01	1.69e+01	1.59e+01	1.55e+01
D	PO	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
D	PO	240	1.04e+01	8.21e-01	6.19e-01	5.41e-01	4.84e-01	3.81e-01	1.20e+01	1.13e+01	1.06e+01	1.00e+01	9.64e+00
D	PO	240	1.04e+01	7.10e-01	5.86e-01	5.23e-01	4.51e-01	3.66e-01	1.17e+01	1.10e+01	1.03e+01	9.87e+00	9.48e+00
D	PO	240	2.03e+01	1.74e+00	1.28e+00	1.09e+00	9.81e-01	8.11e-01	2.30e+01	2.15e+01	2.00e+01	1.90e+01	1.81e+01
D	PO	240	1.75e+01	9.55e-01	6.30e-01	NA	3.90e-01	2.98e-01	NA	NA	1.84e+01	1.80e+01	1.77e+01
D	PO	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
D	PO	720	1.07e+01	5.11e-01	4.56e-01	1.10e-01	2.91e-01	1.53e-01	8.18e+00	7.72e+00	7.61e+00	7.30e+00	7.14e+00
D	PO	720	1.06e+01	1.02e+00	4.64e-01	1.13e-01	1.82e-01	1.64e-01	8.80e+00	8.33e+00	8.21e+00	8.02e+00	7.84e+00
D	PO	720	2.05e+01	1.14e+00	1.05e+00	3.11e-01	4.72e-01	3.75e-01	1.75e+01	1.64e+01	1.61e+01	1.56e+01	1.52e+01
D	PO	720	1.85e+01	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
D	PO	720	0.00e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00

Table E.5 – continued from previous page

MC	S	t_{Ads}	C_{CTRL}	C_A	C_{D1}	C_{D2}	C_{D3}	C_{D4}	q_A	q_{D1}	q_{D2}	q_{D3}	q_{D4}
D	R	2	1.13e+01	9.74e-01	5.54e-01	4.85e-01	4.13e-01	4.01e-01	1.78e+01	1.69e+01	1.60e+01	1.53e+01	1.46e+01
D	R	2	1.13e+01	8.47e-01	4.98e-01	4.81e-01	4.28e-01	3.89e-01	1.82e+01	1.73e+01	1.65e+01	1.57e+01	1.51e+01
D	R	2	2.17e+01	2.03e+00	1.18e+00	1.10e+00	9.42e-01	8.75e-01	3.40e+01	3.20e+01	3.00e+01	2.84e+01	2.69e+01
D	R	2	1.94e+01	1.49e+00	9.72e-01	9.12e-01	7.96e-01	7.38e-01	3.17e+01	3.00e+01	2.84e+01	2.70e+01	2.58e+01
D	R	2	0.00e+00	0.00e+00	0.00e+00	0.00e+00	NA	0.00e+00	NA	NA	NA	0.00e+00	0.00e+00
D	R	48	1.06e+01	4.74e-01	4.06e-01	3.92e-01	3.53e-01	3.39e-01	1.62e+01	1.55e+01	1.48e+01	1.42e+01	1.36e+01
D	R	48	1.06e+01	4.82e-01	4.34e-01	4.36e-01	3.48e-01	3.42e-01	1.67e+01	1.60e+01	1.53e+01	1.47e+01	1.41e+01
D	R	48	2.04e+01	9.97e-01	8.67e-01	8.40e-01	7.50e-01	7.10e-01	3.18e+01	3.03e+01	2.89e+01	2.76e+01	2.64e+01
D	R	48	1.95e+01	1.12e+00	9.73e-01	9.02e-01	7.85e-01	7.32e-01	2.94e+01	2.77e+01	2.61e+01	2.48e+01	2.35e+01
D	R	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
D	R	240	1.06e+01	4.54e-01	3.67e-01	3.38e-01	3.09e-01	2.83e-01	1.42e+01	1.36e+01	1.30e+01	1.25e+01	1.20e+01
D	R	240	1.06e+01	3.77e-01	3.35e-01	2.71e-01	2.79e-01	2.57e-01	1.43e+01	1.38e+01	1.33e+01	1.28e+01	1.24e+01
D	R	240	2.02e+01	7.90e-01	7.27e-01	6.60e-01	6.14e-01	NA	NA	NA	NA	NA	2.29e+01
D	R	240	1.92e+01	7.51e-01	7.01e-01	6.71e-01	6.03e-01	5.60e-01	2.72e+01	2.60e+01	2.48e+01	2.38e+01	2.28e+01
D	R	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
D	R	720	1.06e+01	3.67e-01	2.64e-01	1.01e-01	7.93e-02	8.71e-02	1.82e+01	1.77e+01	1.75e+01	1.74e+01	1.72e+01
D	R	720	1.06e+01	2.26e-01	2.06e-01	7.12e-02	6.38e-02	9.00e-02	1.80e+01	1.77e+01	1.76e+01	1.75e+01	1.73e+01
D	R	720	2.04e+01	6.19e-01	5.43e-01	2.27e-01	1.46e-01	1.11e-01	3.31e+01	3.22e+01	3.18e+01	3.15e+01	3.13e+01
D	R	720	1.92e+01	5.42e-01	5.08e-01	2.28e-01	7.89e-02	2.07e-01	2.95e+01	2.86e+01	2.82e+01	2.81e+01	2.77e+01
D	R	720	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
D	SOU	2	1.09e+01	6.29e+00	2.79e+00	1.62e+00	9.54e-01	5.45e-01	6.96e+00	4.15e+00	2.49e+00	1.49e+00	9.05e-01
D	SOU	2	1.06e+01	6.27e+00	2.85e+00	1.61e+00	9.51e-01	5.34e-01	7.13e+00	4.23e+00	2.60e+00	1.60e+00	1.02e+00
D	SOU	2	2.12e+01	1.26e+01	0.00e+00	3.05e+00	1.72e+00	9.44e-01	7.37e+00	7.37e+00	4.20e+00	2.37e+00	1.36e+00
D	SOU	2	1.86e+01	1.13e+01	5.13e+00	2.62e+00	1.54e+00	8.44e-01	1.19e+01	6.74e+00	4.06e+00	2.42e+00	1.52e+00
D	SOU	2	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
D	SOU	48	1.03e+01	5.41e+00	2.68e+00	1.56e+00	8.38e-01	5.14e-01	7.14e+00	4.31e+00	2.68e+00	1.79e+00	1.24e+00
D	SOU	48	1.03e+01	5.37e+00	2.95e+00	1.67e+00	8.80e-01	5.55e-01	8.38e+00	5.29e+00	3.52e+00	2.58e+00	1.99e+00
D	SOU	48	1.99e+01	1.05e+01	5.49e+00	2.94e+00	1.59e+00	9.74e-01	1.46e+01	8.79e+00	5.66e+00	3.96e+00	2.92e+00
D	SOU	48	1.90e+01	9.85e+00	5.28e+00	2.88e+00	1.62e+00	1.18e+00	1.37e+01	8.03e+00	4.99e+00	3.28e+00	2.06e+00
D	SOU	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
D	SOU	240	1.03e+01	4.85e+00	2.94e+00	1.60e+00	9.31e-01	6.91e-01	9.55e+00	6.51e+00	4.85e+00	3.85e+00	3.16e+00
D	SOU	240	1.04e+01	4.90e+00	3.00e+00	1.66e+00	9.56e-01	NA	NA	NA	NA	NA	0.00e+00
D	SOU	240	1.98e+01	8.79e+00	5.87e+00	3.21e+00	1.81e+00	7.78e-02	1.53e+01	9.22e+00	5.86e+00	3.96e+00	3.88e+00
D	SOU	240	1.87e+01	9.07e+00	4.77e+00	3.05e+00	1.66e+00	1.00e+00	1.48e+01	9.79e+00	6.73e+00	4.98e+00	3.91e+00
D	SOU	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	NA	NA	NA	NA	NA	0.00e+00
D	SOU	720	1.03e+01	4.16e+00	2.06e+00	9.19e-01	2.21e-01	2.37e-01	5.99e+00	3.80e+00	2.82e+00	2.60e+00	2.34e+00
D	SOU	720	1.03e+01	4.73e+00	2.29e+00	1.09e+00	2.48e-01	2.44e-01	7.35e+00	4.91e+00	3.77e+00	3.51e+00	3.25e+00
D	SOU	720	1.98e+01	1.08e+01	5.03e+00	2.33e+00	1.17e+00	6.08e-01	1.53e+01	9.88e+00	7.42e+00	6.22e+00	5.56e+00
D	SOU	720	1.87e+01	8.40e+00	4.36e+00	2.38e+00	5.87e-01	5.37e-02	9.60e+00	5.19e+00	3.70e+00	3.11e+00	3.05e+00
D	SOU	720	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	NA	NA	NA	NA	NA	0.00e+00

Table E.5 – continued from previous page

MC	S	t_{Ads}	C_{CTRL}	C_A	C_{D1}	C_{D2}	C_{D3}	C_{D4}	q_A	q_{D1}	q_{D2}	q_{D3}	q_{D4}
D	SSL1	2	1.07e+01	5.26e+00	2.66e+00	1.54e+00	9.93e-01	6.95e-01	8.26e+00	5.41e+00	3.82e+00	2.78e+00	2.07e+00
D	SSL1	2	1.07e+01	5.24e+00	2.71e+00	1.54e+00	9.94e-01	1.31e+00	9.07e+00	6.13e+00	4.52e+00	3.46e+00	2.09e+00
D	SSL1	2	2.06e+01	1.08e+01	5.29e+00	2.97e+00	1.88e+00	NA	NA	NA	NA	NA	3.41e+00
D	SSL1	2	1.86e+01	9.57e+00	4.77e+00	2.81e+00	1.71e+00	1.22e+00	1.45e+01	9.31e+00	6.36e+00	4.53e+00	3.25e+00
D	SSL1	2	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
D	SSL1	48	1.07e+01	4.40e+00	0.00e+00	1.66e+00	1.05e+00	7.67e-01	6.23e+00	6.23e+00	4.47e+00	3.35e+00	2.55e+00
D	SSL1	48	1.07e+01	4.48e+00	4.73e+00	1.69e+00	1.04e+00	7.65e-01	1.14e+01	6.28e+00	4.48e+00	3.36e+00	2.56e+00
D	SSL1	48	2.05e+01	9.10e+00	5.37e+00	3.19e+00	2.02e+00	1.42e+00	1.69e+01	1.12e+01	7.87e+00	5.71e+00	4.23e+00
D	SSL1	48	1.85e+01	NA	NA	2.97e+00	1.82e+00	1.31e+00	NA	1.07e+01	7.62e+00	5.67e+00	4.30e+00
D	SSL1	48	0.00e+00	0.00e+00	NA	0.00e+00	0.00e+00	0.00e+00	NA	0.00e+00	0.00e+00	0.00e+00	0.00e+00
D	SSL1	240	1.07e+01	3.49e+00	2.26e+00	1.53e+00	1.01e+00	6.54e-01	9.04e+00	6.73e+00	5.02e+00	3.96e+00	3.26e+00
D	SSL1	240	1.08e+01	3.65e+00	2.32e+00	1.58e+00	1.04e+00	6.79e-01	9.38e+00	7.01e+00	5.25e+00	4.16e+00	3.43e+00
D	SSL1	240	2.06e+01	9.66e+00	4.64e+00	NA	1.96e+00	1.33e+00	NA	NA	9.07e+00	7.04e+00	5.63e+00
D	SSL1	240	1.83e+01	4.70e+00	4.02e+00	NA	NA	1.18e+00	NA	NA	NA	6.56e+00	5.30e+00
D	SSL1	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
D	SSL1	720	1.07e+01	3.91e+00	2.33e+00	1.49e+00	1.01e+00	6.71e-01	8.66e+00	6.11e+00	4.56e+00	3.44e+00	2.72e+00
D	SSL1	720	1.07e+01	4.02e+00	2.40e+00	1.53e+00	1.01e+00	6.51e-01	8.20e+00	5.56e+00	3.95e+00	2.82e+00	2.12e+00
D	SSL1	720	2.05e+01	8.31e+00	4.78e+00	3.06e+00	1.98e+00	1.24e+00	1.64e+01	1.14e+01	8.23e+00	6.06e+00	4.72e+00
D	SSL1	720	1.86e+01	NA	4.22e+00	2.70e+00	1.79e+00	1.15e+00	1.42e+01	9.66e+00	6.87e+00	4.87e+00	3.64e+00
D	SSL1	720	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
D	SSL2	2	1.11e+01	5.32e+00	2.70e+00	1.57e+00	9.99e-01	7.12e-01	8.57e+00	5.72e+00	4.08e+00	3.00e+00	2.26e+00
D	SSL2	2	1.12e+01	5.21e+00	2.75e+00	1.62e+00	1.09e+00	7.73e-01	8.98e+00	6.22e+00	4.53e+00	3.34e+00	2.52e+00
D	SSL2	2	2.14e+01	1.11e+01	5.44e+00	3.12e+00	2.01e+00	1.33e+00	1.64e+01	1.06e+01	7.40e+00	5.23e+00	3.85e+00
D	SSL2	2	1.94e+01	9.77e+00	4.83e+00	2.81e+00	1.80e+00	NA	NA	NA	NA	NA	3.45e+00
D	SSL2	2	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
D	SSL2	48	1.12e+01	4.50e+00	2.70e+00	1.69e+00	1.06e+00	7.79e-01	9.42e+00	6.65e+00	4.84e+00	3.72e+00	2.90e+00
D	SSL2	48	1.12e+01	4.52e+00	2.73e+00	1.73e+00	1.10e+00	7.99e-01	9.23e+00	6.42e+00	4.63e+00	3.43e+00	2.61e+00
D	SSL2	48	2.14e+01	9.52e+00	5.40e+00	3.43e+00	2.12e+00	1.45e+00	1.73e+01	1.17e+01	8.20e+00	5.91e+00	4.43e+00
D	SSL2	48	1.93e+01	8.22e+00	4.77e+00	3.01e+00	1.89e+00	1.37e+00	1.58e+01	1.08e+01	7.70e+00	5.65e+00	4.25e+00
D	SSL2	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
D	SSL2	240	1.12e+01	3.50e+00	2.28e+00	1.53e+00	1.03e+00	6.73e-01	7.20e+00	4.93e+00	3.19e+00	2.11e+00	1.40e+00
D	SSL2	240	1.11e+01	3.47e+00	2.32e+00	1.56e+00	1.03e+00	6.74e-01	7.13e+00	4.88e+00	3.16e+00	2.09e+00	1.38e+00
D	SSL2	240	2.15e+01	7.84e+00	4.92e+00	3.24e+00	2.04e+00	1.31e+00	1.43e+01	9.53e+00	5.85e+00	3.70e+00	2.31e+00
D	SSL2	240	1.92e+01	6.37e+00	4.17e+00	2.76e+00	1.78e+00	NA	NA	NA	NA	NA	2.27e+00
D	SSL2	240	0.00e+00	NA	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
D	SSL2	720	1.11e+01	3.93e+00	2.40e+00	1.56e+00	1.03e+00	0.00e+00	8.14e+00	5.51e+00	3.87e+00	2.75e+00	2.75e+00
D	SSL2	720	1.11e+01	4.12e+00	2.44e+00	1.56e+00	1.01e+00	0.00e+00	8.46e+00	5.74e+00	4.08e+00	2.97e+00	2.97e+00
D	SSL2	720	2.13e+01	8.49e+00	4.93e+00	3.11e+00	1.97e+00	0.00e+00	1.53e+01	9.95e+00	6.65e+00	4.51e+00	4.51e+00
D	SSL2	720	1.92e+01	7.43e+00	4.35e+00	2.83e+00	1.80e+00	0.00e+00	1.14e+01	6.55e+00	3.74e+00	1.78e+00	1.78e+00
D	SSL2	720	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00

Table E.5 – continued from previous page

MC	S	t_{Ads}	C_{CTRL}	C_A	C_{D1}	C_{D2}	C_{D3}	C_{D4}	q_A	q_{D1}	q_{D2}	q_{D3}	q_{D4}
D	SSL3	2	1.10e+01	5.21e+00	2.67e+00	1.57e+00	1.02e+00	7.41e-01	8.64e+00	5.81e+00	4.13e+00	3.06e+00	2.29e+00
D	SSL3	2	1.11e+01	5.24e+00	2.72e+00	1.57e+00	1.02e+00	7.45e-01	8.81e+00	5.91e+00	4.23e+00	3.15e+00	2.38e+00
D	SSL3	2	2.12e+01	1.06e+01	5.38e+00	3.11e+00	1.98e+00	1.40e+00	1.66e+01	1.09e+01	7.48e+00	5.38e+00	3.93e+00
D	SSL3	2	1.90e+01	9.46e+00	4.93e+00	2.87e+00	1.79e+00	NA	NA	NA	NA	NA	3.76e+00
D	SSL3	2	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
D	SSL3	48	1.10e+01	4.27e+00	2.65e+00	1.74e+00	1.11e+00	7.90e-01	9.31e+00	6.50e+00	4.68e+00	3.49e+00	2.68e+00
D	SSL3	48	1.10e+01	4.35e+00	2.65e+00	1.70e+00	1.09e+00	7.91e-01	9.36e+00	6.54e+00	4.79e+00	3.61e+00	2.79e+00
D	SSL3	48	2.11e+01	7.74e+00	5.33e+00	3.33e+00	2.11e+00	1.48e+00	1.75e+01	1.18e+01	8.30e+00	6.06e+00	4.54e+00
D	SSL3	48	1.90e+01	8.17e+00	4.85e+00	NA	NA	1.32e+00	NA	NA	NA	5.55e+00	4.19e+00
D	SSL3	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
D	SSL3	240	1.10e+01	3.42e+00	2.28e+00	1.52e+00	1.03e+00	6.86e-01	9.44e+00	7.16e+00	5.43e+00	4.35e+00	3.60e+00
D	SSL3	240	1.09e+01	3.51e+00	2.25e+00	1.56e+00	1.03e+00	6.73e-01	9.15e+00	6.92e+00	5.21e+00	4.13e+00	3.41e+00
D	SSL3	240	2.13e+01	7.47e+00	4.66e+00	3.13e+00	2.05e+00	1.29e+00	1.77e+01	1.31e+01	9.60e+00	7.45e+00	6.07e+00
D	SSL3	240	1.87e+01	6.47e+00	4.02e+00	2.68e+00	1.58e+00	1.02e+00	1.48e+01	1.08e+01	7.75e+00	6.09e+00	5.00e+00
D	SSL3	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
D	SSL3	720	1.06e+01	3.82e+00	2.34e+00	1.55e+00	1.03e+00	6.75e-01	8.41e+00	5.85e+00	4.21e+00	3.08e+00	2.36e+00
D	SSL3	720	1.06e+01	3.88e+00	2.38e+00	1.56e+00	1.03e+00	6.84e-01	8.32e+00	5.77e+00	4.15e+00	3.02e+00	2.29e+00
D	SSL3	720	2.03e+01	8.52e+00	4.84e+00	3.19e+00	2.05e+00	1.30e+00	1.60e+01	1.07e+01	7.46e+00	5.19e+00	3.82e+00
D	SSL3	720	1.84e+01	7.52e+00	4.36e+00	2.82e+00	1.82e+00	1.20e+00	1.46e+01	9.88e+00	6.89e+00	4.92e+00	3.65e+00
D	SSL3	720	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
D	ST	2	9.17e+00	3.92e+00	2.46e+00	1.45e+00	9.43e-01	7.84e-01	1.16e+01	7.43e+00	4.84e+00	3.16e+00	1.83e+00
D	ST	2	9.12e+00	3.98e+00	2.49e+00	1.51e+00	9.58e-01	6.68e-01	1.14e+01	7.19e+00	4.49e+00	2.82e+00	1.67e+00
D	ST	2	1.75e+01	8.53e+00	5.39e+00	3.29e+00	2.24e+00	1.62e+00	2.49e+01	1.58e+01	1.00e+01	6.21e+00	3.48e+00
D	ST	2	1.57e+01	8.12e+00	4.88e+00	3.12e+00	2.03e+00	1.41e+00	2.18e+01	1.34e+01	7.86e+00	4.33e+00	1.92e+00
D	ST	2	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
D	ST	48	9.09e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
D	ST	48	9.10e+00	3.98e+00	2.48e+00	1.76e+00	1.29e+00	9.71e-01	1.34e+01	9.24e+00	6.16e+00	3.88e+00	2.24e+00
D	ST	48	1.74e+01	7.90e+00	4.88e+00	3.09e+00	1.88e+00	1.67e+00	2.44e+01	1.62e+01	1.07e+01	7.37e+00	4.56e+00
D	ST	48	1.57e+01	7.07e+00	4.64e+00	2.83e+00	1.80e+00	1.58e+00	2.26e+01	1.48e+01	9.95e+00	6.77e+00	4.17e+00
D	ST	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
D	ST	240	9.29e+00	3.92e+00	2.42e+00	1.87e+00	1.27e+00	7.87e-01	1.40e+01	1.02e+01	6.94e+00	4.69e+00	3.26e+00
D	ST	240	9.21e+00	4.01e+00	2.34e+00	2.05e+00	1.27e+00	7.62e-01	1.47e+01	1.07e+01	7.14e+00	4.84e+00	3.45e+00
D	ST	240	1.89e+01	7.74e+00	4.98e+00	3.89e+00	2.72e+00	1.83e+00	2.93e+01	2.09e+01	1.40e+01	9.22e+00	5.95e+00
D	ST	240	1.59e+01	6.99e+00	3.66e+00	3.17e+00	2.17e+00	1.35e+00	2.42e+01	1.81e+01	1.25e+01	8.67e+00	6.26e+00
D	ST	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
D	ST	720	8.78e+00	4.10e+00	2.52e+00	1.66e+00	1.04e+00	5.49e-01	1.24e+01	8.14e+00	5.07e+00	3.25e+00	2.28e+00
D	ST	720	8.91e+00	4.13e+00	2.68e+00	1.71e+00	1.06e+00	6.13e-01	1.25e+01	8.10e+00	4.98e+00	3.12e+00	2.03e+00
D	ST	720	1.75e+01	7.89e+00	5.01e+00	3.17e+00	1.84e+00	1.26e+00	2.42e+01	1.58e+01	1.01e+01	6.77e+00	4.60e+00
D	ST	720	1.54e+01	7.23e+00	4.51e+00	2.96e+00	1.67e+00	1.09e+00	2.37e+01	1.61e+01	1.06e+01	7.53e+00	5.57e+00
D	ST	720	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00

Table E.5 – continued from previous page

MC	S	t_{Ads}	C_{CTRL}	C_A	C_{D1}	C_{D2}	C_{D3}	C_{D4}	q_A	q_{D1}	q_{D2}	q_{D3}	q_{D4}
D	W	2	1.08e+01	3.80e+00	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
D	W	2	1.06e+01	3.69e+00	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
D	W	2	2.07e+01	7.61e+00	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
D	W	2	1.88e+01	6.64e+00	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
D	W	2	0.00e+00	0.00e+00	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
D	W	48	8.87e+00	2.86e+00	1.56e+00	1.12e+00	9.08e-01	7.55e-01	8.95e+00	7.36e+00	6.19e+00	5.24e+00	4.40e+00
D	W	48	9.02e+00	2.92e+00	1.87e+00	2.46e+00	9.21e-01	7.99e-01	1.09e+01	8.95e+00	6.46e+00	5.49e+00	4.61e+00
D	W	48	1.81e+01	4.80e+00	3.50e+00	2.43e+00	1.93e+00	1.55e+00	1.85e+01	1.49e+01	1.25e+01	1.05e+01	8.75e+00
D	W	48	1.75e+01	4.64e+00	2.24e+00	1.29e+00	8.39e-01	8.73e-01	1.35e+01	1.11e+01	9.78e+00	8.91e+00	7.96e+00
D	W	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
D	W	240	1.06e+01	2.75e+00	1.88e+00	1.34e+00	8.40e-01	7.77e-01	1.03e+01	8.08e+00	6.27e+00	5.36e+00	4.56e+00
D	W	240	1.05e+01	2.71e+00	1.86e+00	1.32e+00	8.64e-01	7.79e-01	1.02e+01	8.03e+00	6.28e+00	5.33e+00	4.53e+00
D	W	240	2.06e+01	5.51e+00	3.80e+00	2.66e+00	2.00e+00	1.49e+00	2.04e+01	1.59e+01	1.24e+01	1.03e+01	8.68e+00
D	W	240	1.79e+01	4.39e+00	2.78e+00	1.88e+00	1.28e+00	7.90e-01	1.58e+01	1.24e+01	9.95e+00	8.56e+00	7.72e+00
D	W	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
D	W	720	1.09e+01	2.31e+00	1.74e+00	1.36e+00	9.73e-01	4.15e-01	8.19e+00	6.37e+00	4.87e+00	3.84e+00	3.39e+00
D	W	720	1.08e+01	2.38e+00	1.77e+00	1.35e+00	3.86e-01	3.47e-01	7.17e+00	5.33e+00	3.85e+00	3.45e+00	3.06e+00
D	W	720	2.08e+01	5.08e+00	3.69e+00	2.73e+00	1.68e+00	9.90e-01	1.65e+01	1.27e+01	9.72e+00	7.96e+00	6.86e+00
D	W	720	1.87e+01	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
D	W	720	0.00e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
D	W1	2	1.03e+01	5.67e+00	2.60e+00	1.46e+00	9.01e-01	6.37e-01	7.79e+00	5.06e+00	3.43e+00	2.51e+00	1.84e+00
D	W1	2	1.03e+01	5.75e+00	2.60e+00	1.47e+00	8.98e-01	6.37e-01	7.81e+00	5.07e+00	3.45e+00	2.53e+00	1.86e+00
D	W1	2	1.97e+01	1.19e+01	5.29e+00	2.80e+00	1.63e+00	1.10e+00	1.45e+01	8.95e+00	5.86e+00	4.18e+00	3.02e+00
D	W1	2	1.78e+01	1.02e+01	4.73e+00	2.60e+00	1.57e+00	1.06e+00	1.37e+01	8.74e+00	5.86e+00	4.25e+00	3.13e+00
D	W1	2	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
D	W1	48	1.02e+01	5.00e+00	2.64e+00	1.57e+00	9.77e-01	6.73e-01	8.60e+00	5.69e+00	4.10e+00	3.00e+00	2.29e+00
D	W1	48	1.03e+01	4.95e+00	2.68e+00	1.59e+00	9.75e-01	6.87e-01	8.79e+00	5.87e+00	4.24e+00	3.13e+00	2.40e+00
D	W1	48	1.97e+01	1.07e+01	5.50e+00	2.46e+00	1.74e+00	1.21e+00	1.52e+01	9.20e+00	6.70e+00	4.74e+00	3.47e+00
D	W1	48	1.78e+01	9.00e+00	4.85e+00	2.44e+00	1.64e+00	1.13e+00	1.43e+01	8.99e+00	6.53e+00	4.69e+00	3.50e+00
D	W1	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
D	W1	240	1.03e+01	4.38e+00	2.48e+00	1.56e+00	9.45e-01	6.03e-01	8.72e+00	6.28e+00	4.46e+00	3.52e+00	2.88e+00
D	W1	240	1.03e+01	4.42e+00	2.47e+00	1.56e+00	9.38e-01	6.09e-01	8.57e+00	6.16e+00	4.34e+00	3.39e+00	2.75e+00
D	W1	240	1.98e+01	1.02e+01	5.13e+00	3.02e+00	1.78e+00	1.09e+00	1.59e+01	1.09e+01	7.36e+00	5.54e+00	4.40e+00
D	W1	240	1.76e+01	8.26e+00	4.35e+00	2.63e+00	1.59e+00	1.01e+00	1.48e+01	1.06e+01	7.49e+00	5.88e+00	4.82e+00
D	W1	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
D	W1	720	1.01e+01	4.73e+00	2.56e+00	1.50e+00	9.37e-01	6.01e-01	7.84e+00	4.89e+00	3.30e+00	2.31e+00	1.67e+00
D	W1	720	9.96e+00	4.77e+00	2.55e+00	1.56e+00	9.27e-01	5.94e-01	7.76e+00	4.89e+00	3.28e+00	2.30e+00	1.66e+00
D	W1	720	1.91e+01	1.04e+01	5.35e+00	2.86e+00	1.69e+00	1.03e+00	1.46e+01	8.47e+00	5.43e+00	3.63e+00	2.52e+00
D	W1	720	1.72e+01	8.57e+00	4.55e+00	2.53e+00	1.64e+00	1.02e+00	1.37e+01	8.48e+00	5.80e+00	4.07e+00	2.97e+00
D	W1	720	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00

Table E.5 – continued from previous page

MC	S	t_{Ads}	C_{CTRL}	C_A	C_{D1}	C_{D2}	C_{D3}	C_{D4}	q_A	q_{D1}	q_{D2}	q_{D3}	q_{D4}
D	W2	2	1.04e+01	5.57e+00	2.61e+00	1.48e+00	9.11e-01	6.35e-01	7.92e+00	5.17e+00	3.54e+00	2.60e+00	1.94e+00
D	W2	2	1.04e+01	5.63e+00	2.64e+00	1.48e+00	9.12e-01	6.47e-01	7.93e+00	5.14e+00	3.50e+00	2.57e+00	1.88e+00
D	W2	2	2.01e+01	1.20e+01	5.32e+00	2.83e+00	1.69e+00	1.11e+00	1.46e+01	8.96e+00	5.81e+00	4.09e+00	2.88e+00
D	W2	2	1.80e+01	1.04e+01	4.83e+00	2.62e+00	1.55e+00	1.08e+00	1.38e+01	8.76e+00	5.84e+00	4.26e+00	3.10e+00
D	W2	2	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
D	W2	48	1.04e+01	4.85e+00	2.68e+00	1.64e+00	9.92e-01	6.84e-01	8.14e+00	5.18e+00	3.52e+00	2.39e+00	1.66e+00
D	W2	48	1.05e+01	4.99e+00	2.68e+00	1.65e+00	9.94e-01	6.94e-01	8.69e+00	5.68e+00	4.04e+00	2.91e+00	2.19e+00
D	W2	48	2.00e+01	1.07e+01	5.49e+00	3.13e+00	1.79e+00	1.20e+00	1.61e+01	9.89e+00	6.72e+00	4.69e+00	3.44e+00
D	W2	48	1.80e+01	8.97e+00	4.83e+00	2.81e+00	1.67e+00	1.16e+00	1.52e+01	9.71e+00	6.89e+00	5.00e+00	3.78e+00
D	W2	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
D	W2	240	1.04e+01	4.26e+00	2.53e+00	1.54e+00	9.27e-01	6.01e-01	8.55e+00	6.00e+00	4.34e+00	3.42e+00	2.78e+00
D	W2	240	1.05e+01	4.22e+00	2.55e+00	1.55e+00	9.67e-01	6.31e-01	8.86e+00	6.27e+00	4.57e+00	3.61e+00	2.93e+00
D	W2	240	1.92e+01	9.41e+00	5.19e+00	3.04e+00	1.75e+00	1.08e+00	1.56e+01	1.03e+01	6.97e+00	5.22e+00	4.08e+00
D	W2	240	1.79e+01	7.73e+00	4.45e+00	2.69e+00	1.60e+00	1.03e+00	1.49e+01	1.03e+01	7.36e+00	5.77e+00	4.65e+00
D	W2	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
D	W2	720	1.01e+01	4.78e+00	2.57e+00	1.52e+00	9.49e-01	6.18e-01	7.47e+00	4.80e+00	3.29e+00	2.25e+00	1.59e+00
D	W2	720	1.01e+01	4.76e+00	2.62e+00	1.54e+00	9.58e-01	6.12e-01	7.71e+00	4.87e+00	3.33e+00	2.27e+00	1.60e+00
D	W2	720	1.94e+01	1.03e+01	5.25e+00	2.95e+00	1.74e+00	1.07e+00	1.42e+01	8.49e+00	5.52e+00	3.61e+00	2.45e+00
D	W2	720	1.75e+01	8.82e+00	4.63e+00	2.65e+00	1.63e+00	1.05e+00	1.35e+01	8.46e+00	5.79e+00	3.97e+00	2.84e+00
D	W2	720	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
D	Z	2	1.15e+01	7.69e-01	NA	NA	5.40e-01	NA	NA	NA	NA	NA	0.00e+00
D	Z	2	1.16e+01	7.88e-01	5.42e-01	5.58e-01	NA	4.80e-01	NA	NA	NA	1.46e+01	1.39e+01
D	Z	2	2.24e+01	1.83e+00	1.22e+00	1.13e+00	1.11e+00	1.01e+00	3.47e+01	3.26e+01	3.06e+01	2.87e+01	2.70e+01
D	Z	2	2.00e+01	1.45e+00	1.03e+00	9.55e-01	6.48e-01	8.68e-01	3.01e+01	2.84e+01	2.68e+01	2.56e+01	2.41e+01
D	Z	2	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
D	Z	48	1.06e+01	5.11e-01	5.26e-01	4.66e-01	4.04e-01	4.20e-01	1.76e+01	1.67e+01	1.58e+01	1.51e+01	1.44e+01
D	Z	48	1.06e+01	6.29e-01	5.93e-01	5.47e-01	4.26e-01	4.64e-01	1.85e+01	1.75e+01	1.66e+01	1.58e+01	1.50e+01
D	Z	48	2.05e+01	1.07e+00	1.14e+00	1.06e+00	8.59e-01	9.17e-01	3.35e+01	3.16e+01	2.97e+01	2.82e+01	2.66e+01
D	Z	48	1.96e+01	1.32e+00	1.20e+00	1.08e+00	9.39e-01	8.97e-01	3.54e+01	3.33e+01	3.15e+01	2.99e+01	2.82e+01
D	Z	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
D	Z	240	1.06e+01	5.88e-01	5.60e-01	5.23e-01	4.55e-01	4.40e-01	2.04e+01	1.96e+01	1.87e+01	1.79e+01	1.72e+01
D	Z	240	1.06e+01	5.24e-01	5.34e-01	4.82e-01	3.64e-01	4.20e-01	2.10e+01	2.00e+01	1.92e+01	1.86e+01	1.78e+01
D	Z	240	2.04e+01	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
D	Z	240	1.92e+01	1.05e+00	1.01e+00	9.60e-01	6.13e-01	8.12e-01	3.65e+01	3.48e+01	3.32e+01	3.21e+01	3.07e+01
D	Z	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
D	Z	720	1.06e+01	4.88e-01	5.04e-01	3.59e-01	8.50e-02	0.00e+00	1.83e+01	1.74e+01	1.68e+01	1.66e+01	1.66e+01
D	Z	720	1.06e+01	4.64e-01	4.53e-01	3.27e-01	1.81e-01	0.00e+00	1.84e+01	1.76e+01	1.71e+01	1.68e+01	1.68e+01
D	Z	720	2.04e+01	9.57e-01	9.38e-01	1.02e-01	2.98e-01	2.93e-01	3.36e+01	3.20e+01	3.18e+01	3.13e+01	3.08e+01
D	Z	720	1.90e+01	9.40e-01	9.04e-01	7.62e-01	2.34e-01	2.49e-01	3.20e+01	3.04e+01	2.91e+01	2.86e+01	2.82e+01
D	Z	720	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00

Table E.5 – continued from previous page

MC	S	t_{Ads}	C_{CTRL}	C_A	C_{D1}	C_{D2}	C_{D3}	C_{D4}	q_A	q_{D1}	q_{D2}	q_{D3}	q_{D4}
H	AM	2	8.46e-01	3.22e-01	2.12e-01	1.65e-01	1.05e-01	4.54e-02	8.80e-01	6.43e-01	4.70e-01	3.55e-01	3.07e-01
H	AM	2	8.51e-01	3.21e-01	1.95e-01	7.41e-02	9.13e-02	8.01e-02	8.66e-01	6.50e-01	5.74e-01	4.74e-01	3.90e-01
H	AM	2	1.54e+00	6.92e-01	4.02e-01	2.22e-01	1.64e-01	1.20e-01	1.45e+00	1.01e+00	7.82e-01	6.03e-01	4.79e-01
H	AM	2	1.61e+00	7.15e-01	4.24e-01	2.37e-01	NA	1.43e-01	NA	NA	NA	8.17e-01	6.71e-01
H	AM	2	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
H	AM	48	8.55e-01	3.72e-01	2.29e-01	1.56e-01	0.00e+00	7.59e-02	9.40e-01	6.95e-01	5.31e-01	5.31e-01	4.52e-01
H	AM	48	8.62e-01	3.63e-01	2.33e-01	1.62e-01	1.95e-01	7.76e-02	1.16e+00	9.15e-01	7.46e-01	5.38e-01	4.58e-01
H	AM	48	1.52e+00	7.27e-01	4.26e-01	2.67e-01	1.76e-01	1.23e-01	1.68e+00	1.23e+00	9.44e-01	7.59e-01	6.36e-01
H	AM	48	1.61e+00	6.92e-01	4.45e-01	2.96e-01	NA	1.41e-01	NA	NA	NA	7.82e-01	6.37e-01
H	AM	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	NA	0.00e+00	NA	NA	NA	0.00e+00	0.00e+00
H	AM	240	8.26e-01	6.97e-01	2.58e-01	0.00e+00	0.00e+00	5.45e-02	6.96e-01	4.31e-01	4.31e-01	4.31e-01	3.74e-01
H	AM	240	8.22e-01	2.68e-01	3.03e-02	1.26e-01	5.52e-02	5.12e-02	6.45e-01	6.13e-01	4.82e-01	4.25e-01	3.72e-01
H	AM	240	1.30e+00	5.95e-01	3.36e-01	1.54e-01	1.14e-01	7.70e-02	1.21e+00	8.66e-01	7.03e-01	5.87e-01	5.05e-01
H	AM	240	1.58e+00	6.29e-02	3.38e-01	NA	0.00e+00	0.00e+00	NA	NA	1.87e-01	1.87e-01	1.87e-01
H	AM	240	0.00e+00	NA	0.00e+00	0.00e+00	NA	NA	NA	NA	NA	NA	0.00e+00
H	AM	720	8.46e-01	2.45e-01	0.00e+00	1.04e-01	0.00e+00	0.00e+00	2.72e-01	2.72e-01	1.65e-01	1.65e-01	1.65e-01
H	AM	720	8.43e-01	2.32e-01	0.00e+00	9.81e-02	0.00e+00	0.00e+00	2.97e-01	2.97e-01	1.96e-01	1.96e-01	1.96e-01
H	AM	720	1.16e+00	3.90e-01	0.00e+00	1.79e-01	0.00e+00	7.82e-02	5.43e-01	5.43e-01	3.59e-01	3.59e-01	2.76e-01
H	AM	720	1.60e+00	4.83e-01	0.00e+00	0.00e+00	0.00e+00	9.74e-02	1.04e-01	1.04e-01	1.04e-01	1.04e-01	0.00e+00
H	AM	720	0.00e+00	0.00e+00	0.00e+00	NA	NA	0.00e+00	NA	NA	NA	0.00e+00	0.00e+00
H	B	2	9.73e-01	8.01e-01	3.13e-01	NA	NA	NA	NA	NA	NA	NA	0.00e+00
H	B	2	9.78e-01	8.25e-01	4.40e-01	NA	NA	NA	NA	NA	NA	NA	0.00e+00
H	B	2	1.57e+00	1.22e+00	5.06e-01	NA	NA	NA	NA	NA	NA	NA	0.00e+00
H	B	2	1.59e+00	1.37e+00	5.78e-01	NA	NA	NA	NA	NA	NA	NA	0.00e+00
H	B	2	0.00e+00	0.00e+00	0.00e+00	NA	NA	NA	NA	NA	NA	NA	0.00e+00
H	B	48	9.28e-01	1.00e+00	3.04e-01	1.15e-01	5.59e-02	3.48e-02	5.29e-01	2.15e-01	9.40e-02	3.66e-02	0.00e+00
H	B	48	9.31e-01	5.45e-01	2.96e-01	1.13e-01	5.33e-02	3.62e-02	5.19e-01	2.12e-01	9.27e-02	3.82e-02	0.00e+00
H	B	48	1.26e+00	9.49e-01	3.59e-01	2.00e-01	6.95e-02	4.44e-02	7.07e-01	3.30e-01	1.17e-01	4.74e-02	0.00e+00
H	B	48	1.50e+00	1.05e+00	4.34e-01	1.63e-01	6.80e-02	2.85e-02	7.10e-01	2.70e-01	9.89e-02	3.04e-02	0.00e+00
H	B	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
H	B	240	9.06e-01	5.13e-01	1.85e-01	7.96e-02	6.67e-02	2.65e-02	4.21e-01	1.98e-01	9.89e-02	2.76e-02	0.00e+00
H	B	240	8.96e-01	7.37e-01	2.41e-01	1.13e-01	4.05e-02	2.72e-02	4.97e-01	2.15e-01	7.18e-02	2.88e-02	0.00e+00
H	B	240	1.18e+00	8.66e-01	3.41e-01	2.05e-01	8.47e-02	4.06e-02	7.96e-01	3.91e-01	1.34e-01	4.31e-02	0.00e+00
H	B	240	1.54e+00	1.27e+00	5.08e-01	1.76e-01	2.76e-01	0.00e+00	1.10e+00	5.01e-01	2.94e-01	0.00e+00	0.00e+00
H	B	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	NA	0.00e+00	NA	NA	NA	0.00e+00	0.00e+00
H	B	720	9.31e-01	5.17e-01	2.08e-01	1.04e-01	4.71e-02	3.06e-02	4.12e-01	1.95e-01	8.25e-02	3.43e-02	0.00e+00
H	B	720	9.35e-01	7.12e-01	2.42e-01	8.84e-02	3.83e-02	0.00e+00	3.80e-01	1.36e-01	3.96e-02	0.00e+00	0.00e+00
H	B	720	1.66e+00	9.88e-01	3.46e-01	1.36e-01	6.15e-02	3.27e-02	6.06e-01	2.46e-01	1.01e-01	3.58e-02	0.00e+00
H	B	720	1.76e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
H	B	720	0.00e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00

Table E.5 – continued from previous page

MC	S	t_{Ads}	C_{CTRL}	C_A	C_{D1}	C_{D2}	C_{D3}	C_{D4}	q_A	q_{D1}	q_{D2}	q_{D3}	q_{D4}
H	BA	2	9.34e-01	6.84e-01	2.89e-01	1.14e-01	5.75e-02	3.46e-02	5.15e-01	2.18e-01	9.50e-02	3.47e-02	0.00e+00
H	BA	2	9.40e-01	6.96e-01	2.83e-01	1.14e-01	5.88e-02	3.77e-02	5.10e-01	2.21e-01	9.84e-02	3.65e-02	0.00e+00
H	BA	2	1.71e+00	1.23e+00	4.75e-01	1.95e-01	9.37e-02	5.39e-02	9.07e-01	4.21e-01	2.12e-01	1.13e-01	5.83e-02
H	BA	2	1.77e+00	1.27e+00	5.06e-01	2.17e-01	9.97e-02	5.16e-02	9.67e-01	4.49e-01	2.15e-01	1.09e-01	5.60e-02
H	BA	2	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
H	BA	48	9.51e-01	6.92e-01	2.94e-01	1.28e-01	6.14e-02	3.50e-02	5.35e-01	2.35e-01	1.02e-01	3.67e-02	0.00e+00
H	BA	48	9.58e-01	6.75e-01	2.98e-01	1.29e-01	6.18e-02	3.61e-02	5.48e-01	2.38e-01	1.03e-01	3.78e-02	0.00e+00
H	BA	48	1.72e+00	1.28e+00	5.19e-01	2.17e-01	9.41e-02	4.92e-02	9.17e-01	3.82e-01	1.51e-01	5.19e-02	0.00e+00
H	BA	48	1.78e+00	1.35e+00	5.64e-01	2.48e-01	1.06e-01	5.44e-02	1.01e+00	4.28e-01	1.68e-01	5.61e-02	0.00e+00
H	BA	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
H	BA	240	9.20e-01	7.06e-01	2.91e-01	NA	5.05e-02	3.14e-02	NA	NA	8.51e-02	3.38e-02	0.00e+00
H	BA	240	9.20e-01	6.87e-01	2.94e-01	1.17e-01	5.51e-02	3.25e-02	5.17e-01	2.16e-01	9.12e-02	3.47e-02	0.00e+00
H	BA	240	1.49e+00	1.09e+00	4.67e-01	1.97e-01	7.90e-02	3.69e-02	8.16e-01	3.30e-01	1.21e-01	3.94e-02	0.00e+00
H	BA	240	1.75e+00	1.27e+00	5.60e-01	2.25e-01	8.62e-02	4.14e-02	9.49e-01	3.71e-01	1.32e-01	4.46e-02	0.00e+00
H	BA	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
H	BA	720	9.05e-01	9.34e-01	2.73e-01	1.12e-01	4.86e-02	0.00e+00	4.59e-01	1.72e-01	5.30e-02	0.00e+00	0.00e+00
H	BA	720	9.02e-01	7.14e-01	2.71e-01	1.15e-01	4.74e-02	0.00e+00	4.58e-01	1.75e-01	5.17e-02	0.00e+00	0.00e+00
H	BA	720	1.15e+00	9.15e-01	5.01e-01	2.18e-01	7.85e-02	0.00e+00	8.40e-01	3.02e-01	8.42e-02	0.00e+00	0.00e+00
H	BA	720	1.74e+00	1.41e+00	5.31e-01	2.11e-01	8.64e-02	0.00e+00	8.92e-01	3.15e-01	9.36e-02	0.00e+00	0.00e+00
H	BA	720	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
H	BOX	2	9.01e-01	2.98e-01	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
H	BOX	2	8.96e-01	3.28e-01	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
H	BOX	2	1.43e+00	6.09e-01	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
H	BOX	2	1.46e+00	5.91e-01	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
H	BOX	2	0.00e+00	0.00e+00	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
H	BOX	48	8.40e-01	NA	9.74e-02	2.18e-01	1.26e-01	9.59e-02	8.64e-01	7.60e-01	5.27e-01	3.92e-01	2.91e-01
H	BOX	48	8.50e-01	2.77e-01	1.08e-01	2.12e-01	1.31e-01	1.00e-01	8.03e-01	6.89e-01	4.62e-01	3.22e-01	2.16e-01
H	BOX	48	1.14e+00	3.11e-01	2.04e-01	3.08e-01	1.99e-01	0.00e+00	9.72e-01	7.62e-01	4.37e-01	2.25e-01	2.25e-01
H	BOX	48	1.35e+00	7.44e-01	2.12e-01	7.32e-02	8.23e-02	6.62e-02	2.42e+00	2.20e+00	2.13e+00	2.04e+00	1.97e+00
H	BOX	48	0.00e+00	NA	0.00e+00	0.00e+00	0.00e+00	NA	NA	NA	NA	NA	0.00e+00
H	BOX	240	8.21e-01	1.56e-01	3.40e-01	1.49e-01	7.77e-02	6.10e-02	1.02e+00	5.97e-01	3.98e-01	3.17e-01	2.52e-01
H	BOX	240	8.17e-01	1.49e-01	8.51e-02	0.00e+00	7.74e-02	6.46e-02	4.97e-01	3.91e-01	3.91e-01	3.10e-01	2.41e-01
H	BOX	240	1.07e+00	3.13e-01	2.12e-01	1.46e-01	1.27e-01	8.35e-02	1.03e+00	7.71e-01	5.74e-01	4.42e-01	3.53e-01
H	BOX	240	1.39e+00	5.13e-01	2.87e-01	NA	1.11e-01	8.05e-02	NA	NA	5.90e-01	4.74e-01	3.88e-01
H	BOX	240	0.00e+00	0.00e+00	0.00e+00	NA	0.00e+00	0.00e+00	NA	NA	0.00e+00	0.00e+00	0.00e+00
H	BOX	720	8.40e-01	1.26e+00	5.54e-01	1.16e-01	1.48e-01	5.99e-02	1.11e+00	5.27e-01	4.01e-01	2.49e-01	1.84e-01
H	BOX	720	8.39e-01	2.41e-01	9.63e-02	1.20e-01	6.99e-02	5.94e-02	5.51e-01	4.50e-01	3.20e-01	2.48e-01	1.84e-01
H	BOX	720	1.49e+00	2.88e-01	2.14e-01	2.16e-01	1.27e-01	9.12e-02	1.08e+00	8.53e-01	6.18e-01	4.87e-01	3.87e-01
H	BOX	720	1.58e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
H	BOX	720	0.00e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00

Table E.5 – continued from previous page

MC	S	t_{Ads}	C_{CTRL}	C_A	C_{D1}	C_{D2}	C_{D3}	C_{D4}	q_A	q_{D1}	q_{D2}	q_{D3}	q_{D4}
H	BT	2	9.37e-01	6.99e-01	2.57e-01	9.89e-02	4.98e-02	3.62e-02	4.69e-01	1.96e-01	9.04e-02	3.75e-02	0.00e+00
H	BT	2	9.34e-01	7.02e-01	2.60e-01	1.02e-01	5.29e-02	3.14e-02	4.71e-01	1.98e-01	8.93e-02	3.26e-02	0.00e+00
H	BT	2	1.70e+00	1.26e+00	4.54e-01	1.73e-01	8.09e-02	4.24e-02	7.83e-01	3.12e-01	1.29e-01	4.38e-02	0.00e+00
H	BT	2	1.77e+00	1.31e+00	5.01e-01	1.97e-01	8.92e-02	4.69e-02	8.72e-01	3.52e-01	1.44e-01	4.94e-02	0.00e+00
H	BT	2	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
H	BT	48	9.49e-01	7.17e-01	2.70e-01	1.13e-01	5.94e-02	3.99e-02	4.97e-01	2.22e-01	1.05e-01	4.26e-02	0.00e+00
H	BT	48	9.49e-01	7.52e-01	4.15e-01	2.24e-01	1.04e-01	7.75e-02	1.11e+00	7.00e-01	4.68e-01	3.60e-01	2.80e-01
H	BT	48	1.68e+00	1.34e+00	4.87e-01	1.93e-01	8.06e-02	4.23e-02	8.21e-01	3.32e-01	1.28e-01	4.40e-02	0.00e+00
H	BT	48	1.79e+00	1.45e+00	5.56e-01	2.24e-01	1.49e-01	8.59e-02	1.03e+00	4.74e-01	2.44e-01	8.90e-02	0.00e+00
H	BT	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	NA	NA	NA	NA	NA	0.00e+00
H	BT	240	9.20e-01	6.77e-01	2.64e-01	9.58e-02	3.87e-02	0.00e+00	4.14e-01	1.42e-01	4.04e-02	0.00e+00	0.00e+00
H	BT	240	9.23e-01	6.85e-01	2.66e-01	9.53e-02	4.10e-02	0.00e+00	4.16e-01	1.41e-01	4.02e-02	0.00e+00	0.00e+00
H	BT	240	1.50e+00	1.09e+00	4.17e-01	1.51e-01	6.21e-02	0.00e+00	6.48e-01	2.21e-01	6.21e-02	0.00e+00	0.00e+00
H	BT	240	1.76e+00	1.32e+00	5.07e-01	1.86e-01	7.20e-02	0.00e+00	8.01e-01	2.74e-01	7.15e-02	0.00e+00	0.00e+00
H	BT	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
H	BT	720	9.13e-01	6.82e-01	0.00e+00	9.21e-02	4.22e-02	0.00e+00	1.37e-01	1.37e-01	4.75e-02	0.00e+00	0.00e+00
H	BT	720	9.07e-01	6.87e-01	2.40e-01	9.69e-02	4.72e-02	NA	NA	NA	NA	NA	0.00e+00
H	BT	720	1.15e+00	8.75e-01	4.76e-01	1.87e-01	6.57e-02	0.00e+00	7.29e-01	2.65e-01	7.17e-02	0.00e+00	0.00e+00
H	BT	720	1.73e+00	1.06e+00	3.25e-01	1.47e-01	7.89e-02	0.00e+00	5.56e-01	2.30e-01	8.58e-02	0.00e+00	0.00e+00
H	BT	720	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
H	BU	2	9.37e-01	2.59e-01	1.37e-01	NA	NA	NA	NA	NA	NA	NA	0.00e+00
H	BU	2	9.43e-01	2.64e-01	1.05e-01	NA	NA	NA	NA	NA	NA	NA	0.00e+00
H	BU	2	1.51e+00	5.10e-01	2.21e-01	NA	NA	NA	NA	NA	NA	NA	0.00e+00
H	BU	2	1.52e+00	4.36e-01	2.11e-01	NA	NA	NA	NA	NA	NA	NA	0.00e+00
H	BU	2	0.00e+00	0.00e+00	0.00e+00	NA	NA	NA	NA	NA	NA	NA	0.00e+00
H	BU	48	8.36e-01	1.52e-01	8.87e-02	6.41e-02	6.15e-02	5.90e-02	9.52e-01	8.53e-01	7.86e-01	7.21e-01	6.58e-01
H	BU	48	8.64e-01	1.37e-01	6.79e-02	5.04e-02	5.94e-02	5.36e-02	6.54e-01	5.78e-01	5.26e-01	4.64e-01	4.06e-01
H	BU	48	1.20e+00	2.08e-01	1.12e-01	9.84e-02	1.02e-01	9.06e-02	1.35e+00	1.23e+00	1.13e+00	1.02e+00	9.21e-01
H	BU	48	1.45e+00	2.84e-01	2.23e-01	1.41e-01	1.23e-01	1.11e-01	1.63e+00	1.38e+00	1.24e+00	1.11e+00	9.90e-01
H	BU	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
H	BU	240	8.62e-01	1.03e-01	7.94e-02	6.34e-02	5.46e-02	5.59e-02	1.03e+00	9.28e-01	8.44e-01	7.87e-01	7.28e-01
H	BU	240	8.58e-01	7.94e-02	8.14e-02	6.20e-02	5.53e-02	5.64e-02	8.43e-01	7.56e-01	6.75e-01	6.17e-01	5.57e-01
H	BU	240	1.12e+00	1.93e-01	1.32e-01	1.12e-01	8.79e-02	8.14e-02	1.26e+00	1.10e+00	9.88e-01	8.96e-01	8.10e-01
H	BU	240	1.46e+00	2.45e-01	1.01e-01	1.15e-01	8.76e-02	8.12e-02	1.48e+00	1.36e+00	1.24e+00	1.15e+00	1.06e+00
H	BU	240	0.00e+00	0.00e+00	NA	0.00e+00	0.00e+00	0.00e+00	NA	0.00e+00	0.00e+00	0.00e+00	0.00e+00
H	BU	720	8.82e-01	8.21e-02	8.14e-02	NA	7.44e-02	4.59e-02	NA	NA	6.47e-01	5.70e-01	5.20e-01
H	BU	720	8.79e-01	1.19e-01	8.89e-02	NA	7.50e-02	5.43e-02	NA	NA	6.52e-01	5.74e-01	5.15e-01
H	BU	720	1.56e+00	1.88e-01	9.55e-02	NA	1.11e-01	8.19e-02	NA	NA	1.01e+00	8.90e-01	8.00e-01
H	BU	720	1.66e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
H	BU	720	0.00e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00

Table E.5 – continued from previous page

MC	S	t_{Ads}	C_{CTRL}	C_A	C_{D1}	C_{D2}	C_{D3}	C_{D4}	q_A	q_{D1}	q_{D2}	q_{D3}	q_{D4}
H	CM	2	8.86e-01	3.73e-01	NA	NA	NA	NA	NA	NA	NA	NA	NA
H	CM	2	8.77e-01	4.09e-01	NA	NA	NA	NA	NA	NA	NA	NA	NA
H	CM	2	1.37e+00	6.57e-01	NA	NA	NA	NA	NA	NA	NA	NA	NA
H	CM	2	1.41e+00	6.79e-01	NA	NA	NA	NA	NA	NA	NA	NA	NA
H	CM	2	0.00e+00	0.00e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA
H	CM	48	8.19e-01	3.33e-01	3.03e-01	2.33e-01	1.37e-01	9.78e-02	NA	NA	NA	NA	NA
H	CM	48	8.20e-01	3.07e-01	1.14e-01	2.13e-01	1.35e-01	9.57e-02	NA	NA	NA	NA	NA
H	CM	48	1.04e+00	4.62e-01	2.37e-01	2.72e-01	1.93e-01	1.38e-01	NA	NA	NA	NA	NA
H	CM	48	1.32e+00	5.57e-01	3.24e-01	2.21e-01	1.55e-01	1.18e-01	NA	NA	NA	NA	NA
H	CM	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	NA	NA	NA	NA	NA
H	CM	240	9.21e-01	1.31e-01	1.27e-01	1.66e-01	1.26e-01	8.46e-02	NA	NA	NA	NA	NA
H	CM	240	8.01e-01	2.86e-01	8.21e-02	1.19e-01	7.65e-02	6.86e-02	NA	NA	NA	NA	NA
H	CM	240	1.04e+00	4.32e-01	2.30e-01	2.32e-01	1.40e-01	1.13e-01	NA	NA	NA	NA	NA
H	CM	240	1.37e+00	4.92e-01	2.54e-01	2.19e-01	1.35e-01	1.02e-01	NA	NA	NA	NA	NA
H	CM	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	NA	NA	NA	NA	NA
H	CM	720	8.17e-01	1.45e-01	5.17e-01	1.01e-01	7.52e-02	8.62e-02	NA	NA	NA	NA	NA
H	CM	720	8.13e-01	2.59e-01	1.58e-01	8.19e-02	9.10e-02	6.49e-02	NA	NA	NA	NA	NA
H	CM	720	1.46e+00	3.96e-01	2.83e-01	1.53e-01	1.62e-01	1.07e-01	NA	NA	NA	NA	NA
H	CM	720	1.41e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
H	CM	720	0.00e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
H	ELL	2	8.54e-01	0.00e+00	1.52e-01	1.18e-01	9.71e-02	7.83e-02	8.51e-01	6.86e-01	5.64e-01	4.57e-01	3.75e-01
H	ELL	2	8.57e-01	1.68e-01	1.72e-01	1.16e-01	1.01e-01	8.39e-02	8.76e-01	6.90e-01	5.73e-01	4.61e-01	3.74e-01
H	ELL	2	1.55e+00	6.31e-01	3.38e-01	2.16e-01	1.67e-01	1.30e-01	1.43e+00	1.07e+00	8.43e-01	6.60e-01	5.24e-01
H	ELL	2	1.61e+00	5.27e-01	3.52e-01	2.42e-01	1.87e-01	1.46e-01	1.63e+00	1.25e+00	1.00e+00	7.96e-01	6.44e-01
H	ELL	2	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
H	ELL	48	8.69e-01	2.72e-01	1.90e-01	1.33e-01	9.78e-02	7.94e-02	9.43e-01	7.47e-01	6.12e-01	5.01e-01	4.19e-01
H	ELL	48	8.70e-01	3.80e-01	2.06e-01	1.39e-01	1.09e-01	8.26e-02	9.92e-01	7.75e-01	6.34e-01	5.11e-01	4.25e-01
H	ELL	48	1.56e+00	6.82e-01	3.74e-01	2.25e-01	1.78e-01	1.35e-01	1.57e+00	1.17e+00	9.45e-01	7.44e-01	6.03e-01
H	ELL	48	1.63e+00	5.39e-01	3.75e-01	2.56e-01	1.99e-01	1.50e-01	1.74e+00	1.35e+00	1.09e+00	8.64e-01	7.06e-01
H	ELL	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
H	ELL	240	8.57e-01	4.92e-01	1.95e-01	0.00e+00	6.46e-02	4.92e-02	8.24e-01	6.24e-01	6.24e-01	5.56e-01	5.04e-01
H	ELL	240	8.48e-01	1.82e-01	1.67e-01	3.25e-02	6.36e-02	5.25e-02	8.27e-01	6.55e-01	6.21e-01	5.55e-01	4.99e-01
H	ELL	240	1.38e+00	5.84e-02	3.62e-01	1.73e-01	1.26e-01	1.15e-01	1.59e+00	1.22e+00	1.03e+00	8.96e-01	7.74e-01
H	ELL	240	1.62e+00	0.00e+00	6.89e-02	0.00e+00	0.00e+00	0.00e+00	3.20e-01	2.49e-01	2.49e-01	2.49e-01	2.49e-01
H	ELL	240	0.00e+00	NA	NA	0.00e+00	NA	NA	NA	NA	NA	NA	0.00e+00
H	ELL	720	8.39e-01	1.37e-01	0.00e+00	7.13e-02	0.00e+00	0.00e+00	3.00e-01	3.00e-01	2.22e-01	2.22e-01	2.22e-01
H	ELL	720	8.28e-01	1.80e-01	0.00e+00	7.65e-02	0.00e+00	0.00e+00	2.90e-01	2.90e-01	2.05e-01	2.05e-01	2.05e-01
H	ELL	720	1.06e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
H	ELL	720	1.58e+00	0.00e+00	2.74e-01	1.93e-01	0.00e+00	0.00e+00	9.99e-01	7.12e-01	5.01e-01	5.01e-01	5.01e-01
H	ELL	720	0.00e+00	NA	NA	NA	NA	0.00e+00	NA	NA	NA	0.00e+00	0.00e+00

Table E.5 – continued from previous page

MC	S	t_{Ads}	C_{CTRL}	C_A	C_{D1}	C_{D2}	C_{D3}	C_{D4}	q_A	q_{D1}	q_{D2}	q_{D3}	q_{D4}
H	FT	2	9.02e-01	6.43e-01	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
H	FT	2	9.04e-01	5.79e-01	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
H	FT	2	1.42e+00	1.02e+00	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
H	FT	2	1.47e+00	9.65e-01	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
H	FT	2	0.00e+00	0.00e+00	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
H	FT	48	8.37e-01	5.24e-01	2.54e-01	1.44e-01	7.83e-02	4.25e-02	6.23e-01	3.54e-01	2.03e-01	1.22e-01	7.67e-02
H	FT	48	8.37e-01	4.85e-01	2.66e-01	1.29e-01	5.20e-02	4.80e-02	5.67e-01	2.92e-01	1.53e-01	9.93e-02	4.60e-02
H	FT	48	1.16e+00	7.43e-01	3.88e-01	2.06e-01	1.11e-01	0.00e+00	1.02e+00	6.19e-01	3.99e-01	2.86e-01	2.86e-01
H	FT	48	1.38e+00	9.57e-01	3.86e-01	1.86e-01	1.77e-01	5.97e-02	9.15e-01	5.25e-01	3.26e-01	1.43e-01	7.63e-02
H	FT	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
H	FT	240	8.22e-01	4.84e-01	2.44e-01	1.04e-01	6.00e-02	5.82e-02	6.30e-01	3.34e-01	1.92e-01	1.29e-01	6.69e-02
H	FT	240	8.27e-01	4.92e-01	2.36e-01	1.05e-01	6.46e-02	5.31e-02	6.11e-01	3.26e-01	1.84e-01	1.15e-01	5.86e-02
H	FT	240	1.09e+00	6.98e-01	3.31e-01	2.03e-01	1.06e-01	5.74e-02	9.12e-01	5.20e-01	2.42e-01	1.30e-01	6.96e-02
H	FT	240	1.41e+00	1.55e+00	2.77e-01	3.68e-01	7.86e-02	4.76e-02	1.10e+00	7.70e-01	2.79e-01	1.96e-01	1.44e-01
H	FT	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
H	FT	720	8.62e-01	5.30e-01	2.78e-01	1.55e-01	7.89e-02	4.36e-02	6.52e-01	3.62e-01	1.94e-01	1.08e-01	6.19e-02
H	FT	720	8.65e-01	4.14e-01	2.19e-01	1.02e-01	1.26e-01	4.11e-02	5.81e-01	3.55e-01	2.45e-01	1.07e-01	6.39e-02
H	FT	720	1.52e+00	7.13e-01	3.54e-01	1.69e-01	1.07e-01	6.66e-02	8.20e-01	4.50e-01	2.66e-01	1.50e-01	7.93e-02
H	FT	720	1.63e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
H	FT	720	0.00e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
H	GAS	2	9.03e-01	7.65e-02	0.00e+00	NA	NA	NA	NA	NA	NA	NA	0.00e+00
H	GAS	2	8.16e-01	7.94e-02	0.00e+00	NA	NA	NA	NA	NA	NA	NA	0.00e+00
H	GAS	2	1.40e+00	8.82e-02	0.00e+00	NA	NA	NA	NA	NA	NA	NA	0.00e+00
H	GAS	2	1.44e+00	7.76e-02	0.00e+00	NA	NA	NA	NA	NA	NA	NA	0.00e+00
H	GAS	2	0.00e+00	0.00e+00	0.00e+00	NA	NA	NA	NA	NA	NA	NA	0.00e+00
H	GAS	48	8.52e-01	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	2.67e-01	2.67e-01	2.67e-01	2.67e-01	2.67e-01
H	GAS	48	8.56e-01	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	3.20e-01	3.20e-01	3.20e-01	3.20e-01	3.20e-01
H	GAS	48	1.05e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	4.49e-01	4.49e-01	4.49e-01	4.49e-01	4.49e-01
H	GAS	48	1.36e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	3.56e-01	3.56e-01	3.56e-01	3.56e-01	3.56e-01
H	GAS	48	0.00e+00	0.00e+00	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
H	GAS	240	8.12e-01	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
H	GAS	240	8.14e-01	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
H	GAS	240	1.05e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	4.09e-01	4.09e-01	4.09e-01	4.09e-01	4.09e-01
H	GAS	240	1.40e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	6.75e-01	6.75e-01	6.75e-01	6.75e-01	6.75e-01
H	GAS	240	0.00e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
H	GAS	720	8.44e-01	0.00e+00	0.00e+00	2.65e-01	0.00e+00	0.00e+00	2.90e-01	2.90e-01	0.00e+00	0.00e+00	0.00e+00
H	GAS	720	8.48e-01	0.00e+00	0.00e+00	1.19e-01	0.00e+00	0.00e+00	1.31e-01	1.31e-01	0.00e+00	0.00e+00	0.00e+00
H	GAS	720	1.51e+00	0.00e+00	0.00e+00	2.06e-01	0.00e+00	0.00e+00	3.64e-01	3.64e-01	1.37e-01	1.37e-01	1.37e-01
H	GAS	720	1.60e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
H	GAS	720	0.00e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00

Table E.5 – continued from previous page

MC	S	t_{Ads}	C_{CTRL}	C_A	C_{D1}	C_{D2}	C_{D3}	C_{D4}	q_A	q_{D1}	q_{D2}	q_{D3}	q_{D4}
H	GUA	2	8.30e-01	5.18e-01	2.55e-01	1.36e-01	0.00e+00	4.79e-02	5.32e-01	2.66e-01	1.27e-01	1.27e-01	7.93e-02
H	GUA	2	8.30e-01	5.61e-01	2.48e-01	1.37e-01	7.85e-02	4.92e-02	6.08e-01	3.48e-01	2.11e-01	1.26e-01	8.10e-02
H	GUA	2	1.42e+00	8.50e-01	4.06e-01	2.16e-01	1.15e-01	6.86e-02	9.23e-01	4.93e-01	2.73e-01	1.54e-01	8.81e-02
H	GUA	2	1.66e+00	1.03e+00	5.05e-01	2.57e-01	1.44e-01	8.31e-02	1.13e+00	5.91e-01	3.30e-01	1.76e-01	1.05e-01
H	GUA	2	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
H	GUA	48	7.73e-01	4.05e-01	2.51e-01	1.40e-01	7.91e-02	4.97e-02	5.97e-01	3.53e-01	2.05e-01	1.20e-01	6.78e-02
H	GUA	48	7.79e-01	4.59e-01	2.64e-01	NA	7.54e-02	4.89e-02	NA	NA	1.95e-01	1.16e-01	6.37e-02
H	GUA	48	1.12e+00	5.11e-01	3.27e-01	1.84e-01	1.06e-01	6.40e-02	7.97e-01	4.54e-01	2.59e-01	1.46e-01	7.86e-02
H	GUA	48	1.69e+00	1.14e+00	5.33e-01	2.85e-01	1.52e-01	9.23e-02	1.25e+00	6.66e-01	3.69e-01	2.08e-01	1.11e-01
H	GUA	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
H	GUA	240	7.72e-01	7.01e-01	3.22e-01	1.59e-01	8.04e-02	5.19e-02	7.87e-01	4.55e-01	2.90e-01	2.04e-01	1.48e-01
H	GUA	240	7.77e-01	6.61e-01	3.27e-01	1.54e-01	8.06e-02	5.20e-02	7.88e-01	4.51e-01	2.91e-01	2.05e-01	1.50e-01
H	GUA	240	1.12e+00	9.51e-01	4.42e-01	2.24e-01	1.15e-01	6.81e-02	1.04e+00	5.81e-01	3.49e-01	2.28e-01	1.54e-01
H	GUA	240	1.67e+00	1.27e+00	6.08e-01	3.07e-01	1.57e-01	0.00e+00	1.18e+00	5.57e-01	2.30e-01	6.40e-02	6.40e-02
H	GUA	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	NA	NA	NA	NA	NA	0.00e+00
H	GUA	720	7.76e-01	1.14e+00	4.66e-01	1.60e-01	7.05e-02	4.57e-02	9.24e-01	4.33e-01	2.67e-01	1.93e-01	1.45e-01
H	GUA	720	7.79e-01	1.18e+00	4.85e-01	1.37e-01	7.52e-02	4.74e-02	9.20e-01	4.11e-01	2.68e-01	1.89e-01	1.39e-01
H	GUA	720	1.12e+00	2.78e+00	1.06e+00	4.24e-01	2.05e-01	8.11e-02	2.17e+00	1.06e+00	6.23e-01	4.11e-01	3.25e-01
H	GUA	720	1.67e+00	8.98e-01	5.04e-01	1.99e-01	9.53e-02	5.29e-02	9.58e-01	4.54e-01	2.39e-01	1.38e-01	8.30e-02
H	GUA	720	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
H	H	2	9.14e-01	5.00e-01	2.16e-01	1.17e-01	7.97e-02	5.27e-02	5.99e-01	3.72e-01	2.51e-01	1.67e-01	1.11e-01
H	H	2	9.02e-01	5.06e-01	2.22e-01	1.16e-01	8.30e-02	5.39e-02	6.15e-01	3.81e-01	2.60e-01	1.73e-01	1.16e-01
H	H	2	1.56e+00	8.39e-01	3.62e-01	1.83e-01	1.19e-01	8.08e-02	1.01e+00	6.24e-01	4.31e-01	3.05e-01	2.21e-01
H	H	2	1.82e+00	3.39e-01	4.05e-01	2.19e-01	1.22e-01	8.71e-02	1.16e+00	7.32e-01	5.01e-01	3.73e-01	2.82e-01
H	H	2	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
H	H	48	8.23e-01	3.11e-01	1.80e-01	1.62e-01	0.00e+00	7.64e-02	6.10e-01	4.23e-01	2.54e-01	2.54e-01	1.76e-01
H	H	48	7.93e-01	2.80e-01	1.84e-01	1.74e-01	0.00e+00	3.90e-02	5.86e-01	3.92e-01	2.10e-01	2.10e-01	1.70e-01
H	H	48	1.20e+00	4.15e-01	2.49e-01	2.45e-01	0.00e+00	4.49e-02	8.81e-01	6.16e-01	3.56e-01	3.56e-01	3.10e-01
H	H	48	1.80e+00	1.32e+00	6.77e-01	3.94e-01	2.05e-01	0.00e+00	1.58e+00	8.45e-01	4.32e-01	2.18e-01	2.18e-01
H	H	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	NA	0.00e+00	NA	NA	NA	0.00e+00	0.00e+00
H	H	240	8.35e-01	3.34e-01	1.33e-01	1.32e-01	8.13e-02	4.88e-02	6.42e-01	5.06e-01	3.71e-01	2.86e-01	2.35e-01
H	H	240	8.37e-01	0.00e+00	2.07e-01	1.32e-01	6.26e-02	5.28e-02	5.94e-01	3.80e-01	2.43e-01	1.79e-01	1.22e-01
H	H	240	1.21e+00	0.00e+00	2.32e-01	1.92e-01	9.51e-02	1.23e-01	8.40e-01	6.04e-01	4.03e-01	3.04e-01	1.76e-01
H	H	240	1.78e+00	7.97e-01	3.69e-01	2.85e-01	1.61e-01	9.04e-02	1.32e+00	9.36e-01	6.34e-01	4.67e-01	3.74e-01
H	H	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
H	H	720	8.29e-01	2.39e-01	1.50e-01	6.49e-02	5.42e-02	4.10e-02	5.28e-01	3.71e-01	3.04e-01	2.47e-01	2.05e-01
H	H	720	8.35e-01	5.27e-01	2.29e-01	8.90e-02	5.36e-02	4.23e-02	6.08e-01	3.71e-01	2.78e-01	2.23e-01	1.78e-01
H	H	720	1.21e+00	4.53e-01	2.09e-01	8.72e-02	5.38e-02	4.56e-02	7.38e-01	5.16e-01	4.24e-01	3.69e-01	3.22e-01
H	H	720	1.79e+00	9.50e-01	4.95e-01	2.66e-01	1.17e-01	6.48e-02	1.33e+00	8.20e-01	5.45e-01	4.23e-01	3.56e-01
H	H	720	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00

Table E.5 – continued from previous page

MC	S	t_{Ads}	C_{CTRL}	C_A	C_{D1}	C_{D2}	C_{D3}	C_{D4}	q_A	q_{D1}	q_{D2}	q_{D3}	q_{D4}
H	J	2	8.31e-01	2.18e-01	1.34e-01	0.00e+00	6.06e-02	0.00e+00	1.17e+00	9.22e-01	9.22e-01	8.17e-01	8.17e-01
H	J	2	8.33e-01	2.21e-01	1.01e-01	7.38e-02	6.15e-02	4.00e-02	1.27e+00	1.09e+00	9.60e-01	8.54e-01	7.83e-01
H	J	2	1.38e+00	4.13e-01	1.94e-01	1.43e-01	1.15e-01	7.76e-02	2.04e+00	1.69e+00	1.43e+00	1.24e+00	1.10e+00
H	J	2	1.65e+00	4.53e-01	2.29e-01	1.61e-01	1.34e-01	9.70e-02	2.31e+00	1.90e+00	1.62e+00	1.38e+00	1.21e+00
H	J	2	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
H	J	48	7.73e-01	9.99e-02	5.70e-02	0.00e+00	4.40e-02	5.67e-02	1.00e+00	9.00e-01	9.00e-01	8.22e-01	7.24e-01
H	J	48	7.73e-01	1.03e-01	7.63e-02	7.41e-02	6.02e-02	5.63e-02	1.20e+00	1.06e+00	9.32e-01	8.24e-01	7.27e-01
H	J	48	1.12e+00	1.70e-01	1.25e-01	1.10e-01	9.22e-02	7.98e-02	1.86e+00	1.64e+00	1.46e+00	1.29e+00	1.15e+00
H	J	48	1.69e+00	1.33e-01	1.09e-01	1.66e-01	1.28e-01	1.19e-01	2.29e+00	2.09e+00	1.80e+00	1.57e+00	1.36e+00
H	J	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
H	J	240	7.82e-01	4.76e-02	0.00e+00	3.95e-02	4.11e-02	4.14e-02	1.06e+00	1.06e+00	9.92e-01	9.22e-01	8.54e-01
H	J	240	7.81e-01	1.06e-01	5.95e-02	6.41e-02	5.28e-02	5.41e-02	1.36e+00	1.26e+00	1.15e+00	1.06e+00	9.67e-01
H	J	240	1.13e+00	2.31e-01	1.73e-01	1.12e-01	8.27e-02	7.91e-02	2.03e+00	1.73e+00	1.54e+00	1.40e+00	1.27e+00
H	J	240	1.67e+00	2.68e-01	2.09e-01	1.68e-01	1.19e-01	9.86e-02	2.72e+00	2.37e+00	2.08e+00	1.88e+00	1.71e+00
H	J	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
H	J	720	7.82e-01	1.26e-01	6.03e-02	0.00e+00	0.00e+00	0.00e+00	1.23e+00	1.13e+00	1.13e+00	1.13e+00	1.13e+00
H	J	720	7.78e-01	1.16e-01	7.38e-02	0.00e+00	0.00e+00	0.00e+00	1.16e+00	1.03e+00	1.03e+00	1.03e+00	1.03e+00
H	J	720	1.12e+00	2.72e-01	1.48e-01	0.00e+00	0.00e+00	0.00e+00	1.82e+00	1.56e+00	1.56e+00	1.56e+00	1.56e+00
H	J	720	1.67e+00	3.34e-01	2.09e-01	0.00e+00	6.00e-02	5.95e-02	2.72e+00	2.38e+00	2.38e+00	2.28e+00	2.17e+00
H	J	720	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
H	KA	2	8.89e-01	8.00e-01	2.86e-01	1.00e-01	4.34e-02	2.56e-02	8.09e-01	2.98e-01	1.22e-01	4.60e-02	0.00e+00
H	KA	2	8.90e-01	7.14e-01	2.80e-01	9.53e-02	4.12e-02	2.48e-02	7.85e-01	2.85e-01	1.16e-01	4.43e-02	0.00e+00
H	KA	2	1.47e+00	1.16e+00	4.52e-01	1.52e-01	6.12e-02	2.99e-02	1.23e+00	4.32e-01	1.60e-01	5.39e-02	0.00e+00
H	KA	2	1.75e+00	1.51e+00	5.15e-01	1.79e-01	6.94e-02	3.26e-02	1.41e+00	5.00e-01	1.80e-01	5.85e-02	0.00e+00
H	KA	2	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
H	KA	48	8.10e-01	6.88e-01	2.70e-01	9.01e-02	3.99e-02	2.43e-02	7.52e-01	2.72e-01	1.13e-01	4.21e-02	0.00e+00
H	KA	48	8.07e-01	7.39e-01	NA	9.27e-02	4.02e-02	2.47e-02	NA	2.78e-01	1.13e-01	4.32e-02	0.00e+00
H	KA	48	1.17e+00	9.96e-01	3.73e-01	1.36e-01	5.35e-02	2.90e-02	9.73e-01	3.86e-01	1.46e-01	5.10e-02	0.00e+00
H	KA	48	1.75e+00	1.56e+00	5.26e-01	1.81e-01	6.93e-02	3.65e-02	1.45e+00	5.07e-01	1.85e-01	6.34e-02	0.00e+00
H	KA	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
H	KA	240	8.10e-01	6.98e-01	2.39e-01	8.68e-02	3.81e-02	2.86e-02	6.94e-01	2.72e-01	1.17e-01	4.95e-02	0.00e+00
H	KA	240	8.14e-01	6.91e-01	2.41e-01	8.84e-02	3.77e-02	2.47e-02	6.83e-01	2.65e-01	1.09e-01	4.27e-02	0.00e+00
H	KA	240	1.17e+00	9.79e-01	3.43e-01	1.23e-01	4.87e-02	3.05e-02	9.57e-01	3.58e-01	1.39e-01	5.29e-02	0.00e+00
H	KA	240	1.74e+00	1.47e+00	4.94e-01	1.75e-01	5.62e-02	3.50e-02	1.33e+00	4.69e-01	1.61e-01	6.20e-02	0.00e+00
H	KA	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
H	KA	720	8.15e-01	5.74e-01	2.20e-01	6.01e-02	0.00e+00	0.00e+00	5.00e-01	1.05e-01	0.00e+00	0.00e+00	0.00e+00
H	KA	720	8.10e-01	6.52e-01	2.28e-01	6.35e-02	0.00e+00	0.00e+00	5.19e-01	1.13e-01	0.00e+00	0.00e+00	0.00e+00
H	KA	720	1.17e+00	9.22e-01	3.16e-01	9.34e-02	3.66e-02	0.00e+00	7.98e-01	2.27e-01	6.32e-02	0.00e+00	0.00e+00
H	KA	720	1.74e+00	NA	4.91e-01	1.49e-01	0.00e+00	0.00e+00	1.11e+00	2.66e-01	0.00e+00	0.00e+00	0.00e+00
H	KA	720	0.00e+00	0.00e+00	NA	0.00e+00	0.00e+00	0.00e+00	NA	0.00e+00	0.00e+00	0.00e+00	0.00e+00

Table E.5 – continued from previous page

MC	S	t_{Ads}	C_{CTRL}	C_A	C_{D1}	C_{D2}	C_{D3}	C_{D4}	q_A	q_{D1}	q_{D2}	q_{D3}	q_{D4}
H	LCL	2	8.77e-01	4.32e-01	2.98e-01	NA	NA	NA	NA	NA	NA	NA	0.00e+00
H	LCL	2	8.75e-01	4.15e-01	3.07e-01	NA	NA	NA	NA	NA	NA	NA	0.00e+00
H	LCL	2	1.32e+00	5.92e-01	4.30e-01	NA	NA	NA	NA	NA	NA	NA	0.00e+00
H	LCL	2	1.36e+00	6.22e-01	0.00e+00	NA	NA	NA	NA	NA	NA	NA	0.00e+00
H	LCL	2	0.00e+00	0.00e+00	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
H	LCL	48	7.69e-01	3.59e-01	1.37e-01	1.42e-01	1.13e-01	9.23e-02	8.45e-01	6.99e-01	5.48e-01	4.28e-01	3.29e-01
H	LCL	48	7.74e-01	2.54e-01	1.32e-01	1.43e-01	1.17e-01	1.00e-01	1.04e+00	9.00e-01	7.50e-01	6.26e-01	5.22e-01
H	LCL	48	1.07e+00	4.13e-01	2.11e-01	1.50e-01	1.77e-01	1.44e-01	1.46e+00	1.24e+00	1.08e+00	8.87e-01	7.33e-01
H	LCL	48	1.28e+00	4.81e-01	2.60e-01	1.91e-01	1.41e-01	1.29e-01	1.36e+00	1.08e+00	8.84e-01	7.32e-01	5.95e-01
H	LCL	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
H	LCL	240	7.64e-01	2.23e-01	1.31e-01	1.41e-01	1.14e-01	6.76e-02	9.76e-01	8.14e-01	6.68e-01	5.49e-01	4.77e-01
H	LCL	240	7.60e-01	1.86e-01	1.29e-01	1.41e-01	1.18e-01	6.17e-02	8.43e-01	6.83e-01	5.35e-01	4.12e-01	3.46e-01
H	LCL	240	1.00e+00	3.32e-01	1.94e-01	2.34e-01	1.85e-01	7.79e-02	1.29e+00	1.06e+00	8.12e-01	6.14e-01	5.31e-01
H	LCL	240	1.31e+00	3.06e-01	3.59e-01	2.36e-01	1.59e-01	7.94e-02	1.93e+00	1.49e+00	1.24e+00	1.08e+00	9.94e-01
H	LCL	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
H	LCL	720	7.94e-01	1.75e-01	1.17e-01	1.81e-01	6.63e-02	6.10e-02	1.12e+00	9.98e-01	8.01e-01	7.33e-01	6.68e-01
H	LCL	720	7.91e-01	1.50e-01	1.05e-01	1.86e-01	6.16e-02	NA	NA	NA	NA	NA	3.64e-01
H	LCL	720	1.40e+00	2.89e-01	1.68e-01	2.78e-01	1.47e-01	7.91e-02	1.31e+00	1.13e+00	8.21e-01	6.69e-01	5.84e-01
H	LCL	720	1.49e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
H	LCL	720	0.00e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
H	LCO	2	9.27e-01	4.27e-01	2.04e-01	NA	NA	NA	NA	NA	NA	NA	0.00e+00
H	LCO	2	9.50e-01	4.92e-01	1.62e-01	NA	NA	NA	NA	NA	NA	NA	0.00e+00
H	LCO	2	1.48e+00	6.22e-01	2.55e-01	NA	NA	NA	NA	NA	NA	NA	0.00e+00
H	LCO	2	1.52e+00	5.45e-01	3.29e-01	NA	NA	NA	NA	NA	NA	NA	0.00e+00
H	LCO	2	0.00e+00	0.00e+00	0.00e+00	NA	NA	NA	NA	NA	NA	NA	0.00e+00
H	LCO	48	8.40e-01	2.05e-01	4.48e-02	7.00e-02	4.55e-02	9.28e-02	8.21e-01	7.76e-01	7.02e-01	6.52e-01	5.59e-01
H	LCO	48	8.49e-01	2.61e-01	1.23e-01	1.29e-01	5.29e-02	8.52e-02	9.43e-01	8.16e-01	6.83e-01	6.25e-01	5.36e-01
H	LCO	48	1.18e+00	2.40e-01	1.93e-01	1.43e-01	1.03e-01	1.12e-01	1.54e+00	1.35e+00	1.20e+00	1.09e+00	9.71e-01
H	LCO	48	1.44e+00	2.96e-01	1.64e-01	1.28e-01	1.12e-01	9.82e-02	1.54e+00	1.36e+00	1.23e+00	1.11e+00	1.00e+00
H	LCO	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
H	LCO	240	8.49e-01	2.81e-01	9.17e-02	6.54e-02	1.07e-01	7.02e-02	1.05e+00	9.46e-01	8.56e-01	7.48e-01	6.74e-01
H	LCO	240	8.50e-01	1.08e-01	1.04e-01	1.13e-01	9.02e-02	4.88e-02	1.05e+00	9.10e-01	7.53e-01	6.61e-01	6.09e-01
H	LCO	240	1.12e+00	1.91e-01	1.72e-01	1.34e-01	1.15e-01	8.23e-02	1.58e+00	1.38e+00	1.19e+00	1.07e+00	9.86e-01
H	LCO	240	1.44e+00	1.82e-01	1.75e-01	1.54e-01	1.18e-01	7.14e-02	1.33e+00	1.13e+00	9.13e-01	7.93e-01	7.18e-01
H	LCO	240	0.00e+00	NA	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
H	LCO	720	8.83e-01	8.66e-02	8.39e-02	6.94e-02	6.25e-02	5.05e-02	9.05e-01	8.19e-01	7.44e-01	6.77e-01	6.22e-01
H	LCO	720	8.81e-01	1.11e-01	2.06e-01	1.54e-01	1.24e-01	4.19e-02	1.17e+00	9.54e-01	7.87e-01	6.55e-01	6.10e-01
H	LCO	720	1.56e+00	1.51e-01	1.71e-01	1.38e-01	1.31e-01	6.87e-02	1.48e+00	1.30e+00	1.15e+00	1.01e+00	9.36e-01
H	LCO	720	1.66e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
H	LCO	720	0.00e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00

Table E.5 – continued from previous page

MC	S	t_{Ads}	C_{CTRL}	C_A	C_{D1}	C_{D2}	C_{D3}	C_{D4}	q_A	q_{D1}	q_{D2}	q_{D3}	q_{D4}
H	M	2	8.66e-01	4.50e-01	2.10e-01	2.85e-01	1.55e-01	9.17e-02	8.84e-01	6.57e-01	3.75e-01	2.03e-01	1.06e-01
H	M	2	8.74e-01	4.22e-01	1.60e-01	6.97e-02	5.27e-02	4.38e-02	4.64e-01	2.88e-01	2.19e-01	1.60e-01	1.13e-01
H	M	2	1.48e+00	7.28e-01	3.71e-01	1.72e-01	1.04e-01	7.07e-02	8.96e-01	4.90e-01	3.16e-01	2.02e-01	1.26e-01
H	M	2	1.74e+00	8.85e-01	4.62e-01	2.25e-01	1.40e-01	8.45e-02	1.09e+00	5.93e-01	3.68e-01	2.15e-01	1.26e-01
H	M	2	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
H	M	48	7.80e-01	3.18e-01	2.13e-01	1.25e-01	8.42e-02	5.84e-02	6.29e-01	4.11e-01	2.83e-01	1.93e-01	1.35e-01
H	M	48	7.74e-01	3.23e-01	2.15e-01	1.30e-01	8.34e-02	5.80e-02	6.58e-01	4.38e-01	3.00e-01	2.11e-01	1.51e-01
H	M	48	1.12e+00	4.96e-01	2.68e-01	1.83e-01	1.16e-01	7.65e-02	8.54e-01	5.79e-01	3.86e-01	2.63e-01	1.84e-01
H	M	48	1.68e+00	9.72e-01	4.86e-01	2.85e-01	1.61e-01	1.19e-01	1.32e+00	7.83e-01	4.84e-01	3.15e-01	1.88e-01
H	M	48	0.00e+00	NA	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
H	M	240	7.81e-01	5.13e-01	6.95e-02	1.93e-01	1.15e-01	1.14e-01	6.50e-01	5.76e-01	3.72e-01	2.51e-01	1.39e-01
H	M	240	7.80e-01	3.81e-01	2.36e-01	1.30e-01	7.86e-02	5.96e-02	7.16e-01	4.58e-01	3.21e-01	2.37e-01	1.78e-01
H	M	240	1.12e+00	6.19e-01	3.63e-01	1.91e-01	1.06e-01	7.84e-02	9.30e-01	5.36e-01	3.35e-01	2.22e-01	1.44e-01
H	M	240	1.67e+00	8.79e-01	4.87e-01	2.80e-01	1.60e-01	1.01e-01	1.32e+00	8.32e-01	5.33e-01	3.66e-01	2.57e-01
H	M	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
H	M	720	7.79e-01	2.30e-01	1.89e-01	1.01e-01	5.61e-02	4.42e-02	5.45e-01	3.41e-01	2.32e-01	1.75e-01	1.29e-01
H	M	720	7.77e-01	4.45e-01	1.79e-01	NA	5.57e-02	4.01e-02	NA	NA	2.09e-01	1.54e-01	1.11e-01
H	M	720	1.12e+00	6.34e-01	2.68e-01	1.45e-01	6.45e-02	5.59e-02	7.22e-01	4.34e-01	2.79e-01	2.14e-01	1.55e-01
H	M	720	1.68e+00	0.00e+00	4.18e-01	2.32e-01	9.46e-02	NA	NA	NA	NA	NA	2.72e-01
H	M	720	0.00e+00	NA	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
H	N	2	8.62e-01	6.30e-01	3.45e-01	1.19e-01	7.02e-02	4.14e-02	6.77e-01	3.11e-01	1.87e-01	1.16e-01	7.12e-02
H	N	2	8.67e-01	6.01e-01	2.42e-01	1.25e-01	7.26e-02	4.20e-02	5.92e-01	3.34e-01	2.02e-01	1.27e-01	8.25e-02
H	N	2	1.52e+00	1.01e+00	4.20e-01	1.86e-01	1.00e-01	5.41e-02	9.22e-01	4.66e-01	2.67e-01	1.63e-01	1.07e-01
H	N	2	1.73e+00	1.17e+00	4.83e-01	2.17e-01	1.17e-01	6.25e-02	1.01e+00	4.97e-01	2.72e-01	1.52e-01	8.57e-02
H	N	2	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
H	N	48	7.53e-01	4.41e-01	1.80e-01	9.61e-02	6.50e-02	4.45e-02	5.09e-01	3.22e-01	2.18e-01	1.50e-01	1.03e-01
H	N	48	8.01e-01	4.72e-01	2.30e-01	1.21e-01	6.82e-02	4.39e-02	5.56e-01	3.18e-01	1.89e-01	1.16e-01	7.12e-02
H	N	48	1.15e+00	6.37e-01	3.23e-01	1.67e-01	9.22e-02	5.70e-02	7.58e-01	4.24e-01	2.42e-01	1.45e-01	8.47e-02
H	N	48	1.74e+00	1.15e+00	5.12e-01	2.67e-01	1.28e-01	8.22e-02	1.21e+00	6.52e-01	3.68e-01	2.35e-01	1.49e-01
H	N	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
H	N	240	7.98e-01	5.52e-01	2.60e-01	1.28e-01	6.82e-02	4.57e-02	6.08e-01	3.30e-01	1.97e-01	1.24e-01	7.52e-02
H	N	240	8.02e-01	5.33e-01	2.64e-01	1.28e-01	6.78e-02	4.81e-02	6.16e-01	3.34e-01	1.98e-01	1.27e-01	7.57e-02
H	N	240	1.16e+00	8.23e-01	3.89e-01	1.82e-01	9.22e-02	5.71e-02	8.61e-01	4.49e-01	2.56e-01	1.59e-01	9.86e-02
H	N	240	1.72e+00	1.16e+00	5.26e-01	2.79e-01	1.36e-01	7.75e-02	1.21e+00	6.67e-01	3.77e-01	2.33e-01	1.52e-01
H	N	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
H	N	720	7.56e-01	5.56e-01	0.00e+00	1.82e-01	5.36e-02	0.00e+00	2.51e-01	2.51e-01	5.68e-02	0.00e+00	0.00e+00
H	N	720	7.97e-01	7.41e-01	2.44e-01	1.81e-01	7.48e-02	0.00e+00	5.26e-01	2.71e-01	7.77e-02	0.00e+00	0.00e+00
H	N	720	1.16e+00	9.36e-01	3.78e-01	1.59e-01	6.54e-02	3.90e-02	6.86e-01	2.80e-01	1.10e-01	4.06e-02	0.00e+00
H	N	720	1.71e+00	5.96e-01	4.66e-01	2.25e-01	9.28e-02	5.37e-02	8.72e-01	3.98e-01	1.54e-01	5.69e-02	0.00e+00
H	N	720	0.00e+00	NA	0.00e+00	0.00e+00	NA	0.00e+00	NA	NA	NA	0.00e+00	0.00e+00

Table E.5 – continued from previous page

MC	S	t_{Ads}	C_{CTRL}	C_A	C_{D1}	C_{D2}	C_{D3}	C_{D4}	q_A	q_{D1}	q_{D2}	q_{D3}	q_{D4}
H	P	2	8.54e-01	5.45e-02	6.82e-02	0.00e+00	0.00e+00	0.00e+00	2.71e+00	2.59e+00	2.59e+00	2.59e+00	2.59e+00
H	P	2	8.49e-01	5.21e-02	8.54e-02	0.00e+00	0.00e+00	7.96e-02	2.98e+00	2.83e+00	2.83e+00	2.83e+00	2.76e+00
H	P	2	1.48e+00	8.10e-02	9.19e-02	5.09e-02	3.82e-02	0.00e+00	3.42e+00	3.26e+00	3.18e+00	3.11e+00	3.11e+00
H	P	2	1.71e+00	9.43e-01	1.07e-01	0.00e+00	4.79e-02	NA	NA	NA	NA	NA	0.00e+00
H	P	2	0.00e+00	0.00e+00	0.00e+00	NA	NA	NA	NA	NA	NA	NA	0.00e+00
H	P	48	7.89e-01	0.00e+00	0.00e+00	0.00e+00	8.10e-02	0.00e+00	9.74e-01	9.74e-01	9.74e-01	8.30e-01	8.30e-01
H	P	48	7.88e-01	0.00e+00	0.00e+00	0.00e+00	0.00e+00	6.46e-02	1.79e+00	1.79e+00	1.79e+00	1.79e+00	1.68e+00
H	P	48	1.14e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	8.13e-02	2.24e+00	2.24e+00	2.24e+00	2.24e+00	2.10e+00
H	P	48	1.71e+00	0.00e+00	1.94e-01	0.00e+00	0.00e+00	1.33e-01	1.82e+00	1.48e+00	1.48e+00	1.48e+00	1.25e+00
H	P	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
H	P	240	7.84e-01	4.40e-02	4.92e-02	3.51e-02	3.71e-02	0.00e+00	9.39e-01	8.53e-01	7.93e-01	7.29e-01	7.29e-01
H	P	240	7.88e-01	0.00e+00	0.00e+00	4.07e-02	3.15e-02	0.00e+00	2.31e+00	2.31e+00	2.24e+00	2.19e+00	2.19e+00
H	P	240	1.14e+00	0.00e+00	0.00e+00	9.74e-02	2.57e-02	3.61e-02	3.71e+00	3.71e+00	3.54e+00	3.50e+00	3.44e+00
H	P	240	1.69e+00	0.00e+00	0.00e+00	1.17e-01	0.00e+00	5.08e-02	2.42e+00	2.42e+00	2.22e+00	2.22e+00	2.13e+00
H	P	240	0.00e+00	0.00e+00	0.00e+00	NA	0.00e+00	0.00e+00	NA	NA	0.00e+00	0.00e+00	0.00e+00
H	P	720	7.90e-01	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	6.92e-01	6.92e-01	6.92e-01	6.92e-01	6.92e-01
H	P	720	7.90e-01	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	7.11e-01	7.11e-01	7.11e-01	7.11e-01	7.11e-01
H	P	720	1.14e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	1.16e+00	1.16e+00	1.16e+00	1.16e+00	1.16e+00
H	P	720	1.70e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	1.95e+00	1.95e+00	1.95e+00	1.95e+00	1.95e+00
H	P	720	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
H	PO	2	9.02e-01	3.33e-01	5.05e-02	NA	NA	NA	NA	NA	NA	NA	0.00e+00
H	PO	2	8.99e-01	3.86e-01	1.11e-01	NA	NA	NA	NA	NA	NA	NA	0.00e+00
H	PO	2	1.41e+00	6.40e-01	3.10e-01	NA	NA	NA	NA	NA	NA	NA	0.00e+00
H	PO	2	1.44e+00	3.20e-01	2.77e-01	NA	NA	NA	NA	NA	NA	NA	0.00e+00
H	PO	2	0.00e+00	0.00e+00	0.00e+00	NA	NA	NA	NA	NA	NA	NA	0.00e+00
H	PO	48	8.66e-01	1.21e-01	1.19e-01	1.48e-01	7.45e-02	6.18e-02	4.25e-01	3.01e-01	1.44e-01	6.56e-02	0.00e+00
H	PO	48	8.47e-01	9.70e-02	9.84e-02	9.64e-02	7.75e-02	6.45e-02	8.76e-01	7.72e-01	6.71e-01	5.91e-01	5.23e-01
H	PO	48	1.15e+00	2.56e-01	2.00e-01	1.57e-01	1.33e-01	9.85e-02	1.46e+00	1.25e+00	1.09e+00	9.76e-01	8.72e-01
H	PO	48	1.36e+00	4.57e-01	2.65e-01	2.07e-01	1.30e-01	7.95e-02	1.38e+00	1.10e+00	8.78e-01	7.43e-01	6.59e-01
H	PO	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
H	PO	240	8.16e-01	4.38e-01	8.09e-02	8.39e-02	1.02e-01	5.51e-02	6.76e-01	5.76e-01	4.67e-01	3.61e-01	3.02e-01
H	PO	240	8.07e-01	5.28e-01	7.80e-02	7.95e-02	6.64e-02	8.21e-02	6.86e-01	5.89e-01	4.85e-01	4.17e-01	3.30e-01
H	PO	240	1.06e+00	2.27e-01	1.57e-01	1.22e-01	1.13e-01	1.22e-01	1.09e+00	8.98e-01	7.35e-01	6.20e-01	4.90e-01
H	PO	240	1.39e+00	3.90e-01	4.59e-01	NA	8.11e-02	7.86e-02	NA	NA	8.73e-01	7.90e-01	7.06e-01
H	PO	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
H	PO	720	8.55e-01	1.67e-01	8.20e-02	6.24e-02	6.59e-02	5.48e-02	9.56e-01	8.73e-01	8.08e-01	7.39e-01	6.81e-01
H	PO	720	8.57e-01	2.35e-01	8.09e-02	8.12e-02	4.64e-02	5.48e-02	6.61e-01	5.78e-01	4.93e-01	4.44e-01	3.86e-01
H	PO	720	1.51e+00	2.05e-01	1.72e-01	1.36e-01	1.73e-01	8.42e-02	1.11e+00	9.30e-01	7.88e-01	6.08e-01	5.18e-01
H	PO	720	1.59e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
H	PO	720	0.00e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00

Table E.5 – continued from previous page

MC	S	t_{Ads}	C_{CTRL}	C_A	C_{D1}	C_{D2}	C_{D3}	C_{D4}	q_A	q_{D1}	q_{D2}	q_{D3}	q_{D4}
H	R	2	8.45e-01	1.40e-01	7.83e-02	7.92e-02	6.75e-02	1.35e-01	1.28e+00	1.14e+00	1.00e+00	8.84e-01	6.58e-01
H	R	2	8.52e-01	1.54e-01	8.71e-02	8.02e-02	4.80e-02	1.20e-01	1.29e+00	1.14e+00	9.95e-01	9.10e-01	7.08e-01
H	R	2	1.44e+00	2.63e-01	1.67e-01	1.48e-01	1.99e-01	1.59e-01	2.10e+00	1.81e+00	1.55e+00	1.20e+00	9.32e-01
H	R	2	1.68e+00	3.14e-01	2.02e-01	1.71e-01	9.70e-02	7.10e-02	2.17e+00	1.83e+00	1.53e+00	1.36e+00	1.23e+00
H	R	2	0.00e+00	0.00e+00	0.00e+00	0.00e+00	NA	0.00e+00	NA	NA	NA	0.00e+00	0.00e+00
H	R	48	7.72e-01	2.04e-01	8.95e-02	7.44e-02	5.28e-02	0.00e+00	9.76e-01	8.21e-01	6.92e-01	6.00e-01	6.00e-01
H	R	48	7.74e-01	2.02e-01	8.60e-02	7.92e-02	1.42e-01	0.00e+00	1.73e+00	1.59e+00	1.45e+00	1.21e+00	1.21e+00
H	R	48	1.12e+00	1.65e-01	1.16e-01	1.06e-01	1.55e-01	1.36e-01	2.29e+00	2.09e+00	1.91e+00	1.65e+00	1.41e+00
H	R	48	1.65e+00	2.80e-01	5.17e-01	3.62e-01	2.63e-01	2.54e-01	4.23e+00	3.29e+00	2.66e+00	2.22e+00	1.77e+00
H	R	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
H	R	240	7.79e-01	1.24e-01	1.06e-01	9.12e-02	6.98e-02	7.15e-02	1.04e+00	8.58e-01	7.03e-01	5.85e-01	4.67e-01
H	R	240	7.79e-01	1.08e-01	0.00e+00	3.64e-02	4.01e-02	3.55e-02	1.45e+00	1.45e+00	1.39e+00	1.32e+00	1.26e+00
H	R	240	1.12e+00	1.75e-01	4.78e-01	4.48e-02	0.00e+00	NA	NA	NA	NA	NA	1.78e+00
H	R	240	1.67e+00	1.66e-01	5.36e-01	3.77e-01	2.65e-01	1.59e-01	4.64e+00	3.72e+00	3.05e+00	2.60e+00	2.32e+00
H	R	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
H	R	720	7.76e-01	7.75e-02	6.19e-02	0.00e+00	0.00e+00	0.00e+00	8.55e-01	7.46e-01	7.46e-01	7.46e-01	7.46e-01
H	R	720	7.75e-01	7.24e-02	6.11e-02	0.00e+00	0.00e+00	0.00e+00	8.37e-01	7.30e-01	7.30e-01	7.30e-01	7.30e-01
H	R	720	1.12e+00	1.08e-01	7.72e-02	0.00e+00	0.00e+00	0.00e+00	1.09e+00	9.55e-01	9.55e-01	9.55e-01	9.55e-01
H	R	720	1.68e+00	1.30e-01	1.74e-01	0.00e+00	0.00e+00	0.00e+00	1.76e+00	1.47e+00	1.47e+00	1.47e+00	1.47e+00
H	R	720	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
H	SOU	2	8.20e-01	4.77e-01	9.36e-02	1.49e-01	9.57e-02	8.30e-02	4.77e-01	3.83e-01	2.30e-01	1.29e-01	4.07e-02
H	SOU	2	7.85e-01	4.93e-01	2.70e-01	1.62e-01	9.53e-02	5.67e-02	6.96e-01	4.21e-01	2.57e-01	1.56e-01	9.51e-02
H	SOU	2	1.31e+00	7.99e-01	0.00e+00	2.43e-01	1.44e-01	8.39e-02	6.04e-01	6.04e-01	3.52e-01	1.98e-01	1.08e-01
H	SOU	2	1.62e+00	9.44e-01	5.07e-01	2.74e-01	1.70e-01	9.71e-02	1.21e+00	7.01e-01	4.20e-01	2.40e-01	1.37e-01
H	SOU	2	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
H	SOU	48	7.18e-01	4.32e-01	1.66e-01	1.17e-01	7.99e-02	5.36e-02	5.53e-01	3.78e-01	2.56e-01	1.71e-01	1.13e-01
H	SOU	48	7.63e-01	4.06e-01	2.86e-01	1.54e-01	8.59e-02	5.82e-02	7.31e-01	4.32e-01	2.69e-01	1.77e-01	1.15e-01
H	SOU	48	1.10e+00	5.73e-01	3.61e-01	1.91e-01	1.13e-01	7.50e-02	9.24e-01	5.43e-01	3.40e-01	2.18e-01	1.39e-01
H	SOU	48	1.65e+00	9.06e-01	5.13e-01	3.07e-01	1.80e-01	1.18e-01	1.29e+00	7.40e-01	4.16e-01	2.26e-01	1.05e-01
H	SOU	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
H	SOU	240	7.58e-01	4.44e-01	2.52e-01	1.45e-01	8.52e-02	6.33e-02	7.81e-01	5.21e-01	3.70e-01	2.79e-01	2.16e-01
H	SOU	240	7.60e-01	4.65e-01	2.71e-01	1.51e-01	8.79e-02	NA	NA	NA	NA	NA	0.00e+00
H	SOU	240	1.09e+00	5.61e-01	3.65e-01	2.14e-01	1.23e-01	2.50e-02	9.88e-01	6.12e-01	3.88e-01	2.59e-01	2.34e-01
H	SOU	240	1.62e+00	9.37e-01	5.06e-01	3.27e-01	1.80e-01	1.12e-01	1.38e+00	8.53e-01	5.24e-01	3.35e-01	2.16e-01
H	SOU	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	NA	NA	NA	NA	NA	0.00e+00
H	SOU	720	7.58e-01	5.79e-01	2.36e-01	1.27e-01	5.00e-02	4.17e-02	5.59e-01	3.07e-01	1.73e-01	1.22e-01	7.66e-02
H	SOU	720	7.54e-01	5.21e-01	2.60e-01	1.19e-01	5.62e-02	4.50e-02	5.85e-01	3.07e-01	1.82e-01	1.26e-01	7.66e-02
H	SOU	720	1.09e+00	8.05e-01	3.95e-01	1.75e-01	9.51e-02	4.92e-02	8.47e-01	4.22e-01	2.37e-01	1.39e-01	8.60e-02
H	SOU	720	1.62e+00	1.15e+00	5.90e-01	3.28e-01	1.62e-01	0.00e+00	1.18e+00	5.80e-01	3.75e-01	2.11e-01	2.11e-01
H	SOU	720	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	NA	NA	NA	NA	NA	0.00e+00

Table E.5 – continued from previous page

MC	S	t_{Ads}	C_{CTRL}	C_A	C_{D1}	C_{D2}	C_{D3}	C_{D4}	q_A	q_{D1}	q_{D2}	q_{D3}	q_{D4}
H	SSL1	2	8.47e-01	1.89e-01	2.35e-01	1.39e-01	1.14e-01	5.83e-02	6.48e-01	3.97e-01	2.54e-01	1.36e-01	7.55e-02
H	SSL1	2	8.50e-01	2.08e-01	6.12e-02	1.27e-01	8.61e-02	9.38e-02	4.63e-01	3.96e-01	2.64e-01	1.72e-01	7.35e-02
H	SSL1	2	1.55e+00	2.21e-01	2.30e-01	2.32e-01	1.38e-01	NA	NA	NA	NA	NA	9.92e-02
H	SSL1	2	1.61e+00	5.82e-01	1.78e-01	2.66e-01	1.57e-01	1.08e-01	8.65e-01	6.73e-01	3.95e-01	2.28e-01	1.14e-01
H	SSL1	2	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
H	SSL1	48	8.53e-01	3.05e-01	0.00e+00	1.33e-01	9.51e-02	5.87e-02	3.78e-01	3.78e-01	2.38e-01	1.36e-01	7.47e-02
H	SSL1	48	8.60e-01	4.05e-01	4.34e-01	1.50e-01	9.05e-02	5.83e-02	8.62e-01	3.94e-01	2.34e-01	1.37e-01	7.55e-02
H	SSL1	48	1.52e+00	8.64e-01	6.68e-01	2.53e-01	1.54e-01	9.05e-02	1.34e+00	6.28e-01	3.65e-01	2.00e-01	1.07e-01
H	SSL1	48	1.62e+00	NA	NA	3.16e-01	1.70e-01	1.03e-01	NA	8.21e-01	4.92e-01	3.10e-01	2.02e-01
H	SSL1	48	0.00e+00	0.00e+00	NA	0.00e+00	0.00e+00	0.00e+00	NA	0.00e+00	0.00e+00	0.00e+00	0.00e+00
H	SSL1	240	8.29e-01	2.98e-01	2.22e-01	1.24e-01	0.00e+00	4.70e-02	4.17e-01	1.89e-01	5.04e-02	5.04e-02	0.00e+00
H	SSL1	240	8.28e-01	3.59e-01	2.26e-01	0.00e+00	0.00e+00	4.35e-02	2.77e-01	4.65e-02	4.65e-02	4.65e-02	0.00e+00
H	SSL1	240	1.33e+00	6.41e-01	3.27e-01	NA	0.00e+00	6.06e-02	NA	NA	1.64e-01	1.64e-01	9.88e-02
H	SSL1	240	1.57e+00	5.06e-01	3.82e-01	NA	NA	7.42e-02	NA	NA	NA	1.94e-01	1.15e-01
H	SSL1	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
H	SSL1	720	8.42e-01	4.27e-01	0.00e+00	1.32e-01	7.39e-02	5.06e-02	2.74e-01	2.74e-01	1.36e-01	5.44e-02	0.00e+00
H	SSL1	720	8.42e-01	3.69e-01	8.87e-01	1.04e-01	6.45e-02	4.98e-02	1.21e+00	2.36e-01	1.26e-01	5.37e-02	0.00e+00
H	SSL1	720	1.17e+00	1.03e+00	0.00e+00	1.41e-01	1.02e-01	6.37e-02	4.26e-01	4.26e-01	2.81e-01	1.69e-01	1.00e-01
H	SSL1	720	1.61e+00	NA	0.00e+00	1.80e-01	1.30e-01	7.69e-02	5.20e-01	5.20e-01	3.34e-01	1.90e-01	1.07e-01
H	SSL1	720	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
H	SSL2	2	8.81e-01	2.41e-01	2.67e-01	1.35e-01	9.03e-02	6.00e-02	7.18e-01	4.37e-01	2.96e-01	1.99e-01	1.36e-01
H	SSL2	2	8.86e-01	3.73e-01	1.30e-01	1.55e-01	9.42e-02	6.67e-02	6.05e-01	4.74e-01	3.12e-01	2.09e-01	1.39e-01
H	SSL2	2	1.61e+00	4.90e-01	9.11e-02	2.47e-01	1.48e-01	9.59e-02	7.92e-01	6.95e-01	4.38e-01	2.78e-01	1.79e-01
H	SSL2	2	1.67e+00	8.04e-01	7.67e-01	2.69e-01	1.65e-01	NA	NA	NA	NA	NA	1.14e-01
H	SSL2	2	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
H	SSL2	48	8.86e-01	4.97e-01	2.58e-01	1.68e-01	9.92e-02	6.86e-02	7.04e-01	4.40e-01	2.61e-01	1.56e-01	8.42e-02
H	SSL2	48	8.86e-01	4.42e-01	2.28e-01	1.59e-01	9.67e-02	6.01e-02	6.40e-01	4.05e-01	2.40e-01	1.35e-01	7.35e-02
H	SSL2	48	1.58e+00	8.65e-01	6.54e-01	2.75e-01	1.62e-01	9.68e-02	1.42e+00	7.42e-01	4.59e-01	2.84e-01	1.85e-01
H	SSL2	48	1.69e+00	9.09e-01	4.57e-01	3.07e-01	1.82e-01	1.09e-01	1.32e+00	8.41e-01	5.24e-01	3.27e-01	2.16e-01
H	SSL2	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
H	SSL2	240	8.62e-01	0.00e+00	3.89e-01	9.22e-02	8.27e-02	5.09e-02	6.30e-01	2.45e-01	1.40e-01	5.32e-02	0.00e+00
H	SSL2	240	8.60e-01	0.00e+00	1.86e-01	6.52e-01	6.06e-02	4.49e-02	1.01e+00	8.29e-01	1.10e-01	4.74e-02	0.00e+00
H	SSL2	240	1.40e+00	1.45e-01	3.22e-01	6.82e-01	1.04e-01	6.49e-02	1.27e+00	9.50e-01	1.79e-01	6.88e-02	0.00e+00
H	SSL2	240	1.65e+00	4.13e-01	3.78e-01	8.14e-01	9.05e-02	NA	NA	NA	NA	NA	0.00e+00
H	SSL2	240	0.00e+00	NA	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
H	SSL2	720	8.69e-01	3.44e-01	1.78e-01	1.24e-01	6.52e-02	9.79e+01	1.04e+02	1.04e+02	1.04e+02	1.04e+02	0.00e+00
H	SSL2	720	8.80e-01	4.08e-01	9.33e-02	1.07e-01	6.45e-02	2.10e+01	2.26e+01	2.25e+01	2.24e+01	2.23e+01	0.00e+00
H	SSL2	720	1.18e+00	1.34e+00	1.26e+00	1.48e-01	1.12e-01	6.69e+00	8.89e+00	7.52e+00	7.36e+00	7.24e+00	1.05e-01
H	SSL2	720	1.66e+00	1.31e+00	2.43e-01	1.87e-01	1.32e-01	1.30e+00	1.99e+00	1.72e+00	1.53e+00	1.39e+00	0.00e+00
H	SSL2	720	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00

Table E.5 – continued from previous page

MC	S	t_{Ads}	C_{CTRL}	C_A	C_{D1}	C_{D2}	C_{D3}	C_{D4}	q_A	q_{D1}	q_{D2}	q_{D3}	q_{D4}
H	SSL3	2	8.73e-01	4.47e-01	0.00e+00	1.45e-01	8.44e-02	6.39e-02	4.54e-01	4.54e-01	2.99e-01	2.10e-01	1.43e-01
H	SSL3	2	8.86e-01	4.92e-01	0.00e+00	1.44e-01	9.17e-02	7.69e-02	4.97e-01	4.97e-01	3.43e-01	2.46e-01	1.67e-01
H	SSL3	2	1.59e+00	4.20e-01	1.02e-01	2.34e-01	1.46e-01	1.00e-01	7.27e-01	6.18e-01	3.64e-01	2.09e-01	1.06e-01
H	SSL3	2	1.64e+00	3.88e-01	1.22e-01	2.18e-01	1.76e-01	NA	NA	NA	NA	NA	2.24e-01
H	SSL3	2	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
H	SSL3	48	8.80e-01	5.36e-01	1.96e-01	2.09e-01	1.39e-01	7.34e-02	7.32e-01	5.25e-01	3.06e-01	1.57e-01	8.21e-02
H	SSL3	48	8.81e-01	4.33e-01	2.41e-01	1.49e-01	9.50e-02	6.60e-02	6.74e-01	4.18e-01	2.64e-01	1.60e-01	9.16e-02
H	SSL3	48	1.58e+00	6.01e-01	6.55e-01	4.08e-01	1.57e-01	1.02e-01	1.59e+00	8.91e-01	4.62e-01	2.94e-01	1.89e-01
H	SSL3	48	1.66e+00	8.62e-01	4.87e-01	NA	NA	1.10e-01	NA	NA	NA	3.34e-01	2.20e-01
H	SSL3	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
H	SSL3	240	8.49e-01	3.30e-01	2.15e-01	8.38e-02	0.00e+00	4.27e-02	4.39e-01	2.24e-01	1.29e-01	1.29e-01	8.23e-02
H	SSL3	240	8.42e-01	4.40e-01	2.30e-01	0.00e+00	0.00e+00	4.69e-02	3.50e-01	1.22e-01	1.22e-01	1.22e-01	7.16e-02
H	SSL3	240	1.38e+00	5.62e-01	3.77e-01	0.00e+00	7.34e-02	5.65e-02	6.14e-01	2.44e-01	2.44e-01	1.67e-01	1.07e-01
H	SSL3	240	1.61e+00	4.19e-01	3.95e-01	8.67e-01	4.83e-01	7.33e-02	2.10e+00	1.70e+00	7.15e-01	2.07e-01	1.28e-01
H	SSL3	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
H	SSL3	720	8.49e-01	4.00e-01	0.00e+00	1.21e-01	0.00e+00	4.38e-02	1.74e-01	1.74e-01	4.68e-02	4.68e-02	0.00e+00
H	SSL3	720	8.60e-01	2.70e-01	0.00e+00	0.00e+00	0.00e+00	4.91e-02	5.26e-02	5.26e-02	5.26e-02	5.26e-02	0.00e+00
H	SSL3	720	1.05e+00	2.10e+00	1.84e-01	1.27e-01	1.09e-01	6.27e-02	6.17e-01	4.17e-01	2.86e-01	1.66e-01	9.93e-02
H	SSL3	720	1.62e+00	1.48e+00	0.00e+00	1.60e-01	1.24e-01	8.46e-02	5.39e-01	5.39e-01	3.69e-01	2.35e-01	1.45e-01
H	SSL3	720	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
H	ST	2	7.30e-01	3.29e-01	2.04e-01	1.23e-01	8.66e-02	7.21e-02	1.02e+00	6.77e-01	4.57e-01	3.03e-01	1.81e-01
H	ST	2	7.27e-01	3.36e-01	2.07e-01	1.29e-01	8.82e-02	6.48e-02	1.03e+00	6.77e-01	4.48e-01	2.94e-01	1.83e-01
H	ST	2	1.32e+00	7.17e-01	4.33e-01	2.55e-01	1.71e-01	1.24e-01	2.02e+00	1.29e+00	8.43e-01	5.52e-01	3.42e-01
H	ST	2	1.36e+00	7.09e-01	4.37e-01	2.82e-01	1.91e-01	1.33e-01	2.04e+00	1.28e+00	7.80e-01	4.48e-01	2.19e-01
H	ST	2	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
H	ST	48	7.30e-01	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
H	ST	48	7.30e-01	3.45e-01	2.16e-01	1.52e-01	1.15e-01	8.67e-02	1.16e+00	7.93e-01	5.26e-01	3.24e-01	1.77e-01
H	ST	48	1.32e+00	5.26e-01	4.06e-01	2.45e-01	1.50e-01	1.29e-01	1.99e+00	1.31e+00	8.74e-01	6.05e-01	3.89e-01
H	ST	48	1.38e+00	6.52e-01	4.33e-01	2.59e-01	1.69e-01	1.45e-01	2.12e+00	1.38e+00	9.43e-01	6.44e-01	4.06e-01
H	ST	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
H	ST	240	7.12e-01	3.22e-01	2.01e-01	1.44e-01	9.98e-02	6.43e-02	1.32e+00	9.95e-01	7.46e-01	5.71e-01	4.54e-01
H	ST	240	7.06e-01	3.41e-01	1.94e-01	1.58e-01	9.89e-02	6.19e-02	1.42e+00	1.08e+00	8.09e-01	6.30e-01	5.17e-01
H	ST	240	1.22e+00	5.37e-01	3.38e-01	2.51e-01	1.77e-01	1.19e-01	2.22e+00	1.65e+00	1.21e+00	8.98e-01	6.85e-01
H	ST	240	1.35e+00	6.25e-01	3.24e-01	2.65e-01	1.82e-01	1.14e-01	2.35e+00	1.81e+00	1.34e+00	1.02e+00	8.19e-01
H	ST	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
H	ST	720	7.04e-01	3.28e-01	1.93e-01	1.22e-01	7.57e-02	5.79e-02	8.68e-01	5.44e-01	3.20e-01	1.87e-01	8.47e-02
H	ST	720	7.06e-01	3.39e-01	2.05e-01	1.26e-01	7.78e-02	5.43e-02	8.91e-01	5.56e-01	3.27e-01	1.90e-01	9.39e-02
H	ST	720	9.47e-01	4.33e-01	2.64e-01	2.25e-01	1.18e-01	9.17e-02	1.80e+00	1.36e+00	9.56e-01	7.44e-01	5.86e-01
H	ST	720	1.33e+00	6.36e-01	3.94e-01	2.45e-01	1.34e-01	9.17e-02	1.95e+00	1.29e+00	8.38e-01	5.91e-01	4.26e-01
H	ST	720	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00

Table E.5 – continued from previous page

MC	S	t_{Ads}	C_{CTRL}	C_A	C_{D1}	C_{D2}	C_{D3}	C_{D4}	q_A	q_{D1}	q_{D2}	q_{D3}	q_{D4}
H	W	2	9.06e-01	3.03e-01	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
H	W	2	9.09e-01	3.87e-01	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
H	W	2	1.43e+00	7.11e-01	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
H	W	2	1.45e+00	6.63e-01	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
H	W	2	0.00e+00	0.00e+00	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
H	W	48	8.22e-01	1.25e+00	3.85e-01	2.06e-01	1.10e-01	6.01e-02	1.06e+00	6.67e-01	4.50e-01	3.36e-01	2.69e-01
H	W	48	8.34e-01	1.68e-01	1.52e-01	1.71e-01	1.14e-01	6.08e-02	7.48e-01	5.91e-01	4.18e-01	2.99e-01	2.32e-01
H	W	48	1.15e+00	4.99e-01	2.38e-01	2.45e-01	1.71e-01	9.59e-02	1.07e+00	8.24e-01	5.79e-01	4.02e-01	2.96e-01
H	W	48	1.37e+00	5.56e-01	3.67e-01	2.28e-01	1.54e-01	1.07e-01	1.27e+00	8.82e-01	6.50e-01	4.90e-01	3.73e-01
H	W	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
H	W	240	8.24e-01	3.11e-01	3.60e-01	1.74e-01	7.50e-02	6.18e-02	1.03e+00	6.04e-01	3.69e-01	2.87e-01	2.23e-01
H	W	240	8.19e-01	3.73e-01	1.31e-01	1.05e-01	7.96e-02	6.28e-02	6.79e-01	5.24e-01	3.85e-01	2.98e-01	2.33e-01
H	W	240	1.08e+00	4.46e-01	2.64e-01	2.14e-01	1.35e-01	9.62e-02	1.17e+00	8.56e-01	5.79e-01	4.31e-01	3.29e-01
H	W	240	1.40e+00	6.08e-01	3.37e-01	1.96e-01	1.27e-01	8.79e-02	1.23e+00	8.27e-01	5.67e-01	4.28e-01	3.35e-01
H	W	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
H	W	720	8.62e-01	2.98e-01	5.03e-01	2.13e-01	7.29e-02	8.54e-02	1.23e+00	7.04e-01	4.69e-01	3.92e-01	2.98e-01
H	W	720	8.60e-01	3.03e-01	1.82e-01	1.45e-01	7.47e-02	6.07e-02	7.14e-01	5.25e-01	3.66e-01	2.88e-01	2.20e-01
H	W	720	1.52e+00	4.53e-01	2.97e-01	2.50e-01	1.72e-01	9.56e-02	1.23e+00	9.21e-01	6.51e-01	4.71e-01	3.65e-01
H	W	720	1.61e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
H	W	720	0.00e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
H	W1	2	8.14e-01	4.46e-01	2.40e-01	1.44e-01	9.87e-02	6.91e-02	6.74e-01	4.22e-01	2.60e-01	1.59e-01	8.71e-02
H	W1	2	8.14e-01	4.49e-01	2.42e-01	1.47e-01	9.84e-02	6.73e-02	7.41e-01	4.86e-01	3.24e-01	2.23e-01	1.52e-01
H	W1	2	1.48e+00	8.81e-01	4.40e-01	2.48e-01	1.56e-01	1.03e-01	1.21e+00	7.53e-01	4.79e-01	3.17e-01	2.08e-01
H	W1	2	1.54e+00	8.30e-01	4.65e-01	2.80e-01	1.81e-01	1.16e-01	1.35e+00	8.63e-01	5.54e-01	3.68e-01	2.46e-01
H	W1	2	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
H	W1	48	8.18e-01	4.48e-01	2.59e-01	1.56e-01	1.01e-01	6.80e-02	7.87e-01	5.01e-01	3.43e-01	2.30e-01	1.58e-01
H	W1	48	8.25e-01	4.42e-01	2.61e-01	1.57e-01	1.01e-01	6.78e-02	8.03e-01	5.20e-01	3.58e-01	2.44e-01	1.72e-01
H	W1	48	1.48e+00	8.94e-01	4.71e-01	2.12e-01	1.58e-01	1.03e-01	1.21e+00	7.01e-01	4.85e-01	3.07e-01	2.00e-01
H	W1	48	1.55e+00	8.42e-01	5.00e-01	2.57e-01	1.82e-01	1.17e-01	1.35e+00	8.05e-01	5.46e-01	3.42e-01	2.19e-01
H	W1	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
H	W1	240	7.92e-01	2.95e-01	2.44e-01	1.35e-01	8.24e-02	5.48e-02	6.22e-01	3.82e-01	2.25e-01	1.42e-01	8.41e-02
H	W1	240	7.96e-01	4.06e-01	2.44e-01	1.39e-01	8.77e-02	5.68e-02	6.33e-01	3.95e-01	2.33e-01	1.44e-01	8.49e-02
H	W1	240	1.28e+00	7.06e-01	4.04e-01	2.23e-01	1.39e-01	8.58e-02	1.02e+00	6.26e-01	3.65e-01	2.23e-01	1.32e-01
H	W1	240	1.51e+00	8.03e-01	4.70e-01	2.65e-01	1.64e-01	1.01e-01	1.20e+00	7.42e-01	4.31e-01	2.64e-01	1.58e-01
H	W1	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
H	W1	720	8.17e-01	3.51e-01	2.16e-01	1.26e-01	8.23e-02	5.35e-02	5.26e-01	2.78e-01	1.44e-01	5.75e-02	0.00e+00
H	W1	720	8.01e-01	4.19e-01	0.00e+00	1.38e-01	8.24e-02	6.56e-02	3.00e-01	3.00e-01	1.58e-01	7.07e-02	0.00e+00
H	W1	720	1.00e+00	5.31e-01	4.46e-01	2.28e-01	1.30e-01	8.03e-02	1.09e+00	5.77e-01	3.34e-01	1.96e-01	1.10e-01
H	W1	720	1.50e+00	8.11e-01	0.00e+00	2.56e-01	1.57e-01	9.63e-02	6.54e-01	6.54e-01	3.82e-01	2.18e-01	1.13e-01
H	W1	720	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00

Table E.5 – continued from previous page

MC	S	t_{Ads}	C_{CTRL}	C_A	C_{D1}	C_{D2}	C_{D3}	C_{D4}	q_A	q_{D1}	q_{D2}	q_{D3}	q_{D4}
H	W2	2	8.37e-01	5.55e-01	2.18e-01	1.46e-01	1.00e-01	6.82e-02	7.27e-01	4.97e-01	3.36e-01	2.33e-01	1.61e-01
H	W2	2	8.26e-01	4.36e-01	2.44e-01	1.45e-01	1.01e-01	6.90e-02	7.37e-01	4.80e-01	3.19e-01	2.16e-01	1.42e-01
H	W2	2	1.51e+00	8.82e-01	4.43e-01	2.50e-01	1.62e-01	1.03e-01	1.22e+00	7.56e-01	4.77e-01	3.12e-01	2.00e-01
H	W2	2	1.55e+00	8.25e-01	4.73e-01	2.81e-01	1.83e-01	1.19e-01	1.35e+00	8.54e-01	5.42e-01	3.55e-01	2.27e-01
H	W2	2	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
H	W2	48	8.35e-01	4.35e-01	2.58e-01	1.64e-01	1.02e-01	6.95e-02	7.29e-01	4.44e-01	2.79e-01	1.62e-01	8.90e-02
H	W2	48	8.41e-01	4.42e-01	2.60e-01	1.63e-01	1.03e-01	7.04e-02	7.96e-01	5.05e-01	3.43e-01	2.26e-01	1.53e-01
H	W2	48	1.50e+00	8.87e-01	4.71e-01	2.74e-01	1.61e-01	1.02e-01	1.31e+00	7.85e-01	5.07e-01	3.25e-01	2.18e-01
H	W2	48	1.58e+00	8.33e-01	4.97e-01	3.01e-01	1.85e-01	1.21e-01	1.45e+00	8.92e-01	5.90e-01	3.80e-01	2.53e-01
H	W2	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
H	W2	240	8.00e-01	4.07e-01	2.49e-01	1.39e-01	8.66e-02	5.65e-02	6.30e-01	3.79e-01	2.30e-01	1.44e-01	8.32e-02
H	W2	240	8.10e-01	4.12e-01	2.49e-01	1.38e-01	8.97e-02	5.83e-02	6.48e-01	3.94e-01	2.43e-01	1.54e-01	9.04e-02
H	W2	240	1.25e+00	6.84e-01	3.99e-01	2.28e-01	1.37e-01	8.71e-02	1.01e+00	5.98e-01	3.52e-01	2.14e-01	1.23e-01
H	W2	240	1.53e+00	7.84e-01	4.72e-01	2.74e-01	1.65e-01	1.04e-01	1.21e+00	7.28e-01	4.28e-01	2.64e-01	1.51e-01
H	W2	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
H	W2	720	7.99e-01	4.20e-01	2.37e-01	1.38e-01	8.58e-02	5.55e-02	5.37e-01	2.91e-01	1.54e-01	5.96e-02	0.00e+00
H	W2	720	7.97e-01	4.23e-01	2.30e-01	1.36e-01	8.48e-02	5.17e-02	5.35e-01	2.86e-01	1.50e-01	5.62e-02	0.00e+00
H	W2	720	1.00e+00	5.56e-01	4.28e-01	2.28e-01	1.31e-01	8.42e-02	1.04e+00	5.81e-01	3.52e-01	2.07e-01	1.16e-01
H	W2	720	1.52e+00	8.09e-01	4.56e-01	2.66e-01	1.62e-01	1.00e-01	1.19e+00	6.91e-01	4.23e-01	2.43e-01	1.34e-01
H	W2	720	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
H	Z	2	8.54e-01	8.28e-02	NA	NA	6.65e-02	NA	NA	NA	NA	NA	0.00e+00
H	Z	2	8.63e-01	9.21e-02	0.00e+00	4.26e-02	NA	4.89e-02	NA	NA	NA	7.07e-01	6.35e-01
H	Z	2	1.39e+00	9.44e-02	0.00e+00	5.79e-02	8.59e-02	8.27e-02	1.36e+00	1.36e+00	1.26e+00	1.10e+00	9.62e-01
H	Z	2	1.73e+00	1.49e-01	0.00e+00	9.05e-02	7.96e-02	1.02e-01	2.03e+00	2.03e+00	1.87e+00	1.73e+00	1.56e+00
H	Z	2	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
H	Z	48	7.36e-01	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	1.46e+00	1.46e+00	1.46e+00	1.46e+00	1.46e+00
H	Z	48	7.35e-01	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	1.99e+00	1.99e+00	1.99e+00	1.99e+00	1.99e+00
H	Z	48	1.06e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	2.70e+00	2.70e+00	2.70e+00	2.70e+00	2.70e+00
H	Z	48	1.69e+00	2.03e-01	1.11e-01	2.01e-01	6.53e-02	0.00e+00	3.17e+00	2.97e+00	2.64e+00	2.52e+00	2.52e+00
H	Z	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
H	Z	240	7.76e-01	7.17e-02	6.40e-02	8.28e-02	5.67e-02	0.00e+00	1.22e+00	1.13e+00	9.83e-01	8.84e-01	8.84e-01
H	Z	240	7.75e-01	8.11e-02	5.71e-02	4.00e-02	5.16e-02	0.00e+00	8.27e-01	7.28e-01	6.60e-01	5.69e-01	5.69e-01
H	Z	240	1.13e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
H	Z	240	1.66e+00	1.87e-01	6.81e-02	0.00e+00	6.35e-02	0.00e+00	1.81e+00	1.69e+00	1.69e+00	1.59e+00	1.59e+00
H	Z	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
H	Z	720	7.76e-01	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	5.97e-01	5.97e-01	5.97e-01	5.97e-01	5.97e-01
H	Z	720	7.77e-01	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	7.15e-01	7.15e-01	7.15e-01	7.15e-01	7.15e-01
H	Z	720	1.12e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	1.07e+00	1.07e+00	1.07e+00	1.07e+00	1.07e+00
H	Z	720	1.69e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	1.65e+00	1.65e+00	1.65e+00	1.65e+00	1.65e+00
H	Z	720	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00

Table E.5 – continued from previous page

MC	S	t_{Ads}	C_{CTRL}	C_A	C_{D1}	C_{D2}	C_{D3}	C_{D4}	q_A	q_{D1}	q_{D2}	q_{D3}	q_{D4}
N	AM	2	4.71e+00	2.96e+00	1.38e+00	7.29e-01	3.09e-01	1.70e-01	3.98e+00	2.44e+00	1.67e+00	1.34e+00	1.16e+00
N	AM	2	4.75e+00	2.90e+00	1.34e+00	7.44e-01	3.24e-01	1.93e-01	3.27e+00	1.79e+00	1.03e+00	6.72e-01	4.70e-01
N	AM	2	9.67e+00	6.25e+00	2.87e+00	1.45e+00	6.53e-01	3.61e-01	5.85e+00	2.73e+00	1.22e+00	5.16e-01	1.43e-01
N	AM	2	1.06e+01	6.84e+00	3.21e+00	1.67e+00	NA	4.39e-01	NA	NA	NA	6.34e-01	1.85e-01
N	AM	2	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	AM	48	4.53e+00	2.05e+00	1.02e+00	5.68e-01	0.00e+00	1.55e-01	1.84e+00	7.58e-01	1.62e-01	1.62e-01	0.00e+00
N	AM	48	4.57e+00	2.07e+00	1.06e+00	6.14e-01	7.04e-01	1.76e-01	2.69e+00	1.57e+00	9.29e-01	1.83e-01	0.00e+00
N	AM	48	9.32e+00	4.77e+00	2.21e+00	1.20e+00	6.48e-01	3.30e-01	4.83e+00	2.46e+00	1.20e+00	5.20e-01	1.91e-01
N	AM	48	1.02e+01	5.47e+00	2.45e+00	1.34e+00	NA	3.70e-01	NA	NA	NA	5.88e-01	2.07e-01
N	AM	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	NA	0.00e+00	NA	NA	NA	0.00e+00	0.00e+00
N	AM	240	4.86e+00	1.06e+00	8.27e-02	0.00e+00	0.00e+00	0.00e+00	8.48e-02	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	AM	240	4.81e+00	2.83e-01	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	AM	240	1.06e+01	2.15e-01	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	AM	240	1.06e+01	1.56e-01	0.00e+00	NA	0.00e+00	0.00e+00	NA	NA	0.00e+00	0.00e+00	0.00e+00
N	AM	240	0.00e+00	NA	0.00e+00	0.00e+00	NA	NA	NA	NA	NA	NA	0.00e+00
N	AM	720	4.31e+00	9.62e-01	3.11e-01	2.05e-01	2.76e-01	0.00e+00	8.58e-01	5.16e-01	3.04e-01	0.00e+00	0.00e+00
N	AM	720	4.29e+00	1.21e+00	3.99e-01	2.11e-01	1.39e-01	0.00e+00	8.08e-01	3.71e-01	1.53e-01	0.00e+00	0.00e+00
N	AM	720	8.56e+00	2.71e+00	9.73e-01	5.05e-01	0.00e+00	0.00e+00	1.56e+00	5.18e-01	0.00e+00	0.00e+00	0.00e+00
N	AM	720	9.75e+00	1.04e+00	3.24e-01	0.00e+00	0.00e+00	0.00e+00	3.52e-01	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	AM	720	0.00e+00	0.00e+00	0.00e+00	NA	NA	0.00e+00	NA	NA	NA	0.00e+00	0.00e+00
N	B	2	4.50e+00	4.02e+00	1.04e+00	NA	NA	NA	NA	NA	NA	NA	0.00e+00
N	B	2	5.32e+00	4.61e+00	1.31e+00	NA	NA	NA	NA	NA	NA	NA	0.00e+00
N	B	2	8.79e+00	7.21e+00	1.99e+00	NA	NA	NA	NA	NA	NA	NA	0.00e+00
N	B	2	1.09e+01	9.56e+00	2.32e+00	NA	NA	NA	NA	NA	NA	NA	0.00e+00
N	B	2	0.00e+00	0.00e+00	0.00e+00	NA	NA	NA	NA	NA	NA	NA	0.00e+00
N	B	48	5.09e+00	6.15e+00	9.77e-01	2.55e-01	6.19e-02	0.00e+00	1.82e+00	8.12e-01	5.44e-01	4.80e-01	4.80e-01
N	B	48	5.03e+00	5.74e+00	9.54e-01	3.11e-01	6.24e-02	0.00e+00	1.38e+00	3.91e-01	6.37e-02	0.00e+00	0.00e+00
N	B	48	9.39e+00	8.53e+00	2.17e+00	4.56e-01	1.25e-01	8.21e-02	2.97e+00	6.98e-01	2.14e-01	8.77e-02	0.00e+00
N	B	48	1.03e+01	9.98e+00	3.03e+00	8.50e-01	2.90e-01	6.40e-02	4.33e+00	1.25e+00	3.60e-01	6.82e-02	0.00e+00
N	B	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	B	240	4.57e+00	4.54e+00	1.13e+00	2.05e-01	1.10e-01	4.03e-02	1.78e+00	4.16e-01	1.60e-01	4.20e-02	0.00e+00
N	B	240	4.54e+00	4.48e+00	1.15e+00	2.18e-01	9.51e-02	5.95e-02	1.78e+00	4.38e-01	1.64e-01	6.31e-02	0.00e+00
N	B	240	8.75e+00	8.42e+00	2.16e+00	4.95e-01	2.02e-01	1.00e-01	3.50e+00	9.46e-01	3.24e-01	1.06e-01	0.00e+00
N	B	240	1.13e+01	9.32e+00	2.62e+00	5.50e-01	2.52e+01	0.00e+00	3.07e+01	2.76e+01	2.69e+01	0.00e+00	0.00e+00
N	B	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	NA	0.00e+00	NA	NA	NA	0.00e+00	0.00e+00
N	B	720	5.23e+00	4.34e+00	1.38e+00	4.40e-01	4.29e-01	0.00e+00	2.36e+00	9.16e-01	4.39e-01	0.00e+00	0.00e+00
N	B	720	5.24e+00	4.24e+00	1.36e+00	4.04e-01	0.00e+00	0.00e+00	1.81e+00	4.40e-01	0.00e+00	0.00e+00	0.00e+00
N	B	720	1.11e+01	9.39e+00	2.69e+00	8.02e-01	1.62e-01	0.00e+00	3.83e+00	1.03e+00	1.70e-01	0.00e+00	0.00e+00
N	B	720	1.17e+01	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
N	B	720	0.00e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00

Table E.5 – continued from previous page

MC	S	t_{Ads}	C_{CTRL}	C_A	C_{D1}	C_{D2}	C_{D3}	C_{D4}	q_A	q_{D1}	q_{D2}	q_{D3}	q_{D4}
N	BA	2	5.18e+00	4.93e+00	1.35e+00	3.51e-01	9.68e-02	5.20e-02	2.03e+00	6.51e-01	2.73e-01	1.72e-01	1.20e-01
N	BA	2	5.22e+00	4.96e+00	1.33e+00	3.53e-01	9.96e-02	4.94e-02	1.89e+00	5.32e-01	1.53e-01	4.78e-02	0.00e+00
N	BA	2	1.06e+01	9.76e+00	2.62e+00	7.12e-01	2.08e-01	8.74e-02	3.75e+00	1.07e+00	3.09e-01	8.87e-02	0.00e+00
N	BA	2	1.16e+01	1.09e+01	2.92e+00	7.87e-01	2.23e-01	9.45e-02	4.17e+00	1.18e+00	3.35e-01	9.64e-02	0.00e+00
N	BA	2	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	BA	48	5.05e+00	4.85e+00	1.33e+00	3.92e-01	1.11e-01	6.11e-02	1.95e+00	5.91e-01	1.82e-01	6.40e-02	0.00e+00
N	BA	48	5.05e+00	4.70e+00	1.34e+00	3.97e-01	1.14e-01	5.96e-02	1.99e+00	5.99e-01	1.82e-01	6.23e-02	0.00e+00
N	BA	48	1.04e+01	9.49e+00	2.62e+00	7.72e-01	2.18e-01	8.65e-02	3.84e+00	1.14e+00	3.21e-01	9.13e-02	0.00e+00
N	BA	48	1.12e+01	1.07e+01	2.97e+00	9.07e-01	2.64e-01	1.08e-01	4.40e+00	1.34e+00	3.90e-01	1.12e-01	0.00e+00
N	BA	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	BA	240	5.38e+00	4.83e+00	1.36e+00	NA	9.24e-02	0.00e+00	NA	NA	9.40e-02	0.00e+00	0.00e+00
N	BA	240	5.36e+00	4.87e+00	1.38e+00	3.78e-01	9.52e-02	0.00e+00	1.91e+00	5.00e-01	9.76e-02	0.00e+00	0.00e+00
N	BA	240	1.21e+01	1.08e+01	3.11e+00	9.02e-01	2.53e-01	0.00e+00	4.45e+00	1.22e+00	2.62e-01	0.00e+00	0.00e+00
N	BA	240	1.17e+01	1.07e+01	3.06e+00	8.83e-01	2.09e-01	0.00e+00	4.31e+00	1.15e+00	2.12e-01	0.00e+00	0.00e+00
N	BA	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	BA	720	5.03e+00	4.37e+00	1.15e+00	3.54e-01	9.83e-02	0.00e+00	1.69e+00	4.83e-01	1.07e-01	0.00e+00	0.00e+00
N	BA	720	5.02e+00	4.49e+00	1.16e+00	3.58e-01	8.20e-02	0.00e+00	1.69e+00	4.73e-01	8.95e-02	0.00e+00	0.00e+00
N	BA	720	9.81e+00	8.85e+00	2.32e+00	7.86e-01	1.59e-01	0.00e+00	3.44e+00	9.55e-01	1.71e-01	0.00e+00	0.00e+00
N	BA	720	1.17e+01	1.06e+01	2.91e+00	8.61e-01	2.84e-01	0.00e+00	4.36e+00	1.21e+00	3.07e-01	0.00e+00	0.00e+00
N	BA	720	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	BOX	2	4.15e+00	2.62e+00	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
N	BOX	2	4.93e+00	2.84e+00	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
N	BOX	2	7.90e+00	4.62e+00	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
N	BOX	2	9.61e+00	5.77e+00	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
N	BOX	2	0.00e+00	0.00e+00	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
N	BOX	48	4.50e+00	NA	7.63e-01	2.90e-01	2.40e-01	1.11e-01	1.50e+00	6.83e-01	3.74e-01	1.18e-01	0.00e+00
N	BOX	48	4.56e+00	2.82e+00	7.29e-01	3.14e-01	2.86e-01	1.15e-01	1.54e+00	7.63e-01	4.28e-01	1.22e-01	0.00e+00
N	BOX	48	8.48e+00	4.65e+00	1.71e+00	7.78e-01	3.47e-01	0.00e+00	2.95e+00	1.19e+00	3.69e-01	0.00e+00	0.00e+00
N	BOX	48	9.03e+00	7.01e+00	2.35e+00	6.23e-01	6.86e-01	4.36e-01	7.08e+00	4.63e+00	3.98e+00	3.26e+00	2.80e+00
N	BOX	48	0.00e+00	NA	0.00e+00	0.00e+00	0.00e+00	NA	NA	NA	NA	NA	0.00e+00
N	BOX	240	4.19e+00	1.86e+00	8.87e-01	1.01e+00	2.76e-01	1.50e-01	3.55e+00	2.44e+00	1.09e+00	8.02e-01	6.42e-01
N	BOX	240	4.16e+00	1.99e+00	8.89e-01	0.00e+00	2.54e-01	1.47e-01	1.98e+00	8.73e-01	8.73e-01	6.08e-01	4.50e-01
N	BOX	240	7.89e+00	3.86e+00	1.52e+00	7.96e-01	4.97e-01	3.00e-01	4.57e+00	2.68e+00	1.61e+00	1.09e+00	7.73e-01
N	BOX	240	1.01e+01	4.64e+00	2.19e+00	NA	5.92e-01	2.90e-01	NA	NA	9.31e-01	3.12e-01	0.00e+00
N	BOX	240	0.00e+00	0.00e+00	0.00e+00	NA	0.00e+00	0.00e+00	NA	NA	0.00e+00	0.00e+00	0.00e+00
N	BOX	720	4.72e+00	8.14e-01	3.52e-01	1.85e-01	7.68e-02	0.00e+00	6.49e-01	2.79e-01	7.86e-02	0.00e+00	0.00e+00
N	BOX	720	4.71e+00	8.40e-01	4.45e-01	2.48e-01	0.00e+00	0.00e+00	7.34e-01	2.70e-01	0.00e+00	0.00e+00	0.00e+00
N	BOX	720	9.90e+00	2.05e+00	1.01e+00	5.43e-01	3.27e-01	2.60e-01	2.26e+00	1.21e+00	6.23e-01	2.88e-01	0.00e+00
N	BOX	720	1.05e+01	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
N	BOX	720	0.00e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00

Table E.5 – continued from previous page

MC	S	t_{Ads}	C_{CTRL}	C_A	C_{D1}	C_{D2}	C_{D3}	C_{D4}	q_A	q_{D1}	q_{D2}	q_{D3}	q_{D4}
N	BT	2	5.24e+00	4.89e+00	1.27e+00	3.24e-01	8.79e-02	3.88e-02	1.83e+00	4.79e-01	1.33e-01	4.01e-02	0.00e+00
N	BT	2	5.19e+00	4.91e+00	1.30e+00	3.21e-01	9.48e-02	4.77e-02	1.86e+00	4.91e-01	1.51e-01	4.95e-02	0.00e+00
N	BT	2	1.07e+01	9.65e+00	2.53e+00	6.55e-01	1.92e-01	9.49e-02	3.62e+00	9.90e-01	3.01e-01	9.79e-02	0.00e+00
N	BT	2	1.17e+01	1.09e+01	3.01e+00	7.77e-01	2.30e-01	8.58e-02	4.28e+00	1.16e+00	3.34e-01	9.03e-02	0.00e+00
N	BT	2	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	BT	48	5.05e+00	4.68e+00	1.18e+00	3.27e-01	8.45e-02	4.27e-02	1.67e+00	4.73e-01	1.34e-01	4.55e-02	0.00e+00
N	BT	48	5.05e+00	4.93e+00	1.26e+00	4.30e-01	7.08e-02	3.87e-02	3.29e+00	2.03e+00	1.58e+00	1.51e+00	1.47e+00
N	BT	48	1.02e+01	9.60e+00	2.38e+00	6.99e-01	1.88e-01	6.86e-02	3.39e+00	1.01e+00	2.68e-01	7.13e-02	0.00e+00
N	BT	48	1.13e+01	1.10e+01	2.76e+00	8.12e-01	2.21e-01	7.31e-02	3.89e+00	1.14e+00	3.06e-01	7.57e-02	0.00e+00
N	BT	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	NA	NA	NA	NA	NA	0.00e+00
N	BT	240	5.41e+00	4.73e+00	1.12e+00	2.50e-01	0.00e+00	0.00e+00	1.42e+00	2.66e-01	0.00e+00	0.00e+00	0.00e+00
N	BT	240	5.43e+00	4.79e+00	1.14e+00	2.46e-01	0.00e+00	0.00e+00	1.44e+00	2.61e-01	0.00e+00	0.00e+00	0.00e+00
N	BT	240	1.21e+01	1.06e+01	2.48e+00	6.05e-01	1.23e-01	0.00e+00	3.39e+00	8.53e-01	2.14e-01	9.12e-02	9.12e-02
N	BT	240	1.19e+01	1.06e+01	2.55e+00	6.18e-01	1.16e-01	0.00e+00	3.44e+00	7.87e-01	1.15e-01	0.00e+00	0.00e+00
N	BT	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	BT	720	5.00e+00	4.18e+00	9.06e-01	2.34e-01	0.00e+00	0.00e+00	3.27e+00	2.30e+00	2.07e+00	2.07e+00	2.07e+00
N	BT	720	4.96e+00	4.33e+00	9.31e-01	2.55e-01	0.00e+00	NA	NA	NA	NA	NA	0.00e+00
N	BT	720	9.88e+00	8.39e+00	1.86e+00	5.71e-01	1.30e-01	0.00e+00	2.54e+00	7.32e-01	1.41e-01	0.00e+00	0.00e+00
N	BT	720	1.16e+01	1.04e+01	2.46e+00	6.48e-01	1.94e-01	0.00e+00	3.31e+00	8.46e-01	2.10e-01	0.00e+00	0.00e+00
N	BT	720	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	BU	2	4.38e+00	1.59e+00	6.99e-01	NA	NA	NA	NA	NA	NA	NA	0.00e+00
N	BU	2	5.16e+00	1.74e+00	7.75e-01	NA	NA	NA	NA	NA	NA	NA	0.00e+00
N	BU	2	8.33e+00	3.07e+00	1.39e+00	NA	NA	NA	NA	NA	NA	NA	0.00e+00
N	BU	2	1.03e+01	3.37e+00	1.57e+00	NA	NA	NA	NA	NA	NA	NA	0.00e+00
N	BU	2	0.00e+00	0.00e+00	0.00e+00	NA	NA	NA	NA	NA	NA	NA	0.00e+00
N	BU	48	4.39e+00	1.13e+00	3.11e-01	3.69e-01	2.64e-01	1.63e-01	2.45e+00	2.10e+00	1.72e+00	1.44e+00	1.27e+00
N	BU	48	4.46e+00	9.96e-01	3.92e-01	3.01e-01	2.19e-01	1.42e-01	2.40e+00	1.97e+00	1.66e+00	1.43e+00	1.27e+00
N	BU	48	8.93e+00	2.20e+00	8.15e-01	5.24e-01	3.95e-01	3.66e-01	4.75e+00	3.85e+00	3.30e+00	2.89e+00	2.49e+00
N	BU	48	9.81e+00	2.10e+00	1.30e+00	8.48e-01	6.23e-01	3.78e-01	7.86e+00	6.40e+00	5.52e+00	4.87e+00	4.46e+00
N	BU	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	BU	240	4.41e+00	6.53e-01	4.30e-01	2.74e-01	2.13e-01	1.89e-01	3.40e+00	2.86e+00	2.50e+00	2.28e+00	2.08e+00
N	BU	240	4.40e+00	6.71e-01	4.64e-01	2.84e-01	2.25e-01	2.10e-01	3.66e+00	3.16e+00	2.79e+00	2.56e+00	2.33e+00
N	BU	240	8.34e+00	1.48e+00	9.74e-01	6.79e-01	0.00e+00	4.33e-01	6.46e+00	5.27e+00	4.58e+00	4.58e+00	4.12e+00
N	BU	240	1.05e+01	1.85e+00	1.27e+00	9.02e-01	6.70e-01	4.46e-01	6.88e+00	5.33e+00	4.41e+00	3.70e+00	3.23e+00
N	BU	240	0.00e+00	0.00e+00	NA	0.00e+00	0.00e+00	0.00e+00	NA	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	BU	720	4.95e+00	3.08e-01	2.53e-01	NA	1.25e-01	1.25e-01	NA	NA	1.18e+00	1.05e+00	9.18e-01
N	BU	720	4.94e+00	3.18e-01	2.42e-01	NA	1.57e-01	8.93e-02	NA	NA	1.18e+00	1.01e+00	9.16e-01
N	BU	720	1.04e+01	8.13e-01	5.41e-01	NA	3.96e-01	2.63e-01	NA	NA	2.40e+00	1.99e+00	1.70e+00
N	BU	720	1.09e+01	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
N	BU	720	0.00e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00

Table E.5 – continued from previous page

MC	S	t_{Ads}	C_{CTRL}	C_A	C_{D1}	C_{D2}	C_{D3}	C_{D4}	q_A	q_{D1}	q_{D2}	q_{D3}	q_{D4}
N	CM	2	4.28e+00	3.67e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA
N	CM	2	4.44e+00	2.81e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA
N	CM	2	7.93e+00	6.82e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA
N	CM	2	9.71e+00	8.45e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA
N	CM	2	0.00e+00	0.00e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA
N	CM	48	4.44e+00	2.82e+00	1.03e+00	3.53e-01	2.79e-01	7.53e-02	NA	NA	NA	NA	NA
N	CM	48	4.46e+00	2.72e+00	1.01e+00	3.33e-01	2.12e-01	6.41e-02	NA	NA	NA	NA	NA
N	CM	48	8.60e+00	5.67e+00	2.28e+00	8.70e-01	3.25e-01	1.92e-01	NA	NA	NA	NA	NA
N	CM	48	8.89e+00	6.59e+00	3.08e+00	1.40e+00	6.07e-01	3.59e-01	NA	NA	NA	NA	NA
N	CM	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	NA	NA	NA	NA	NA
N	CM	240	4.11e+00	3.02e+00	1.11e+00	4.94e-01	2.17e-01	1.26e-01	NA	NA	NA	NA	NA
N	CM	240	4.06e+00	3.10e+00	1.11e+00	4.60e-01	2.02e-01	1.32e-01	NA	NA	NA	NA	NA
N	CM	240	7.80e+00	5.99e+00	2.20e+00	9.88e-01	3.92e-01	2.57e-01	NA	NA	NA	NA	NA
N	CM	240	1.00e+01	7.01e+00	2.81e+00	1.32e+00	6.05e-01	2.26e-01	NA	NA	NA	NA	NA
N	CM	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	NA	NA	NA	NA	NA
N	CM	720	4.57e+00	2.62e+00	1.18e+00	0.00e+00	3.60e-01	1.39e-01	NA	NA	NA	NA	NA
N	CM	720	4.57e+00	2.58e+00	1.18e+00	0.00e+00	3.77e-01	1.73e-01	NA	NA	NA	NA	NA
N	CM	720	9.64e+00	5.79e+00	2.56e+00	1.95e-01	4.62e-01	2.04e-01	NA	NA	NA	NA	NA
N	CM	720	9.37e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
N	CM	720	0.00e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
N	ELL	2	4.80e+00	3.49e+00	1.43e+00	6.81e-01	3.20e-01	1.79e-01	2.79e+00	1.24e+00	5.38e-01	1.87e-01	0.00e+00
N	ELL	2	4.74e+00	3.31e+00	1.53e+00	7.03e-01	3.40e-01	1.93e-01	2.94e+00	1.28e+00	5.78e-01	1.99e-01	0.00e+00
N	ELL	2	9.78e+00	6.97e+00	3.03e+00	1.36e+00	6.77e-01	3.55e-01	5.95e+00	2.67e+00	1.26e+00	5.19e-01	1.48e-01
N	ELL	2	1.06e+01	7.55e+00	3.35e+00	1.55e+00	8.45e-01	4.09e-01	6.74e+00	3.13e+00	1.53e+00	5.93e-01	1.68e-01
N	ELL	2	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	ELL	48	4.60e+00	3.17e+00	1.58e+00	6.61e-01	3.44e-01	1.77e-01	3.05e+00	1.42e+00	7.48e-01	3.60e-01	1.76e-01
N	ELL	48	4.61e+00	2.92e+00	1.46e+00	6.86e-01	3.62e-01	1.88e-01	4.35e+00	2.81e+00	2.11e+00	1.70e+00	1.50e+00
N	ELL	48	9.29e+00	5.91e+00	2.95e+00	1.40e+00	7.30e-01	3.72e-01	5.91e+00	2.82e+00	1.39e+00	5.64e-01	1.75e-01
N	ELL	48	1.03e+01	6.60e+00	3.27e+00	1.68e+00	8.20e-01	4.13e-01	6.77e+00	3.32e+00	1.60e+00	6.83e-01	2.48e-01
N	ELL	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	ELL	240	5.04e+00	1.95e+00	7.20e-01	1.16e-01	0.00e+00	0.00e+00	8.63e-01	1.26e-01	0.00e+00	0.00e+00	0.00e+00
N	ELL	240	4.98e+00	7.82e-02	6.31e-01	1.04e-01	0.00e+00	0.00e+00	7.60e-01	1.11e-01	0.00e+00	0.00e+00	0.00e+00
N	ELL	240	1.12e+01	2.59e+00	8.59e-01	0.00e+00	0.00e+00	0.00e+00	8.91e-01	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	ELL	240	1.10e+01	1.29e+00	4.78e-01	9.29e-02	0.00e+00	0.00e+00	1.05e+00	5.51e-01	4.52e-01	4.52e-01	4.52e-01
N	ELL	240	0.00e+00	NA	NA	0.00e+00	NA	NA	NA	NA	NA	NA	0.00e+00
N	ELL	720	4.69e+00	2.40e+00	1.02e+00	5.57e-01	2.64e-01	0.00e+00	1.95e+00	8.87e-01	2.78e-01	0.00e+00	0.00e+00
N	ELL	720	4.63e+00	2.35e+00	1.02e+00	5.66e-01	2.58e-01	0.00e+00	1.95e+00	8.99e-01	2.72e-01	0.00e+00	0.00e+00
N	ELL	720	9.11e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
N	ELL	720	1.06e+01	0.00e+00	2.48e+00	1.36e+00	0.00e+00	0.00e+00	4.09e+00	1.48e+00	0.00e+00	0.00e+00	0.00e+00
N	ELL	720	0.00e+00	NA	NA	NA	NA	0.00e+00	NA	NA	NA	0.00e+00	0.00e+00

Table E.5 – continued from previous page

MC	S	t_{Ads}	C_{CTRL}	C_A	C_{D1}	C_{D2}	C_{D3}	C_{D4}	q_A	q_{D1}	q_{D2}	q_{D3}	q_{D4}
N	FT	2	4.96e+00	3.38e+00	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
N	FT	2	4.31e+00	4.21e+00	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
N	FT	2	9.37e+00	6.07e+00	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
N	FT	2	1.14e+01	7.93e+00	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
N	FT	2	0.00e+00	0.00e+00	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
N	FT	48	4.26e+00	3.59e+00	1.27e+00	3.18e-01	1.72e-01	3.98e-02	1.90e+00	5.53e-01	2.19e-01	4.25e-02	0.00e+00
N	FT	48	4.22e+00	3.44e+00	1.30e+00	3.23e-01	1.65e-01	4.91e-02	1.92e+00	5.73e-01	2.25e-01	5.44e-02	0.00e+00
N	FT	48	8.36e+00	7.44e+00	2.74e+00	8.09e-01	3.29e-01	0.00e+00	4.04e+00	1.20e+00	3.34e-01	0.00e+00	0.00e+00
N	FT	48	9.58e+00	8.69e+00	3.41e+00	1.31e+00	4.41e-01	0.00e+00	5.30e+00	1.85e+00	4.57e-01	0.00e+00	0.00e+00
N	FT	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	FT	240	4.20e+00	4.02e+00	1.25e+00	3.44e-01	1.16e-01	1.04e-01	2.38e+00	8.63e-01	3.93e-01	2.71e-01	1.60e-01
N	FT	240	4.23e+00	3.98e+00	1.24e+00	3.46e-01	1.23e-01	1.11e-01	2.36e+00	8.66e-01	3.98e-01	2.66e-01	1.49e-01
N	FT	240	7.96e+00	7.51e+00	2.40e+00	7.83e-01	2.67e-01	1.37e-01	4.48e+00	1.64e+00	5.69e-01	2.85e-01	1.42e-01
N	FT	240	1.03e+01	9.18e+00	3.05e+00	1.03e+00	3.77e-01	1.70e-01	5.60e+00	1.95e+00	5.88e-01	1.86e-01	0.00e+00
N	FT	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	FT	720	4.79e+00	3.84e+00	1.40e+00	5.47e-01	3.11e-01	5.68e-02	2.45e+00	9.93e-01	3.99e-01	6.02e-02	0.00e+00
N	FT	720	4.81e+00	3.89e+00	1.44e+00	4.58e-01	3.02e-01	0.00e+00	2.31e+00	8.22e-01	3.29e-01	0.00e+00	0.00e+00
N	FT	720	1.01e+01	8.31e+00	3.00e+00	9.73e-01	4.06e-01	1.42e-01	4.79e+00	1.65e+00	5.92e-01	1.51e-01	0.00e+00
N	FT	720	1.08e+01	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
N	FT	720	0.00e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
N	GAS	2	4.68e+00	5.29e-01	1.10e-01	NA	NA	NA	NA	NA	NA	NA	0.00e+00
N	GAS	2	4.34e+00	3.31e-01	6.19e-02	NA	NA	NA	NA	NA	NA	NA	0.00e+00
N	GAS	2	9.27e+00	6.61e-01	2.28e-01	NA	NA	NA	NA	NA	NA	NA	0.00e+00
N	GAS	2	1.13e+01	1.09e+00	2.59e-01	NA	NA	NA	NA	NA	NA	NA	0.00e+00
N	GAS	2	0.00e+00	0.00e+00	0.00e+00	NA	NA	NA	NA	NA	NA	NA	0.00e+00
N	GAS	48	4.64e+00	1.83e-01	0.00e+00	0.00e+00	0.00e+00	2.88e-02	1.08e+00	1.08e+00	1.08e+00	1.08e+00	1.05e+00
N	GAS	48	4.64e+00	1.37e-01	0.00e+00	0.00e+00	0.00e+00	4.56e-02	1.04e+00	1.04e+00	1.04e+00	1.04e+00	9.90e-01
N	GAS	48	8.69e+00	3.97e-01	6.97e-02	5.20e-02	6.02e-02	5.93e-02	1.63e+00	1.56e+00	1.51e+00	1.44e+00	1.38e+00
N	GAS	48	9.42e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	4.18e+00	4.18e+00	4.18e+00	4.18e+00	4.18e+00
N	GAS	48	0.00e+00	0.00e+00	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
N	GAS	240	4.11e+00	7.66e-02	5.77e-02	4.76e-02	4.78e-02	4.23e-02	2.24e+00	2.17e+00	2.11e+00	2.06e+00	2.02e+00
N	GAS	240	4.14e+00	5.65e-02	4.64e-02	3.35e-02	3.89e-02	4.05e-02	1.49e+00	1.44e+00	1.40e+00	1.36e+00	1.32e+00
N	GAS	240	7.80e+00	1.37e-01	9.85e-02	9.80e-02	8.81e-02	9.32e-02	3.40e+00	3.30e+00	3.17e+00	3.08e+00	2.98e+00
N	GAS	240	1.01e+01	1.41e-01	0.00e+00	0.00e+00	0.00e+00	0.00e+00	3.35e+00	3.35e+00	3.35e+00	3.35e+00	3.35e+00
N	GAS	240	0.00e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
N	GAS	720	4.75e+00	0.00e+00	0.00e+00	5.57e-01	0.00e+00	0.00e+00	6.08e-01	6.08e-01	0.00e+00	0.00e+00	0.00e+00
N	GAS	720	4.75e+00	0.00e+00	0.00e+00	5.51e-01	0.00e+00	0.00e+00	6.05e-01	6.05e-01	0.00e+00	0.00e+00	0.00e+00
N	GAS	720	1.01e+01	0.00e+00	0.00e+00	1.20e+00	0.00e+00	0.00e+00	1.33e+00	1.33e+00	0.00e+00	0.00e+00	0.00e+00
N	GAS	720	1.06e+01	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
N	GAS	720	0.00e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00

Table E.5 – continued from previous page

MC	S	t_{Ads}	C_{CTRL}	C_A	C_{D1}	C_{D2}	C_{D3}	C_{D4}	q_A	q_{D1}	q_{D2}	q_{D3}	q_{D4}
N	GUA	2	4.79e+00	3.94e+00	1.38e+00	4.75e-01	1.60e-01	7.08e-02	2.16e+00	7.26e-01	2.42e-01	7.12e-02	0.00e+00
N	GUA	2	4.80e+00	4.07e+00	1.31e+00	4.94e-01	1.69e-01	6.84e-02	2.11e+00	7.41e-01	2.44e-01	6.30e-02	0.00e+00
N	GUA	2	1.09e+01	8.91e+00	3.03e+00	1.06e+00	3.41e-01	1.10e-01	4.75e+00	1.54e+00	4.59e-01	1.05e-01	0.00e+00
N	GUA	2	1.06e+01	8.57e+00	2.95e+00	1.06e+00	3.64e-01	1.24e-01	4.71e+00	1.57e+00	4.94e-01	1.07e-01	0.00e+00
N	GUA	2	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	GUA	48	4.64e+00	3.22e+00	1.22e+00	5.12e-01	1.52e-01	6.96e-02	2.12e+00	9.37e-01	3.96e-01	2.34e-01	1.61e-01
N	GUA	48	4.64e+00	3.51e+00	1.34e+00	NA	1.37e-01	6.26e-02	NA	NA	2.10e-01	6.69e-02	0.00e+00
N	GUA	48	1.14e+01	6.72e+00	3.14e+00	1.12e+00	4.05e-01	1.50e-01	5.13e+00	1.84e+00	6.49e-01	2.16e-01	5.80e-02
N	GUA	48	1.07e+01	9.06e+00	3.23e+00	1.17e+00	4.51e-01	2.08e-01	5.57e+00	2.02e+00	8.07e-01	3.29e-01	1.12e-01
N	GUA	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	GUA	240	4.56e+00	2.44e+00	9.40e-01	2.41e-01	1.01e-01	5.56e-02	1.39e+00	4.17e-01	1.67e-01	5.99e-02	0.00e+00
N	GUA	240	4.59e+00	2.53e+00	1.05e+00	3.99e-01	1.01e-01	5.55e-02	1.67e+00	5.84e-01	1.67e-01	5.90e-02	0.00e+00
N	GUA	240	1.12e+01	7.46e+00	2.76e+00	1.03e+00	3.52e-01	1.30e-01	4.45e+00	1.58e+00	5.12e-01	1.40e-01	0.00e+00
N	GUA	240	1.03e+01	7.32e+00	2.64e+00	9.93e-01	3.33e-01	0.00e+00	4.11e+00	1.41e+00	3.51e-01	0.00e+00	0.00e+00
N	GUA	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	NA	NA	NA	NA	NA	0.00e+00
N	GUA	720	4.61e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	GUA	720	4.63e+00	1.12e-01	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	GUA	720	1.13e+01	1.78e-01	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	GUA	720	1.05e+01	8.95e-02	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	GUA	720	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	H	2	5.22e+00	2.62e+00	1.00e+00	4.73e-01	2.15e-01	9.37e-02	2.18e+00	1.12e+00	6.32e-01	4.05e-01	3.06e-01
N	H	2	5.21e+00	2.71e+00	1.00e+00	5.00e-01	2.22e-01	9.49e-02	2.16e+00	1.11e+00	5.86e-01	3.53e-01	2.54e-01
N	H	2	1.18e+01	5.87e+00	2.20e+00	1.07e+00	4.92e-01	2.56e-01	4.68e+00	2.31e+00	1.17e+00	6.54e-01	3.89e-01
N	H	2	1.15e+01	9.95e-01	2.08e+00	1.10e+00	5.02e-01	2.79e-01	4.94e+00	2.75e+00	1.59e+00	1.06e+00	7.65e-01
N	H	2	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	H	48	4.99e+00	1.16e+00	5.97e-01	3.26e-01	1.99e-01	1.35e-01	2.29e+00	1.67e+00	1.32e+00	1.12e+00	9.82e-01
N	H	48	5.00e+00	1.17e+00	6.23e-01	3.07e-01	1.81e-01	1.17e-01	2.67e+00	2.01e+00	1.69e+00	1.50e+00	1.38e+00
N	H	48	1.23e+01	2.99e+00	1.62e+00	8.51e-01	5.17e-01	3.28e-01	4.87e+00	3.14e+00	2.24e+00	1.69e+00	1.36e+00
N	H	48	1.15e+01	3.06e+00	1.58e+00	8.37e-01	4.70e-01	2.87e-01	4.48e+00	2.77e+00	1.89e+00	1.40e+00	1.10e+00
N	H	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	NA	0.00e+00	NA	NA	NA	0.00e+00	0.00e+00
N	H	240	4.95e+00	1.30e-01	0.00e+00	0.00e+00	0.00e+00	0.00e+00	5.01e-02	5.01e-02	5.01e-02	5.01e-02	5.01e-02
N	H	240	4.97e+00	1.03e-01	0.00e+00	0.00e+00	0.00e+00	0.00e+00	5.43e-02	5.43e-02	5.43e-02	5.43e-02	5.43e-02
N	H	240	1.21e+01	2.78e-01	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	H	240	1.14e+01	2.07e-01	1.24e-01	0.00e+00	0.00e+00	0.00e+00	1.28e-01	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	H	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	H	720	4.96e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	H	720	4.98e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	H	720	1.22e+01	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	H	720	1.14e+01	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	H	720	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00

Table E.5 – continued from previous page

MC	S	t_{Ads}	C_{CTRL}	C_A	C_{D1}	C_{D2}	C_{D3}	C_{D4}	q_A	q_{D1}	q_{D2}	q_{D3}	q_{D4}
N	J	2	4.82e+00	2.17e+00	1.04e+00	5.98e-01	3.87e-01	2.01e-01	6.20e+00	4.23e+00	3.17e+00	2.50e+00	2.15e+00
N	J	2	4.81e+00	2.02e+00	8.89e-01	5.38e-01	3.76e-01	1.81e-01	5.88e+00	4.27e+00	3.33e+00	2.68e+00	2.36e+00
N	J	2	1.05e+01	5.38e+00	2.41e+00	1.38e+00	9.11e-01	5.33e-01	1.31e+01	8.71e+00	6.24e+00	4.67e+00	3.73e+00
N	J	2	1.05e+01	5.02e+00	2.31e+00	1.27e+00	8.64e-01	5.27e-01	1.21e+01	7.99e+00	5.76e+00	4.28e+00	3.35e+00
N	J	2	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	J	48	4.61e+00	1.18e+00	7.22e-01	5.05e-01	3.35e-01	2.47e-01	5.77e+00	4.48e+00	3.61e+00	3.01e+00	2.58e+00
N	J	48	4.61e+00	1.24e+00	7.61e-01	5.29e-01	3.37e-01	2.63e-01	5.46e+00	4.12e+00	3.18e+00	2.58e+00	2.12e+00
N	J	48	1.14e+01	3.63e+00	2.03e+00	1.41e+00	8.93e-01	6.65e-01	1.46e+01	1.09e+01	8.53e+00	6.95e+00	5.78e+00
N	J	48	1.07e+01	3.78e+00	2.13e+00	1.34e+00	8.71e-01	7.95e-01	1.68e+01	1.29e+01	1.06e+01	9.07e+00	7.67e+00
N	J	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	J	240	4.61e+00	8.25e-01	5.40e-01	3.54e-01	2.55e-01	2.42e-01	5.68e+00	4.77e+00	4.15e+00	3.71e+00	3.32e+00
N	J	240	4.60e+00	7.68e-01	5.33e-01	3.31e-01	2.35e-01	2.33e-01	5.69e+00	4.79e+00	4.21e+00	3.81e+00	3.43e+00
N	J	240	1.14e+01	2.73e+00	1.70e+00	1.05e+00	7.15e-01	6.56e-01	1.33e+01	1.04e+01	8.54e+00	7.31e+00	6.23e+00
N	J	240	1.07e+01	2.50e+00	1.47e+00	1.10e+00	7.10e-01	5.15e-01	1.33e+01	1.09e+01	9.02e+00	7.82e+00	6.93e+00
N	J	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	J	720	4.60e+00	1.29e-01	0.00e+00	0.00e+00	0.00e+00	0.00e+00	8.51e-01	8.51e-01	8.51e-01	8.51e-01	8.51e-01
N	J	720	4.62e+00	1.36e-01	7.83e-02	0.00e+00	0.00e+00	0.00e+00	1.17e+00	1.03e+00	1.03e+00	1.03e+00	1.03e+00
N	J	720	1.13e+01	2.78e-01	1.53e-01	0.00e+00	0.00e+00	0.00e+00	3.15e+00	2.88e+00	2.88e+00	2.88e+00	2.88e+00
N	J	720	1.05e+01	1.37e-01	1.40e-01	0.00e+00	0.00e+00	0.00e+00	1.07e+00	8.40e-01	8.40e-01	8.40e-01	8.40e-01
N	J	720	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	KA	2	5.10e+00	4.62e+00	1.33e+00	4.09e-01	8.68e-02	3.41e-02	3.31e+00	9.35e-01	2.13e-01	6.12e-02	0.00e+00
N	KA	2	5.07e+00	4.66e+00	1.30e+00	4.00e-01	8.83e-02	2.94e-02	3.23e+00	9.17e-01	2.06e-01	5.25e-02	0.00e+00
N	KA	2	1.12e+01	1.04e+01	2.97e+00	9.23e-01	2.36e-01	7.54e-02	7.42e+00	2.20e+00	5.44e-01	1.36e-01	0.00e+00
N	KA	2	1.12e+01	1.03e+01	2.83e+00	8.92e-01	2.23e-01	6.43e-02	7.10e+00	2.10e+00	5.05e-01	1.15e-01	0.00e+00
N	KA	2	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	KA	48	4.84e+00	4.26e+00	1.37e+00	3.32e-01	7.98e-02	3.15e-02	3.21e+00	7.80e-01	1.96e-01	5.45e-02	0.00e+00
N	KA	48	4.83e+00	4.63e+00	NA	3.41e-01	8.18e-02	2.96e-02	NA	8.01e-01	1.94e-01	5.18e-02	0.00e+00
N	KA	48	1.19e+01	1.06e+01	3.31e+00	9.20e-01	2.46e-01	8.21e-02	7.41e+00	2.20e+00	5.79e-01	1.44e-01	0.00e+00
N	KA	48	1.11e+01	1.08e+01	3.05e+00	8.67e-01	2.31e-01	7.86e-02	7.57e+00	2.08e+00	5.42e-01	1.37e-01	0.00e+00
N	KA	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	KA	240	4.80e+00	4.34e+00	1.23e+00	3.43e-01	9.71e-02	1.64e-02	2.98e+00	8.13e-01	2.00e-01	2.84e-02	0.00e+00
N	KA	240	4.81e+00	4.29e+00	1.23e+00	3.43e-01	1.16e-01	4.05e-02	3.02e+00	8.80e-01	2.73e-01	6.99e-02	0.00e+00
N	KA	240	1.18e+01	1.02e+01	3.01e+00	8.52e-01	2.45e-01	8.64e-02	7.36e+00	2.10e+00	5.83e-01	1.50e-01	0.00e+00
N	KA	240	1.12e+01	1.01e+01	2.91e+00	8.18e-01	1.92e-01	8.16e-02	6.98e+00	1.92e+00	4.82e-01	1.45e-01	0.00e+00
N	KA	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	KA	720	4.83e+00	4.00e+00	1.11e+00	1.25e-01	3.76e-02	0.00e+00	2.27e+00	2.83e-01	6.48e-02	0.00e+00	0.00e+00
N	KA	720	4.80e+00	4.11e+00	1.15e+00	1.25e-01	5.63e-02	0.00e+00	2.37e+00	3.19e-01	9.70e-02	0.00e+00	0.00e+00
N	KA	720	1.18e+01	9.71e+00	2.78e+00	3.01e-01	1.02e-01	0.00e+00	5.73e+00	7.04e-01	1.77e-01	0.00e+00	0.00e+00
N	KA	720	1.10e+01	NA	2.84e+00	5.89e-01	1.02e-01	0.00e+00	6.11e+00	1.24e+00	1.83e-01	0.00e+00	0.00e+00
N	KA	720	0.00e+00	0.00e+00	NA	0.00e+00	0.00e+00	0.00e+00	NA	0.00e+00	0.00e+00	0.00e+00	0.00e+00

Table E.5 – continued from previous page

MC	S	t_{Ads}	C_{CTRL}	C_A	C_{D1}	C_{D2}	C_{D3}	C_{D4}	q_A	q_{D1}	q_{D2}	q_{D3}	q_{D4}
N	LCL	2	4.44e+00	2.07e+00	1.14e+00	NA	NA	NA	NA	NA	NA	NA	0.00e+00
N	LCL	2	3.80e+00	2.56e+00	9.19e-01	NA	NA	NA	NA	NA	NA	NA	0.00e+00
N	LCL	2	8.66e+00	3.64e+00	2.20e+00	NA	NA	NA	NA	NA	NA	NA	0.00e+00
N	LCL	2	1.06e+01	4.73e+00	0.00e+00	NA	NA	NA	NA	NA	NA	NA	0.00e+00
N	LCL	2	0.00e+00	0.00e+00	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
N	LCL	48	3.93e+00	1.95e+00	6.06e-01	3.17e-01	2.52e-01	1.61e-01	2.15e+00	1.51e+00	1.17e+00	9.02e-01	7.30e-01
N	LCL	48	3.91e+00	1.91e+00	5.84e-01	3.02e-01	2.58e-01	1.55e-01	2.00e+00	1.37e+00	1.06e+00	7.84e-01	6.24e-01
N	LCL	48	7.92e+00	3.50e+00	1.47e+00	7.95e-01	4.34e-01	3.51e-01	4.28e+00	2.74e+00	1.89e+00	1.43e+00	1.06e+00
N	LCL	48	8.70e+00	4.53e+00	2.06e+00	1.20e+00	8.42e-01	5.39e-01	7.32e+00	5.18e+00	3.92e+00	3.02e+00	2.44e+00
N	LCL	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	LCL	240	3.92e+00	1.34e+00	7.43e-01	4.27e-01	2.73e-01	2.14e-01	3.18e+00	2.26e+00	1.82e+00	1.54e+00	1.31e+00
N	LCL	240	3.90e+00	1.36e+00	7.42e-01	4.34e-01	2.82e-01	2.28e-01	3.01e+00	2.09e+00	1.64e+00	1.34e+00	1.10e+00
N	LCL	240	7.39e+00	2.78e+00	1.53e+00	9.09e-01	5.87e-01	3.77e-01	6.08e+00	4.22e+00	3.27e+00	2.64e+00	2.24e+00
N	LCL	240	9.52e+00	3.29e+00	1.82e+00	1.22e+00	7.86e-01	4.52e-01	7.32e+00	5.08e+00	3.81e+00	2.99e+00	2.51e+00
N	LCL	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	LCL	720	4.42e+00	5.55e-01	3.59e-01	2.42e-01	1.28e-01	0.00e+00	1.36e+00	9.83e-01	7.20e-01	5.87e-01	5.87e-01
N	LCL	720	4.42e+00	5.62e-01	3.56e-01	2.45e-01	1.90e-01	NA	NA	NA	NA	NA	6.14e-01
N	LCL	720	9.34e+00	1.43e+00	8.95e-01	6.12e-01	2.96e-01	2.87e-01	3.29e+00	2.34e+00	1.66e+00	1.35e+00	1.05e+00
N	LCL	720	9.87e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
N	LCL	720	0.00e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
N	LCO	2	4.26e+00	2.49e+00	7.81e-01	NA	NA	NA	NA	NA	NA	NA	0.00e+00
N	LCO	2	4.93e+00	2.17e+00	5.92e-01	NA	NA	NA	NA	NA	NA	NA	0.00e+00
N	LCO	2	8.22e+00	4.31e+00	1.73e+00	NA	NA	NA	NA	NA	NA	NA	0.00e+00
N	LCO	2	9.99e+00	4.85e+00	2.26e+00	NA	NA	NA	NA	NA	NA	NA	0.00e+00
N	LCO	2	0.00e+00	0.00e+00	0.00e+00	NA	NA	NA	NA	NA	NA	NA	0.00e+00
N	LCO	48	4.38e+00	1.25e+00	3.63e-01	2.42e-01	1.87e-01	9.89e-02	1.87e+00	1.50e+00	1.25e+00	1.04e+00	9.43e-01
N	LCO	48	4.41e+00	1.97e+00	3.12e-01	2.92e-01	2.02e-01	1.15e-01	2.41e+00	2.09e+00	1.78e+00	1.56e+00	1.44e+00
N	LCO	48	8.65e+00	2.49e+00	7.15e-01	4.01e-01	2.56e-01	2.23e-01	2.19e+00	1.50e+00	1.08e+00	8.02e-01	5.67e-01
N	LCO	48	9.82e+00	1.23e+00	9.24e-01	4.86e-01	5.08e-01	3.90e-01	4.62e+00	3.64e+00	3.13e+00	2.57e+00	2.16e+00
N	LCO	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	LCO	240	4.33e+00	7.25e-01	3.85e-01	2.53e-01	1.92e-01	1.72e-01	3.73e+00	3.28e+00	2.94e+00	2.74e+00	2.56e+00
N	LCO	240	4.35e+00	7.06e-01	3.75e-01	2.41e-01	1.77e-01	1.70e-01	3.95e+00	3.43e+00	3.10e+00	2.92e+00	2.74e+00
N	LCO	240	8.22e+00	1.40e+00	7.14e-01	4.66e-01	3.12e-01	2.71e-01	4.32e+00	3.49e+00	2.84e+00	2.52e+00	2.24e+00
N	LCO	240	1.06e+01	1.74e+00	1.05e+00	7.30e-01	4.88e-01	2.82e-01	5.40e+00	4.17e+00	3.16e+00	2.66e+00	2.36e+00
N	LCO	240	0.00e+00	NA	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	LCO	720	4.96e+00	1.49e-01	1.14e-01	9.21e-02	7.30e-02	0.00e+00	9.86e-01	8.70e-01	7.70e-01	6.91e-01	6.91e-01
N	LCO	720	4.93e+00	2.35e-01	1.51e-01	1.13e-01	9.13e-02	0.00e+00	1.35e+00	1.19e+00	1.07e+00	9.74e-01	9.74e-01
N	LCO	720	1.04e+01	4.13e-01	2.38e-01	1.62e-01	1.17e-01	8.23e-02	1.58e+00	1.34e+00	1.17e+00	1.04e+00	9.52e-01
N	LCO	720	1.10e+01	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
N	LCO	720	0.00e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00

Table E.5 – continued from previous page

MC	S	t_{Ads}	C_{CTRL}	C_A	C_{D1}	C_{D2}	C_{D3}	C_{D4}	q_A	q_{D1}	q_{D2}	q_{D3}	q_{D4}
N	M	2	5.04e+00	3.79e+00	1.47e+00	5.90e-01	2.25e-01	1.12e-01	2.59e+00	1.00e+00	4.18e-01	1.67e-01	4.89e-02
N	M	2	5.01e+00	3.88e+00	1.43e+00	5.80e-01	2.26e-01	8.21e-02	2.52e+00	9.44e-01	3.66e-01	1.15e-01	2.70e-02
N	M	2	1.13e+01	8.50e+00	3.33e+00	1.31e+00	5.31e-01	2.07e-01	5.82e+00	2.18e+00	8.61e-01	2.78e-01	5.74e-02
N	M	2	1.10e+01	8.47e+00	3.26e+00	1.31e+00	5.17e-01	2.06e-01	5.59e+00	2.10e+00	7.82e-01	2.17e-01	0.00e+00
N	M	2	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	M	48	4.61e+00	3.18e+00	1.22e+00	4.94e-01	2.12e-01	9.32e-02	2.14e+00	8.92e-01	3.84e-01	1.59e-01	6.53e-02
N	M	48	4.61e+00	3.19e+00	1.35e+00	4.98e-01	2.08e-01	9.20e-02	2.34e+00	9.60e-01	4.33e-01	2.12e-01	1.17e-01
N	M	48	1.13e+01	7.75e+00	3.08e+00	1.26e+00	5.43e-01	2.47e-01	5.60e+00	2.45e+00	1.12e+00	5.43e-01	2.89e-01
N	M	48	1.08e+01	8.15e+00	3.25e+00	1.43e+00	5.76e-01	3.29e-01	6.57e+00	3.00e+00	1.50e+00	8.93e-01	5.43e-01
N	M	48	0.00e+00	NA	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	M	240	4.62e+00	2.93e+00	1.19e+00	4.85e-01	1.62e-01	7.84e-02	2.61e+00	1.33e+00	8.23e-01	6.52e-01	5.75e-01
N	M	240	4.60e+00	2.91e+00	1.18e+00	4.88e-01	1.60e-01	8.14e-02	2.44e+00	1.15e+00	6.34e-01	4.64e-01	3.82e-01
N	M	240	1.13e+01	7.42e+00	2.91e+00	1.15e+00	4.49e-01	2.12e-01	5.52e+00	2.36e+00	1.15e+00	6.75e-01	4.64e-01
N	M	240	1.06e+01	7.14e+00	2.91e+00	1.24e+00	5.70e-01	2.13e-01	5.92e+00	2.98e+00	1.66e+00	1.06e+00	8.31e-01
N	M	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	M	720	4.61e+00	2.00e+00	7.49e-01	3.31e-01	9.36e-02	0.00e+00	1.26e+00	4.51e-01	9.48e-02	0.00e+00	0.00e+00
N	M	720	4.60e+00	1.93e+00	7.35e-01	NA	9.15e-02	0.00e+00	NA	NA	9.15e-02	0.00e+00	0.00e+00
N	M	720	1.13e+01	5.66e+00	2.13e+00	8.09e-01	1.72e-01	0.00e+00	3.33e+00	1.04e+00	1.72e-01	0.00e+00	0.00e+00
N	M	720	1.05e+01	0.00e+00	2.26e+00	8.85e-01	2.84e-01	NA	NA	NA	NA	NA	0.00e+00
N	M	720	0.00e+00	NA	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	N	2	4.97e+00	4.11e+00	1.26e+00	4.70e-01	1.58e-01	7.49e-02	2.06e+00	7.30e-01	2.41e-01	8.01e-02	0.00e+00
N	N	2	5.02e+00	4.02e+00	1.27e+00	4.63e-01	1.46e-01	6.31e-02	2.06e+00	7.06e-01	2.18e-01	6.69e-02	0.00e+00
N	N	2	1.14e+01	9.31e+00	2.91e+00	9.66e-01	3.07e-01	9.06e-02	4.61e+00	1.45e+00	4.13e-01	9.44e-02	0.00e+00
N	N	2	1.11e+01	9.05e+00	2.73e+00	9.43e-01	3.16e-01	9.67e-02	4.28e+00	1.41e+00	4.28e-01	1.02e-01	0.00e+00
N	N	2	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	N	48	4.76e+00	3.45e+00	1.20e+00	4.13e-01	1.45e-01	6.46e-02	1.96e+00	7.17e-01	2.67e-01	1.15e-01	4.69e-02
N	N	48	4.77e+00	3.83e+00	1.28e+00	4.20e-01	1.41e-01	6.58e-02	2.06e+00	7.28e-01	2.81e-01	1.31e-01	6.37e-02
N	N	48	1.17e+01	8.92e+00	3.05e+00	1.06e+00	3.72e-01	1.46e-01	4.96e+00	1.81e+00	6.49e-01	2.58e-01	1.04e-01
N	N	48	1.11e+01	8.74e+00	2.90e+00	1.18e+00	3.79e-01	1.83e-01	5.02e+00	1.84e+00	5.85e-01	1.90e-01	0.00e+00
N	N	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	N	240	4.74e+00	3.11e+00	1.10e+00	4.14e-01	1.17e-01	5.61e-02	2.00e+00	8.29e-01	3.96e-01	2.72e-01	2.12e-01
N	N	240	4.74e+00	3.14e+00	1.16e+00	3.67e-01	1.21e-01	5.80e-02	2.04e+00	7.98e-01	4.09e-01	2.81e-01	2.20e-01
N	N	240	1.16e+01	7.62e+00	2.69e+00	9.65e-01	3.06e-01	1.25e-01	4.42e+00	1.57e+00	5.45e-01	2.24e-01	9.20e-02
N	N	240	1.09e+01	7.31e+00	2.60e+00	1.04e+00	3.28e-01	1.24e-01	4.68e+00	1.99e+00	9.17e-01	5.70e-01	4.40e-01
N	N	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	N	720	4.76e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	N	720	4.71e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	N	720	1.18e+01	9.38e-02	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	N	720	1.09e+01	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	N	720	0.00e+00	NA	0.00e+00	0.00e+00	NA	0.00e+00	NA	NA	NA	0.00e+00	0.00e+00

Table E.5 – continued from previous page

MC	S	t_{Ads}	C_{CTRL}	C_A	C_{D1}	C_{D2}	C_{D3}	C_{D4}	q_A	q_{D1}	q_{D2}	q_{D3}	q_{D4}
N	P	2	4.92e+00	5.66e-01	2.21e-01	1.84e-01	9.93e-02	7.83e-02	3.16e+00	2.79e+00	2.47e+00	2.29e+00	2.19e+00
N	P	2	4.90e+00	5.39e-01	1.90e-01	1.68e-01	9.44e-02	0.00e+00	2.70e+00	2.38e+00	2.08e+00	1.91e+00	1.91e+00
N	P	2	1.12e+01	1.48e+00	5.60e-01	4.74e-01	2.66e-01	2.19e-01	5.75e+00	4.76e+00	3.96e+00	3.48e+00	3.21e+00
N	P	2	1.09e+01	5.49e+00	4.10e-01	3.72e-01	1.95e-01	NA	NA	NA	NA	NA	0.00e+00
N	P	2	0.00e+00	0.00e+00	0.00e+00	NA	NA	NA	NA	NA	NA	NA	0.00e+00
N	P	48	4.71e+00	1.64e-01	1.50e-01	1.28e-01	1.05e-01	9.51e-02	5.66e+00	5.40e+00	5.18e+00	5.00e+00	4.84e+00
N	P	48	4.71e+00	1.51e-01	1.67e-01	1.13e-01	9.42e-02	9.10e-02	2.76e+00	2.48e+00	2.28e+00	2.12e+00	1.96e+00
N	P	48	1.15e+01	4.70e-01	4.33e-01	3.33e-01	2.90e-01	2.69e-01	6.70e+00	5.96e+00	5.39e+00	4.89e+00	4.41e+00
N	P	48	1.09e+01	2.38e-01	2.16e-01	2.72e-01	1.12e-01	7.43e-02	4.50e+00	4.13e+00	3.68e+00	3.49e+00	3.36e+00
N	P	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	P	240	4.64e+00	8.12e-02	4.65e-02	0.00e+00	0.00e+00	0.00e+00	1.09e+00	1.01e+00	1.01e+00	1.01e+00	1.01e+00
N	P	240	4.66e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	6.12e-01	6.12e-01	6.12e-01	6.12e-01	6.12e-01
N	P	240	1.16e+01	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	P	240	1.08e+01	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	P	240	0.00e+00	0.00e+00	0.00e+00	NA	0.00e+00	0.00e+00	NA	NA	0.00e+00	0.00e+00	0.00e+00
N	P	720	4.68e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	P	720	4.66e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	P	720	1.15e+01	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	P	720	1.08e+01	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	P	720	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	PO	2	4.91e+00	1.51e+00	4.19e-01	NA	NA	NA	NA	NA	NA	NA	0.00e+00
N	PO	2	4.07e+00	1.60e+00	6.84e-01	NA	NA	NA	NA	NA	NA	NA	0.00e+00
N	PO	2	9.15e+00	3.56e+00	1.08e+00	NA	NA	NA	NA	NA	NA	NA	0.00e+00
N	PO	2	1.13e+01	4.72e+00	1.38e+00	NA	NA	NA	NA	NA	NA	NA	0.00e+00
N	PO	2	0.00e+00	0.00e+00	0.00e+00	NA	NA	NA	NA	NA	NA	NA	0.00e+00
N	PO	48	4.65e+00	1.08e+00	2.48e-01	2.07e-01	2.02e-01	1.67e-01	8.69e-01	6.09e-01	3.89e-01	1.77e-01	0.00e+00
N	PO	48	4.51e+00	1.06e+00	2.95e-01	1.63e-01	1.64e-01	1.11e-01	1.14e+00	8.28e-01	6.58e-01	4.88e-01	3.70e-01
N	PO	48	8.53e+00	2.19e+00	4.20e-01	3.82e-01	3.68e-01	1.70e-01	2.91e+00	2.47e+00	2.07e+00	1.76e+00	1.58e+00
N	PO	48	9.16e+00	2.25e+00	8.10e-01	4.73e-01	0.00e+00	3.96e-01	3.32e+00	2.47e+00	1.97e+00	1.97e+00	1.55e+00
N	PO	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	PO	240	4.14e+00	4.07e-01	1.86e-01	1.51e-01	1.24e-01	1.43e-01	2.17e+00	1.94e+00	1.74e+00	1.61e+00	1.46e+00
N	PO	240	4.14e+00	3.97e-01	1.95e-01	1.15e-01	1.66e-01	1.26e-01	1.85e+00	1.61e+00	1.46e+00	1.29e+00	1.16e+00
N	PO	240	7.88e+00	1.00e+00	5.10e-01	3.79e-01	3.18e-01	2.07e-01	3.40e+00	2.77e+00	2.27e+00	1.94e+00	1.72e+00
N	PO	240	1.01e+01	1.13e+00	6.28e-01	NA	3.14e-01	2.76e-01	NA	NA	2.03e+00	1.71e+00	1.41e+00
N	PO	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	PO	720	4.69e+00	2.34e-01	0.00e+00	1.97e-01	0.00e+00	0.00e+00	2.05e-01	2.05e-01	0.00e+00	0.00e+00	0.00e+00
N	PO	720	4.71e+00	2.06e-01	2.17e-01	2.01e-01	0.00e+00	0.00e+00	4.33e-01	2.11e-01	0.00e+00	0.00e+00	0.00e+00
N	PO	720	9.88e+00	2.77e-01	2.62e-01	4.97e-01	0.00e+00	0.00e+00	7.87e-01	5.19e-01	0.00e+00	0.00e+00	0.00e+00
N	PO	720	1.05e+01	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
N	PO	720	0.00e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00

Table E.5 – continued from previous page

MC	S	t_{Ads}	C_{CTRL}	C_A	C_{D1}	C_{D2}	C_{D3}	C_{D4}	q_A	q_{D1}	q_{D2}	q_{D3}	q_{D4}
N	R	2	4.85e+00	9.70e-01	6.06e-01	4.93e-01	3.45e-01	2.75e-01	6.00e+00	4.96e+00	4.08e+00	3.48e+00	3.02e+00
N	R	2	4.87e+00	9.17e-01	5.42e-01	4.52e-01	3.24e-01	2.56e-01	5.26e+00	4.34e+00	3.53e+00	2.96e+00	2.54e+00
N	R	2	1.10e+01	2.28e+00	1.40e+00	1.16e+00	8.03e-01	6.69e-01	1.26e+01	1.01e+01	8.10e+00	6.70e+00	5.57e+00
N	R	2	1.07e+01	2.07e+00	1.32e+00	1.09e+00	7.73e-01	6.31e-01	1.21e+01	9.92e+00	7.98e+00	6.64e+00	5.55e+00
N	R	2	0.00e+00	0.00e+00	0.00e+00	0.00e+00	NA	0.00e+00	NA	NA	NA	0.00e+00	0.00e+00
N	R	48	4.63e+00	5.23e-01	4.25e-01	3.77e-01	3.21e-01	2.81e-01	4.80e+00	4.06e+00	3.40e+00	2.85e+00	2.36e+00
N	R	48	4.64e+00	5.22e-01	4.70e-01	3.95e-01	2.99e-01	2.63e-01	4.43e+00	3.64e+00	2.96e+00	2.45e+00	2.00e+00
N	R	48	1.14e+01	1.37e+00	1.10e+00	9.51e-01	7.87e-01	6.71e-01	1.33e+01	1.13e+01	9.76e+00	8.41e+00	7.26e+00
N	R	48	1.07e+01	1.42e+00	1.15e+00	9.35e-01	7.43e-01	5.97e-01	1.14e+01	9.36e+00	7.74e+00	6.50e+00	5.44e+00
N	R	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	R	240	4.60e+00	2.29e-01	9.18e-02	8.43e-02	5.67e-02	5.51e-02	8.90e-01	7.32e-01	5.89e-01	4.93e-01	4.02e-01
N	R	240	4.60e+00	1.84e-01	1.12e-01	5.27e-02	6.58e-02	4.56e-02	1.05e+00	8.57e-01	7.67e-01	6.52e-01	5.76e-01
N	R	240	1.12e+01	5.31e-01	2.74e-01	2.11e-01	1.89e-01	NA	NA	NA	NA	NA	8.51e-01
N	R	240	1.06e+01	4.36e-01	3.86e-01	3.00e-01	2.49e-01	2.08e-01	3.35e+00	2.69e+00	2.15e+00	1.74e+00	1.37e+00
N	R	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	R	720	4.63e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	R	720	4.61e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	R	720	1.14e+01	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	R	720	1.06e+01	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	R	720	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	SOU	2	4.71e+00	3.89e+00	1.41e+00	5.69e-01	2.00e-01	1.08e-01	2.37e+00	9.43e-01	3.60e-01	1.50e-01	3.47e-02
N	SOU	2	4.54e+00	3.85e+00	1.43e+00	5.67e-01	1.97e-01	9.11e-02	2.33e+00	8.82e-01	3.06e-01	9.77e-02	0.00e+00
N	SOU	2	1.07e+01	8.72e+00	0.00e+00	1.23e+00	4.50e-01	1.56e-01	1.93e+00	1.93e+00	6.47e-01	1.68e-01	0.00e+00
N	SOU	2	1.02e+01	8.65e+00	3.23e+00	1.18e+00	4.48e-01	1.58e-01	5.08e+00	1.86e+00	6.45e-01	1.67e-01	0.00e+00
N	SOU	2	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	SOU	48	4.52e+00	3.74e+00	1.30e+00	5.43e-01	1.91e-01	0.00e+00	2.14e+00	7.72e-01	2.03e-01	0.00e+00	0.00e+00
N	SOU	48	4.52e+00	3.77e+00	1.42e+00	5.69e-01	1.94e-01	7.69e-02	2.37e+00	8.90e-01	2.89e-01	8.15e-02	0.00e+00
N	SOU	48	1.11e+01	8.99e+00	3.47e+00	1.31e+00	4.94e-01	2.07e-01	5.82e+00	2.15e+00	7.50e-01	2.20e-01	0.00e+00
N	SOU	48	1.04e+01	8.49e+00	3.45e+00	1.42e+00	5.63e-01	2.98e-01	6.09e+00	2.40e+00	9.01e-01	3.06e-01	0.00e+00
N	SOU	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	SOU	240	4.49e+00	3.17e+00	1.36e+00	5.48e-01	1.90e-01	9.14e-02	2.27e+00	8.65e-01	2.94e-01	9.23e-02	0.00e+00
N	SOU	240	4.48e+00	3.26e+00	1.39e+00	4.63e-01	1.90e-01	NA	NA	NA	NA	NA	0.00e+00
N	SOU	240	1.10e+01	7.01e+00	3.38e+00	1.34e+00	5.12e-01	3.79e-02	5.46e+00	1.98e+00	5.74e-01	3.83e-02	0.00e+00
N	SOU	240	1.04e+01	8.26e+00	3.21e+00	1.44e+00	5.09e-01	2.22e-01	5.58e+00	2.22e+00	7.75e-01	2.36e-01	0.00e+00
N	SOU	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	NA	NA	NA	NA	NA	0.00e+00
N	SOU	720	4.49e+00	1.47e+00	5.09e-01	0.00e+00	0.00e+00	0.00e+00	7.29e-01	1.87e-01	1.87e-01	1.87e-01	1.87e-01
N	SOU	720	4.48e+00	2.27e+00	8.30e-01	0.00e+00	0.00e+00	0.00e+00	8.85e-01	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	SOU	720	1.10e+01	7.08e+00	2.52e+00	0.00e+00	0.00e+00	7.73e-02	2.80e+00	8.34e-02	8.34e-02	8.34e-02	0.00e+00
N	SOU	720	1.02e+01	5.73e+00	2.33e+00	9.11e-01	0.00e+00	0.00e+00	3.15e+00	7.92e-01	2.23e-01	2.23e-01	2.23e-01
N	SOU	720	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	NA	NA	NA	NA	NA	0.00e+00

Table E.5 – continued from previous page

MC	S	t_{Ads}	C_{CTRL}	C_A	C_{D1}	C_{D2}	C_{D3}	C_{D4}	q_A	q_{D1}	q_{D2}	q_{D3}	q_{D4}
N	SSL1	2	4.70e+00	3.68e+00	1.25e+00	5.47e-01	1.37e-01	6.65e-02	2.34e+00	9.98e-01	4.36e-01	2.93e-01	2.25e-01
N	SSL1	2	4.75e+00	3.64e+00	1.26e+00	5.39e-01	1.36e-01	1.24e-01	2.24e+00	8.75e-01	3.13e-01	1.67e-01	3.75e-02
N	SSL1	2	9.70e+00	7.41e+00	2.41e+00	9.77e-01	3.10e-01	NA	NA	NA	NA	NA	1.32e-01
N	SSL1	2	1.07e+01	8.04e+00	2.69e+00	1.12e+00	3.38e-01	1.27e-01	4.67e+00	1.76e+00	5.95e-01	2.36e-01	1.03e-01
N	SSL1	2	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	SSL1	48	4.53e+00	1.46e+00	0.00e+00	1.85e-01	7.49e-02	3.99e-02	3.17e-01	3.17e-01	1.22e-01	4.19e-02	0.00e+00
N	SSL1	48	4.56e+00	1.55e+00	1.38e+00	1.96e-01	8.47e-02	4.53e-02	1.84e+00	3.48e-01	1.38e-01	4.77e-02	0.00e+00
N	SSL1	48	9.31e+00	4.25e+00	1.30e+00	4.56e-01	1.99e-01	7.31e-02	2.16e+00	7.63e-01	2.88e-01	7.57e-02	0.00e+00
N	SSL1	48	1.02e+01	NA	NA	4.83e-01	1.99e-01	6.23e-02	NA	9.87e-01	4.82e-01	2.69e-01	2.04e-01
N	SSL1	48	0.00e+00	0.00e+00	NA	0.00e+00	0.00e+00	0.00e+00	NA	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	SSL1	240	4.80e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	SSL1	240	4.85e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	SSL1	240	1.09e+01	0.00e+00	0.00e+00	NA	0.00e+00	0.00e+00	NA	NA	0.00e+00	0.00e+00	0.00e+00
N	SSL1	240	1.06e+01	0.00e+00	0.00e+00	NA	NA	0.00e+00	NA	NA	NA	0.00e+00	0.00e+00
N	SSL1	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	SSL1	720	4.32e+00	2.44e-01	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	SSL1	720	4.28e+00	2.55e-01	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	SSL1	720	8.58e+00	8.72e-01	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	SSL1	720	9.87e+00	NA	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	SSL1	720	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	SSL2	2	4.93e+00	3.80e+00	1.30e+00	5.62e-01	1.31e-01	6.84e-02	2.19e+00	8.28e-01	2.41e-01	9.88e-02	2.80e-02
N	SSL2	2	4.92e+00	3.74e+00	1.27e+00	5.75e-01	1.41e-01	8.02e-02	2.18e+00	9.04e-01	3.02e-01	1.48e-01	6.27e-02
N	SSL2	2	1.01e+01	7.80e+00	2.67e+00	1.09e+00	3.52e-01	1.38e-01	4.64e+00	1.79e+00	6.55e-01	2.73e-01	1.31e-01
N	SSL2	2	1.10e+01	8.51e+00	2.99e+00	1.23e+00	3.67e-01	NA	NA	NA	NA	NA	8.46e-02
N	SSL2	2	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	SSL2	48	4.77e+00	1.76e+00	6.00e-01	2.04e-01	7.97e-02	2.44e-02	9.73e-01	3.57e-01	1.40e-01	5.58e-02	3.03e-02
N	SSL2	48	4.76e+00	1.76e+00	5.98e-01	2.07e-01	9.01e-02	3.57e-02	1.01e+00	3.92e-01	1.79e-01	8.07e-02	4.42e-02
N	SSL2	48	9.70e+00	3.73e+00	1.27e+00	4.58e-01	1.86e-01	5.42e-02	2.11e+00	7.89e-01	3.17e-01	1.16e-01	6.03e-02
N	SSL2	48	1.06e+01	4.38e+00	1.23e+00	4.13e-01	1.68e-01	6.65e-02	2.03e+00	7.31e-01	3.04e-01	1.22e-01	5.41e-02
N	SSL2	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	SSL2	240	5.10e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	SSL2	240	5.01e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	SSL2	240	1.14e+01	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	SSL2	240	1.11e+01	0.00e+00	0.00e+00	0.00e+00	0.00e+00	NA	NA	NA	NA	NA	0.00e+00
N	SSL2	240	0.00e+00	NA	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	SSL2	720	4.50e+00	1.78e-01	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	SSL2	720	4.51e+00	3.52e-01	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	SSL2	720	8.93e+00	1.20e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	SSL2	720	1.02e+01	1.03e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	SSL2	720	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00

Table E.5 – continued from previous page

MC	S	t_{Ads}	C_{CTRL}	C_A	C_{D1}	C_{D2}	C_{D3}	C_{D4}	q_A	q_{D1}	q_{D2}	q_{D3}	q_{D4}
N	SSL3	2	4.88e+00	3.74e+00	1.28e+00	5.59e-01	1.44e-01	6.13e-02	2.26e+00	9.07e-01	3.07e-01	1.55e-01	9.09e-02
N	SSL3	2	4.84e+00	3.74e+00	1.27e+00	5.56e-01	1.45e-01	6.50e-02	2.25e+00	9.01e-01	3.06e-01	1.53e-01	8.60e-02
N	SSL3	2	9.93e+00	7.45e+00	2.47e+00	1.03e+00	3.27e-01	1.32e-01	4.36e+00	1.72e+00	6.00e-01	2.54e-01	1.17e-01
N	SSL3	2	1.09e+01	8.32e+00	2.95e+00	1.25e+00	3.89e-01	NA	NA	NA	NA	NA	2.12e-01
N	SSL3	2	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	SSL3	48	4.68e+00	1.60e+00	5.94e-01	2.44e-01	1.18e-01	5.49e-02	1.07e+00	4.38e-01	1.83e-01	5.64e-02	0.00e+00
N	SSL3	48	4.67e+00	1.46e+00	5.36e-01	1.97e-01	9.04e-02	4.95e-02	9.24e-01	3.54e-01	1.50e-01	5.14e-02	0.00e+00
N	SSL3	48	9.60e+00	3.18e+00	1.21e+00	4.16e-01	1.86e-01	6.02e-02	1.98e+00	6.97e-01	2.60e-01	6.19e-02	0.00e+00
N	SSL3	48	1.05e+01	5.23e+00	1.63e+00	NA	NA	7.60e-02	NA	NA	NA	7.81e-02	0.00e+00
N	SSL3	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	SSL3	240	4.99e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	SSL3	240	4.92e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	SSL3	240	1.12e+01	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	SSL3	240	1.08e+01	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	SSL3	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	SSL3	720	4.57e+00	2.40e-01	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	SSL3	720	4.57e+00	2.50e-01	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	SSL3	720	8.95e+00	8.20e-01	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	SSL3	720	1.08e+01	1.21e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	SSL3	720	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	ST	2	4.05e+00	3.50e+00	1.45e+00	5.33e-01	2.47e-01	1.95e-01	4.38e+00	1.92e+00	9.64e-01	5.26e-01	1.94e-01
N	ST	2	4.00e+00	3.53e+00	1.33e+00	5.27e-01	2.35e-01	1.42e-01	4.01e+00	1.75e+00	8.13e-01	4.04e-01	1.60e-01
N	ST	2	8.26e+00	7.40e+00	3.08e+00	1.14e+00	5.55e-01	3.46e-01	8.95e+00	3.74e+00	1.73e+00	7.85e-01	2.01e-01
N	ST	2	9.04e+00	8.32e+00	3.44e+00	1.36e+00	6.11e-01	3.27e-01	9.98e+00	4.02e+00	1.62e+00	5.60e-01	0.00e+00
N	ST	2	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	ST	48	3.88e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
N	ST	48	3.87e+00	3.42e+00	1.45e+00	7.82e-01	4.32e-01	2.64e-01	5.33e+00	2.88e+00	1.51e+00	7.54e-01	3.06e-01
N	ST	48	7.82e+00	6.94e+00	3.01e+00	1.40e+00	6.38e-01	5.26e-01	1.03e+01	5.30e+00	2.81e+00	1.67e+00	7.86e-01
N	ST	48	8.68e+00	7.66e+00	3.47e+00	1.53e+00	7.24e-01	5.59e-01	1.14e+01	5.55e+00	2.94e+00	1.66e+00	7.43e-01
N	ST	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	ST	240	4.22e+00	3.34e+00	1.46e+00	8.70e-01	4.26e-01	1.61e-01	4.89e+00	2.55e+00	1.04e+00	2.94e-01	0.00e+00
N	ST	240	4.18e+00	3.46e+00	1.44e+00	9.20e-01	4.07e-01	1.48e-01	5.07e+00	2.60e+00	1.01e+00	2.69e-01	0.00e+00
N	ST	240	1.00e+01	7.75e+00	3.34e+00	1.90e+00	8.89e-01	3.41e-01	1.12e+01	5.54e+00	2.16e+00	6.11e-01	0.00e+00
N	ST	240	9.18e+00	7.49e+00	2.82e+00	2.09e+00	1.03e+00	4.25e-01	1.10e+01	6.25e+00	2.58e+00	7.59e-01	0.00e+00
N	ST	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	ST	720	3.82e+00	3.16e+00	1.33e+00	6.95e-01	2.82e-01	1.10e-01	4.21e+00	1.97e+00	6.90e-01	1.94e-01	0.00e+00
N	ST	720	3.89e+00	3.20e+00	1.38e+00	7.01e-01	2.89e-01	1.15e-01	4.23e+00	1.99e+00	7.13e-01	2.04e-01	0.00e+00
N	ST	720	7.95e+00	6.22e+00	2.67e+00	1.32e+00	4.69e-01	2.33e-01	8.10e+00	3.62e+00	1.25e+00	4.02e-01	0.00e+00
N	ST	720	8.96e+00	7.21e+00	3.21e+00	1.65e+00	6.49e-01	3.19e-01	1.02e+01	4.82e+00	1.77e+00	5.75e-01	0.00e+00
N	ST	720	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00

Table E.5 – continued from previous page

MC	S	t_{Ads}	C_{CTRL}	C_A	C_{D1}	C_{D2}	C_{D3}	C_{D4}	q_A	q_{D1}	q_{D2}	q_{D3}	q_{D4}
N	W	2	4.88e+00	3.12e+00	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
N	W	2	4.21e+00	2.66e+00	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
N	W	2	9.39e+00	5.95e+00	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
N	W	2	1.14e+01	7.51e+00	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
N	W	2	0.00e+00	0.00e+00	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
N	W	48	4.28e+00	2.65e+00	8.98e-01	3.96e-01	3.43e-01	1.70e-01	2.15e+00	1.24e+00	8.22e-01	4.64e-01	2.76e-01
N	W	48	4.32e+00	2.64e+00	9.01e-01	6.98e-01	3.28e-01	1.79e-01	2.43e+00	1.50e+00	7.94e-01	4.49e-01	2.52e-01
N	W	48	8.53e+00	4.36e+00	2.09e+00	9.51e-01	4.93e-01	2.85e-01	5.77e+00	3.59e+00	2.64e+00	2.13e+00	1.82e+00
N	W	48	9.37e+00	5.49e+00	2.81e+00	1.44e+00	7.59e-01	3.60e-01	6.32e+00	3.37e+00	1.90e+00	1.11e+00	7.18e-01
N	W	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	W	240	4.24e+00	2.28e+00	1.11e+00	4.37e-01	4.32e-01	1.95e-01	3.08e+00	1.76e+00	1.17e+00	6.95e-01	4.94e-01
N	W	240	4.20e+00	2.26e+00	1.11e+00	4.18e-01	5.75e-01	2.05e-01	3.31e+00	1.99e+00	1.43e+00	8.01e-01	5.91e-01
N	W	240	8.01e+00	4.38e+00	2.17e+00	9.81e-01	6.89e-01	3.79e-01	5.87e+00	3.30e+00	2.03e+00	1.28e+00	8.75e-01
N	W	240	1.03e+01	5.27e+00	2.48e+00	1.23e+00	7.33e-01	3.43e-01	5.75e+00	2.80e+00	1.16e+00	3.63e-01	0.00e+00
N	W	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	W	720	4.81e+00	1.54e+00	8.65e-01	5.22e-01	2.84e-01	1.65e-01	2.57e+00	1.66e+00	1.08e+00	7.83e-01	6.02e-01
N	W	720	4.82e+00	1.52e+00	8.47e-01	4.97e-01	0.00e+00	0.00e+00	2.07e+00	1.19e+00	6.42e-01	6.42e-01	6.42e-01
N	W	720	1.01e+01	3.59e+00	1.95e+00	1.12e+00	6.23e-01	3.95e-01	5.10e+00	3.08e+00	1.87e+00	1.22e+00	7.80e-01
N	W	720	1.07e+01	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
N	W	720	0.00e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
N	W1	2	4.49e+00	4.16e+00	1.36e+00	4.52e-01	1.43e-01	7.46e-02	2.15e+00	7.29e-01	2.24e-01	7.80e-02	0.00e+00
N	W1	2	4.54e+00	4.19e+00	1.34e+00	4.36e-01	1.42e-01	8.70e-02	2.13e+00	7.18e-01	2.37e-01	9.15e-02	0.00e+00
N	W1	2	9.28e+00	8.48e+00	2.75e+00	8.91e-01	2.93e-01	1.05e-01	4.28e+00	1.40e+00	4.14e-01	1.11e-01	0.00e+00
N	W1	2	1.01e+01	9.24e+00	3.08e+00	1.02e+00	3.46e-01	1.19e-01	4.84e+00	1.61e+00	4.81e-01	1.25e-01	0.00e+00
N	W1	2	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	W1	48	4.35e+00	3.99e+00	1.31e+00	4.40e-01	1.55e-01	6.09e-02	2.12e+00	6.83e-01	2.38e-01	6.46e-02	0.00e+00
N	W1	48	4.38e+00	3.99e+00	1.35e+00	4.66e-01	1.62e-01	9.23e-02	2.23e+00	7.62e-01	2.82e-01	9.80e-02	0.00e+00
N	W1	48	8.84e+00	8.07e+00	2.69e+00	7.07e-01	3.05e-01	9.96e-02	4.10e+00	1.17e+00	4.47e-01	1.04e-01	0.00e+00
N	W1	48	9.80e+00	8.81e+00	2.98e+00	8.64e-01	3.46e-01	1.12e-01	4.63e+00	1.38e+00	5.06e-01	1.18e-01	0.00e+00
N	W1	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	W1	240	4.65e+00	3.86e+00	1.16e+00	3.94e-01	1.09e-01	0.00e+00	1.71e+00	5.69e-01	1.10e-01	0.00e+00	0.00e+00
N	W1	240	4.66e+00	3.92e+00	1.17e+00	4.04e-01	1.11e-01	0.00e+00	1.72e+00	5.82e-01	1.12e-01	0.00e+00	0.00e+00
N	W1	240	1.04e+01	9.11e+00	2.67e+00	9.44e-01	2.76e-01	1.06e-01	4.09e+00	1.50e+00	3.94e-01	1.12e-01	0.00e+00
N	W1	240	1.01e+01	8.80e+00	2.68e+00	9.42e-01	2.81e-01	1.11e-01	4.11e+00	1.51e+00	4.02e-01	1.17e-01	0.00e+00
N	W1	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	W1	720	4.37e+00	3.62e+00	1.13e+00	3.24e-01	1.32e-01	0.00e+00	1.79e+00	4.83e-01	1.40e-01	0.00e+00	0.00e+00
N	W1	720	4.33e+00	4.02e+00	1.37e+00	4.91e-01	0.00e+00	0.00e+00	2.04e+00	5.08e-01	0.00e+00	0.00e+00	0.00e+00
N	W1	720	8.48e+00	7.34e+00	2.29e+00	6.48e-01	2.37e-01	0.00e+00	3.57e+00	9.41e-01	2.51e-01	0.00e+00	0.00e+00
N	W1	720	1.01e+01	8.26e+00	2.76e+00	8.07e-01	2.71e-01	0.00e+00	4.30e+00	1.14e+00	2.85e-01	0.00e+00	0.00e+00
N	W1	720	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00

Table E.5 – continued from previous page

MC	S	t_{Ads}	C_{CTRL}	C_A	C_{D1}	C_{D2}	C_{D3}	C_{D4}	q_A	q_{D1}	q_{D2}	q_{D3}	q_{D4}
N	W2	2	4.60e+00	4.26e+00	1.43e+00	4.90e-01	1.69e-01	1.12e-01	2.34e+00	8.32e-01	2.91e-01	1.18e-01	0.00e+00
N	W2	2	4.60e+00	4.35e+00	1.46e+00	4.87e-01	1.69e-01	1.05e-01	2.37e+00	8.25e-01	2.85e-01	1.12e-01	0.00e+00
N	W2	2	9.47e+00	8.72e+00	2.82e+00	9.28e-01	3.16e-01	1.18e-01	4.47e+00	1.48e+00	4.51e-01	1.29e-01	0.00e+00
N	W2	2	1.02e+01	9.38e+00	3.14e+00	1.04e+00	3.42e-01	1.27e-01	4.92e+00	1.64e+00	4.87e-01	1.37e-01	0.00e+00
N	W2	2	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	W2	48	4.43e+00	4.04e+00	1.37e+00	5.01e-01	1.78e-01	6.76e-02	2.30e+00	7.81e-01	2.73e-01	7.14e-02	0.00e+00
N	W2	48	4.47e+00	4.04e+00	1.34e+00	4.63e-01	1.58e-01	8.34e-02	2.23e+00	7.24e-01	2.65e-01	8.67e-02	0.00e+00
N	W2	48	8.97e+00	8.10e+00	2.73e+00	9.26e-01	3.14e-01	9.95e-02	4.46e+00	1.40e+00	4.58e-01	1.04e-01	0.00e+00
N	W2	48	9.92e+00	8.90e+00	3.07e+00	1.03e+00	3.57e-01	1.22e-01	5.03e+00	1.57e+00	5.33e-01	1.28e-01	0.00e+00
N	W2	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	W2	240	4.65e+00	4.01e+00	1.25e+00	3.51e-01	9.45e-02	0.00e+00	1.73e+00	4.73e-01	9.41e-02	0.00e+00	0.00e+00
N	W2	240	4.73e+00	4.00e+00	1.22e+00	3.65e-01	1.02e-01	0.00e+00	1.75e+00	5.01e-01	1.01e-01	0.00e+00	0.00e+00
N	W2	240	1.01e+01	9.19e+00	2.82e+00	8.91e-01	2.60e-01	0.00e+00	4.12e+00	1.23e+00	2.61e-01	0.00e+00	0.00e+00
N	W2	240	1.03e+01	8.94e+00	2.81e+00	9.01e-01	2.65e-01	0.00e+00	4.12e+00	1.25e+00	2.63e-01	0.00e+00	0.00e+00
N	W2	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	W2	720	4.37e+00	3.82e+00	1.10e+00	3.48e-01	1.15e-01	0.00e+00	1.62e+00	4.71e-01	1.25e-01	0.00e+00	0.00e+00
N	W2	720	4.34e+00	3.75e+00	1.14e+00	3.59e-01	1.05e-01	0.00e+00	1.71e+00	4.76e-01	1.15e-01	0.00e+00	0.00e+00
N	W2	720	8.58e+00	7.33e+00	2.22e+00	7.11e-01	2.74e-01	0.00e+00	3.42e+00	1.02e+00	3.01e-01	0.00e+00	0.00e+00
N	W2	720	1.02e+01	8.62e+00	2.74e+00	9.04e-01	3.65e-01	0.00e+00	4.32e+00	1.32e+00	4.06e-01	0.00e+00	0.00e+00
N	W2	720	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	Z	2	4.94e+00	8.77e-01	NA	NA	2.28e-01	NA	NA	NA	NA	NA	0.00e+00
N	Z	2	5.00e+00	9.04e-01	4.46e-01	3.96e-01	NA	1.86e-01	NA	NA	NA	1.52e+00	1.25e+00
N	Z	2	1.13e+01	2.25e+00	1.12e+00	9.54e-01	6.03e-01	4.73e-01	9.14e+00	7.20e+00	5.55e+00	4.47e+00	3.67e+00
N	Z	2	1.10e+01	2.06e+00	1.11e+00	9.16e-01	4.05e-01	4.88e-01	1.02e+01	8.32e+00	6.78e+00	6.05e+00	5.21e+00
N	Z	2	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	Z	48	4.64e+00	3.51e-01	3.31e-01	2.61e-01	2.21e-01	2.33e-01	3.43e+00	2.86e+00	2.40e+00	2.01e+00	1.60e+00
N	Z	48	4.64e+00	4.43e-01	3.81e-01	3.08e-01	2.24e-01	2.12e-01	3.75e+01	3.68e+01	3.63e+01	3.59e+01	3.55e+01
N	Z	48	1.14e+01	1.08e+00	1.03e+00	8.49e-01	6.37e-01	5.98e-01	5.09e+01	4.92e+01	4.77e+01	4.65e+01	4.55e+01
N	Z	48	1.07e+01	1.10e+00	8.91e-01	7.01e-01	5.36e-01	3.64e-01	8.62e+00	7.06e+00	5.88e+00	4.94e+00	4.28e+00
N	Z	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	Z	240	4.59e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	6.30e-01	6.30e-01	6.30e-01	6.30e-01	6.30e-01
N	Z	240	4.59e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	4.29e-01	4.29e-01	4.29e-01	4.29e-01	4.29e-01
N	Z	240	1.13e+01	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
N	Z	240	1.05e+01	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	Z	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	Z	720	4.60e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	3.50e+01	3.50e+01	3.50e+01	3.50e+01	3.50e+01
N	Z	720	4.60e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	Z	720	1.13e+01	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	Z	720	1.03e+01	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
N	Z	720	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00

Table E.5 – continued from previous page

MC	S	t_{Ads}	C_{CTRL}	C_A	C_{D1}	C_{D2}	C_{D3}	C_{D4}	q_A	q_{D1}	q_{D2}	q_{D3}	q_{D4}
R	AM	2	4.53e+00	2.71e+00	1.39e+00	7.60e-01	4.34e-01	2.60e-01	3.54e+00	1.99e+00	1.19e+00	7.10e-01	4.37e-01
R	AM	2	4.58e+00	2.66e+00	1.38e+00	7.92e-01	4.59e-01	2.96e-01	3.69e+00	2.17e+00	1.35e+00	8.52e-01	5.42e-01
R	AM	2	1.19e+01	7.50e+00	3.73e+00	1.96e+00	1.08e+00	6.49e-01	8.84e+00	4.79e+00	2.74e+00	1.56e+00	8.92e-01
R	AM	2	1.11e+01	6.96e+00	3.45e+00	1.88e+00	NA	6.43e-01	NA	NA	NA	1.81e+00	1.15e+00
R	AM	2	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
R	AM	48	4.53e+00	2.58e+00	1.38e+00	7.96e-01	0.00e+00	2.86e-01	2.69e+00	1.22e+00	3.81e-01	3.81e-01	8.19e-02
R	AM	48	4.56e+00	2.54e+00	1.37e+00	8.25e-01	1.02e+00	2.91e-01	3.70e+00	2.25e+00	1.39e+00	3.02e-01	0.00e+00
R	AM	48	1.18e+01	6.68e+00	3.66e+00	2.00e+00	1.14e+00	7.26e-01	9.86e+00	5.95e+00	3.84e+00	2.65e+00	1.92e+00
R	AM	48	1.09e+01	6.24e+00	3.38e+00	1.85e+00	NA	6.42e-01	NA	NA	NA	1.73e+00	1.06e+00
R	AM	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	NA	0.00e+00	NA	NA	NA	0.00e+00	0.00e+00
R	AM	240	4.54e+00	9.03e-01	6.83e-01	8.02e-01	5.09e-01	3.16e-01	2.40e+00	1.70e+00	8.59e-01	3.31e-01	0.00e+00
R	AM	240	4.53e+00	8.19e-01	6.71e-01	7.53e-01	4.51e-01	2.86e-01	3.36e+00	2.66e+00	1.88e+00	1.42e+00	1.12e+00
R	AM	240	1.15e+01	7.34e+00	3.72e+00	1.93e+00	1.10e+00	6.55e-01	9.26e+00	5.42e+00	3.37e+00	2.26e+00	1.56e+00
R	AM	240	1.09e+01	1.31e+00	3.41e+00	NA	1.77e-01	1.31e-01	NA	NA	6.79e-01	4.97e-01	3.61e-01
R	AM	240	0.00e+00	NA	0.00e+00	0.00e+00	NA	NA	NA	NA	NA	NA	0.00e+00
R	AM	720	4.49e+00	2.48e+00	1.25e+00	6.90e-01	4.00e-01	3.05e-01	2.85e+00	1.48e+00	7.67e-01	3.27e-01	0.00e+00
R	AM	720	4.48e+00	2.37e+00	0.00e+00	6.82e-01	4.02e-01	2.59e-01	1.61e+00	1.61e+00	9.00e-01	4.56e-01	1.79e-01
R	AM	720	1.17e+01	6.90e+00	0.00e+00	2.19e+00	1.28e+00	7.54e-01	6.25e+00	6.25e+00	4.01e+00	2.61e+00	1.81e+00
R	AM	720	1.09e+01	6.39e+00	0.00e+00	0.00e+00	0.00e+00	7.07e-01	7.54e-01	7.54e-01	7.54e-01	7.54e-01	0.00e+00
R	AM	720	0.00e+00	0.00e+00	0.00e+00	NA	NA	0.00e+00	NA	NA	NA	0.00e+00	0.00e+00
R	B	2	4.87e+00	4.71e+00	1.37e+00	NA	NA	NA	NA	NA	NA	NA	0.00e+00
R	B	2	5.05e+00	4.72e+00	1.40e+00	NA	NA	NA	NA	NA	NA	NA	0.00e+00
R	B	2	1.30e+01	1.14e+01	3.60e+00	NA	NA	NA	NA	NA	NA	NA	0.00e+00
R	B	2	1.18e+01	1.02e+01	2.96e+00	NA	NA	NA	NA	NA	NA	NA	0.00e+00
R	B	2	0.00e+00	0.00e+00	0.00e+00	NA	NA	NA	NA	NA	NA	NA	0.00e+00
R	B	48	4.98e+00	6.10e+00	1.42e+00	4.45e-01	1.50e-01	6.15e-02	2.15e+00	6.87e-01	2.19e-01	6.47e-02	0.00e+00
R	B	48	4.98e+00	5.57e+00	1.39e+00	4.31e-01	1.39e-01	5.76e-02	2.10e+00	6.57e-01	2.03e-01	6.07e-02	0.00e+00
R	B	48	1.31e+01	1.16e+01	3.65e+00	1.16e+00	3.74e-01	1.71e-01	5.88e+00	2.04e+00	8.10e-01	4.34e-01	2.51e-01
R	B	48	1.19e+01	1.05e+01	3.35e+00	1.05e+00	3.76e-01	1.64e-01	5.06e+00	1.65e+00	5.53e-01	1.75e-01	0.00e+00
R	B	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
R	B	240	5.01e+00	5.07e+00	1.41e+00	4.67e-01	1.73e-01	5.29e-02	2.52e+00	8.23e-01	2.40e-01	5.52e-02	0.00e+00
R	B	240	4.98e+00	4.50e+00	1.29e+00	3.86e-01	1.25e-01	4.66e-02	2.18e+00	6.68e-01	1.82e-01	4.95e-02	0.00e+00
R	B	240	1.31e+01	1.17e+01	3.32e+00	1.01e+00	3.58e-01	1.15e-01	5.81e+00	1.88e+00	6.07e-01	2.22e-01	9.99e-02
R	B	240	1.21e+01	9.98e+00	3.04e+00	8.60e-01	0.00e+00	9.05e-02	4.70e+00	1.10e+00	9.70e-02	9.70e-02	0.00e+00
R	B	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	NA	0.00e+00	NA	NA	NA	0.00e+00	0.00e+00
R	B	720	5.02e+00	5.43e+00	1.96e+00	6.70e-01	2.19e-01	7.31e-02	3.08e+00	1.03e+00	3.06e-01	8.20e-02	0.00e+00
R	B	720	5.04e+00	4.47e+00	1.57e+00	5.05e-01	1.45e-01	4.80e-02	2.34e+00	7.52e-01	2.02e-01	5.22e-02	0.00e+00
R	B	720	1.32e+01	1.23e+01	3.90e+00	1.27e+00	4.05e-01	1.19e-01	5.98e+00	1.92e+00	5.57e-01	1.30e-01	0.00e+00
R	B	720	1.22e+01	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
R	B	720	0.00e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00

Table E.5 – continued from previous page

MC	S	t_{Ads}	C_{CTRL}	C_A	C_{D1}	C_{D2}	C_{D3}	C_{D4}	q_A	q_{D1}	q_{D2}	q_{D3}	q_{D4}
R	BA	2	4.98e+00	4.33e+00	1.38e+00	4.51e-01	1.47e-01	4.97e-02	2.11e+00	6.89e-01	2.04e-01	4.98e-02	0.00e+00
R	BA	2	5.01e+00	4.35e+00	1.38e+00	4.46e-01	1.47e-01	4.97e-02	2.09e+00	6.82e-01	2.03e-01	4.81e-02	0.00e+00
R	BA	2	1.31e+01	1.12e+01	3.58e+00	1.18e+00	4.03e-01	1.45e-01	5.57e+00	1.90e+00	6.34e-01	2.07e-01	5.98e-02
R	BA	2	1.21e+01	1.05e+01	3.31e+00	1.10e+00	3.62e-01	1.20e-01	5.15e+00	1.75e+00	5.71e-01	1.84e-01	6.18e-02
R	BA	2	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
R	BA	48	5.02e+00	4.25e+00	1.40e+00	4.67e-01	1.56e-01	5.11e-02	2.14e+00	7.07e-01	2.18e-01	5.36e-02	0.00e+00
R	BA	48	5.02e+00	4.14e+00	1.41e+00	4.79e-01	1.55e-01	5.02e-02	2.18e+00	7.20e-01	2.16e-01	5.25e-02	0.00e+00
R	BA	48	1.33e+01	1.10e+01	3.67e+00	1.22e+00	3.99e-01	1.32e-01	5.64e+00	1.86e+00	5.61e-01	1.40e-01	0.00e+00
R	BA	48	1.21e+01	1.05e+01	3.42e+00	1.14e+00	4.03e-01	1.28e-01	5.28e+00	1.76e+00	5.57e-01	1.31e-01	0.00e+00
R	BA	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
R	BA	240	5.04e+00	4.46e+00	1.46e+00	NA	1.66e-01	7.75e-02	NA	NA	2.52e-01	8.34e-02	0.00e+00
R	BA	240	5.06e+00	4.50e+00	1.49e+00	5.07e-01	1.69e-01	7.58e-02	2.32e+00	7.95e-01	2.54e-01	8.11e-02	0.00e+00
R	BA	240	1.32e+01	1.16e+01	3.87e+00	1.33e+00	4.64e-01	2.08e-01	6.14e+00	2.12e+00	7.02e-01	2.22e-01	0.00e+00
R	BA	240	1.21e+01	1.07e+01	3.60e+00	1.22e+00	6.76e-01	5.29e-01	6.26e+00	2.54e+00	1.25e+00	5.70e-01	0.00e+00
R	BA	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
R	BA	720	5.00e+00	4.38e+00	1.43e+00	4.91e-01	1.63e-01	2.34e-01	2.46e+00	9.46e-01	4.24e-01	2.47e-01	0.00e+00
R	BA	720	4.99e+00	4.50e+00	1.46e+00	4.94e-01	1.68e-01	2.11e-01	2.46e+00	9.35e-01	4.06e-01	2.23e-01	0.00e+00
R	BA	720	1.30e+01	1.16e+01	3.81e+00	1.38e+00	4.54e-01	2.33e-01	6.20e+00	2.11e+00	7.35e-01	2.48e-01	0.00e+00
R	BA	720	1.22e+01	1.15e+01	3.71e+00	1.20e+00	4.11e-01	1.34e-01	5.88e+00	1.85e+00	5.88e-01	1.43e-01	0.00e+00
R	BA	720	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
R	BOX	2	4.45e+00	3.29e+00	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
R	BOX	2	4.55e+00	3.03e+00	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
R	BOX	2	1.18e+01	7.54e+00	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
R	BOX	2	1.07e+01	6.52e+00	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
R	BOX	2	0.00e+00	0.00e+00	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
R	BOX	48	4.51e+00	NA	1.88e+00	1.06e+00	4.20e-01	4.13e-01	4.01e+00	2.01e+00	8.86e-01	4.36e-01	0.00e+00
R	BOX	48	4.53e+00	3.83e+00	1.26e+00	6.98e-01	4.07e-01	3.94e-01	3.89e+00	2.55e+00	1.81e+00	1.37e+00	9.55e-01
R	BOX	48	1.18e+01	6.75e+00	4.09e+00	2.26e+00	1.31e+00	0.00e+00	7.99e+00	3.78e+00	1.40e+00	0.00e+00	0.00e+00
R	BOX	48	1.07e+01	9.39e+00	4.09e+00	2.07e+00	5.52e-01	2.46e-01	3.26e+01	2.83e+01	2.62e+01	2.56e+01	2.53e+01
R	BOX	48	0.00e+00	NA	0.00e+00	0.00e+00	0.00e+00	NA	NA	NA	NA	NA	0.00e+00
R	BOX	240	4.54e+00	3.85e+00	1.99e+00	1.54e+00	5.70e-01	3.52e-01	5.50e+00	3.03e+00	9.70e-01	3.77e-01	0.00e+00
R	BOX	240	4.53e+00	2.63e+00	1.29e+00	0.00e+00	5.47e-01	3.25e-01	2.96e+00	1.36e+00	1.36e+00	7.91e-01	4.42e-01
R	BOX	240	1.18e+01	6.50e+00	3.14e+00	1.56e+00	1.04e+00	6.34e-01	8.75e+00	4.88e+00	2.78e+00	1.69e+00	1.01e+00
R	BOX	240	1.09e+01	7.67e+00	3.68e+00	NA	1.02e+00	5.85e-01	NA	NA	2.54e+00	1.47e+00	8.41e-01
R	BOX	240	0.00e+00	0.00e+00	0.00e+00	NA	0.00e+00	0.00e+00	NA	NA	0.00e+00	0.00e+00	0.00e+00
R	BOX	720	4.52e+00	3.62e+00	2.01e+00	7.63e-01	6.36e-01	3.41e-01	4.44e+00	2.34e+00	1.51e+00	8.59e-01	4.89e-01
R	BOX	720	4.50e+00	4.19e+00	2.19e+00	8.63e-01	6.35e-01	3.53e-01	4.81e+00	2.53e+00	1.59e+00	9.38e-01	5.53e-01
R	BOX	720	1.18e+01	7.72e+00	4.13e+00	2.29e+00	1.29e+00	6.99e-01	1.01e+01	5.84e+00	3.35e+00	2.02e+00	1.25e+00
R	BOX	720	1.09e+01	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
R	BOX	720	0.00e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00

Table E.5 – continued from previous page

MC	S	t_{Ads}	C_{CTRL}	C_A	C_{D1}	C_{D2}	C_{D3}	C_{D4}	q_A	q_{D1}	q_{D2}	q_{D3}	q_{D4}
R	BT	2	5.01e+00	4.46e+00	1.31e+00	3.83e-01	1.16e-01	3.64e-02	1.96e+00	5.68e-01	1.61e-01	3.77e-02	0.00e+00
R	BT	2	5.00e+00	4.48e+00	1.33e+00	3.96e-01	1.22e-01	3.85e-02	1.99e+00	5.90e-01	1.70e-01	3.99e-02	0.00e+00
R	BT	2	1.32e+01	1.15e+01	3.37e+00	1.03e+00	3.20e-01	9.97e-02	5.02e+00	1.52e+00	4.42e-01	1.03e-01	0.00e+00
R	BT	2	1.22e+01	1.07e+01	3.30e+00	9.96e-01	3.12e-01	9.67e-02	4.91e+00	1.48e+00	4.33e-01	1.02e-01	0.00e+00
R	BT	2	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
R	BT	48	5.00e+00	4.33e+00	1.26e+00	3.84e-01	1.26e-01	3.43e-02	1.85e+00	5.66e-01	1.68e-01	3.66e-02	0.00e+00
R	BT	48	5.00e+00	4.58e+00	1.15e+00	3.36e-01	9.81e-02	3.02e-02	1.63e+00	4.82e-01	1.33e-01	3.11e-02	0.00e+00
R	BT	48	1.31e+01	1.16e+01	3.31e+00	1.03e+00	3.14e-01	9.58e-02	4.83e+00	1.51e+00	4.28e-01	9.96e-02	0.00e+00
R	BT	48	1.21e+01	1.06e+01	3.00e+00	9.15e-01	3.01e-01	9.00e-02	4.34e+00	1.34e+00	4.07e-01	9.31e-02	0.00e+00
R	BT	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	NA	NA	NA	NA	NA	0.00e+00
R	BT	240	5.03e+00	4.44e+00	1.23e+00	3.49e-01	1.03e-01	3.50e-02	1.78e+00	5.16e-01	1.44e-01	3.61e-02	0.00e+00
R	BT	240	5.05e+00	4.53e+00	1.25e+00	3.53e-01	1.04e-01	4.02e-02	1.81e+00	5.18e-01	1.45e-01	4.22e-02	0.00e+00
R	BT	240	1.31e+01	1.16e+01	3.16e+00	9.00e-01	2.54e-01	7.79e-02	4.52e+00	1.29e+00	3.37e-01	8.29e-02	0.00e+00
R	BT	240	1.21e+01	1.09e+01	3.02e+00	8.56e-01	2.28e-01	1.17e-01	4.42e+00	1.28e+00	3.49e-01	1.23e-01	0.00e+00
R	BT	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
R	BT	720	5.00e+00	4.38e+00	0.00e+00	3.32e-01	1.02e-01	1.23e-01	5.66e-01	5.66e-01	2.41e-01	1.27e-01	0.00e+00
R	BT	720	4.98e+00	4.50e+00	0.00e+00	3.62e-01	1.07e-01	NA	NA	NA	NA	NA	0.00e+00
R	BT	720	1.32e+01	1.15e+01	0.00e+00	1.02e+00	3.28e-01	2.08e-01	1.62e+00	1.62e+00	5.69e-01	2.12e-01	0.00e+00
R	BT	720	1.21e+01	1.31e+01	0.00e+00	1.36e+00	4.46e-01	1.98e-01	2.02e+00	2.02e+00	6.92e-01	2.07e-01	0.00e+00
R	BT	720	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
R	BU	2	4.70e+00	2.00e+00	9.57e-01	NA	NA	NA	NA	NA	NA	NA	0.00e+00
R	BU	2	4.80e+00	1.87e+00	8.92e-01	NA	NA	NA	NA	NA	NA	NA	0.00e+00
R	BU	2	1.24e+01	5.44e+00	2.56e+00	NA	NA	NA	NA	NA	NA	NA	0.00e+00
R	BU	2	1.14e+01	4.71e+00	2.30e+00	NA	NA	NA	NA	NA	NA	NA	0.00e+00
R	BU	2	0.00e+00	0.00e+00	0.00e+00	NA	NA	NA	NA	NA	NA	NA	0.00e+00
R	BU	48	4.71e+00	1.47e+00	7.94e-01	5.87e-01	4.66e-01	4.05e-01	4.68e+00	3.79e+00	3.18e+00	2.69e+00	2.25e+00
R	BU	48	4.73e+00	1.27e+00	7.31e-01	5.68e-01	4.50e-01	3.94e-01	5.69e+00	4.88e+00	4.30e+00	3.82e+00	3.40e+00
R	BU	48	1.25e+01	3.79e+00	2.27e+00	1.60e+00	1.27e+00	1.04e+00	1.29e+01	1.04e+01	8.75e+00	7.43e+00	6.30e+00
R	BU	48	1.14e+01	3.30e+00	1.96e+00	1.39e+00	1.11e+00	9.13e-01	1.07e+01	8.53e+00	7.09e+00	5.93e+00	4.95e+00
R	BU	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
R	BU	240	4.77e+00	1.00e+00	6.99e-01	4.99e-01	3.93e-01	2.89e-01	4.49e+00	3.62e+00	2.97e+00	2.56e+00	2.25e+00
R	BU	240	4.77e+00	1.10e+00	7.36e-01	5.31e-01	4.19e-01	3.23e-01	4.58e+00	3.79e+00	3.09e+00	2.65e+00	2.31e+00
R	BU	240	1.25e+01	3.22e+00	2.11e+00	1.55e+00	1.15e+00	8.51e-01	1.20e+01	9.38e+00	7.80e+00	6.60e+00	5.70e+00
R	BU	240	1.14e+01	2.95e+00	1.94e+00	1.42e+00	1.05e+00	7.52e-01	1.03e+01	7.94e+00	6.50e+00	5.40e+00	4.60e+00
R	BU	240	0.00e+00	0.00e+00	NA	0.00e+00	0.00e+00	0.00e+00	NA	0.00e+00	0.00e+00	0.00e+00	0.00e+00
R	BU	720	4.73e+00	7.68e-01	6.68e-01	NA	3.89e-01	2.95e-01	NA	NA	3.23e+00	2.82e+00	2.50e+00
R	BU	720	4.73e+00	7.64e-01	6.94e-01	NA	4.07e-01	3.17e-01	NA	NA	3.14e+00	2.72e+00	2.37e+00
R	BU	720	1.24e+01	2.49e+00	1.64e+00	NA	1.08e+00	7.70e-01	NA	NA	8.13e+00	7.00e+00	6.16e+00
R	BU	720	1.14e+01	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
R	BU	720	0.00e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00

Table E.5 – continued from previous page

MC	S	t_{Ads}	C_{CTRL}	C_A	C_{D1}	C_{D2}	C_{D3}	C_{D4}	q_A	q_{D1}	q_{D2}	q_{D3}	q_{D4}
R	CM	2	4.33e+00	3.06e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA
R	CM	2	4.38e+00	2.86e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA
R	CM	2	1.14e+01	7.85e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA
R	CM	2	1.04e+01	7.07e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA
R	CM	2	0.00e+00	0.00e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA
R	CM	48	4.37e+00	2.94e+00	1.46e+00	7.76e-01	4.32e-01	2.63e-01	NA	NA	NA	NA	NA
R	CM	48	4.38e+00	2.85e+00	1.47e+00	7.76e-01	4.32e-01	2.50e-01	NA	NA	NA	NA	NA
R	CM	48	1.16e+01	7.50e+00	3.87e+00	2.01e+00	1.12e+00	6.64e-01	NA	NA	NA	NA	NA
R	CM	48	1.05e+01	6.73e+00	3.52e+00	1.84e+00	9.84e-01	5.82e-01	NA	NA	NA	NA	NA
R	CM	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	NA	NA	NA	NA	NA
R	CM	240	4.43e+00	3.01e+00	1.34e+00	7.26e-01	4.05e-01	2.38e-01	NA	NA	NA	NA	NA
R	CM	240	4.44e+00	2.89e+00	1.33e+00	7.31e-01	3.93e-01	2.29e-01	NA	NA	NA	NA	NA
R	CM	240	1.17e+01	7.74e+00	3.56e+00	1.92e+00	1.01e+00	5.66e-01	NA	NA	NA	NA	NA
R	CM	240	1.07e+01	6.94e+00	3.32e+00	1.79e+00	9.54e-01	5.14e-01	NA	NA	NA	NA	NA
R	CM	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	NA	NA	NA	NA	NA
R	CM	720	4.37e+00	2.71e+00	1.46e+00	6.20e-01	4.14e-01	2.31e-01	NA	NA	NA	NA	NA
R	CM	720	4.37e+00	2.78e+00	1.48e+00	8.40e-01	4.45e-01	2.32e-01	NA	NA	NA	NA	NA
R	CM	720	1.14e+01	7.19e+00	3.82e+00	1.96e+00	1.10e+00	6.19e-01	NA	NA	NA	NA	NA
R	CM	720	9.71e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
R	CM	720	0.00e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
R	ELL	2	4.57e+00	2.78e+00	1.38e+00	7.90e-01	4.36e-01	2.78e-01	3.61e+00	2.12e+00	1.30e+00	8.21e-01	5.31e-01
R	ELL	2	4.58e+00	2.61e+00	1.41e+00	7.93e-01	4.50e-01	2.86e-01	3.56e+00	2.04e+00	1.24e+00	7.38e-01	4.43e-01
R	ELL	2	1.20e+01	7.27e+00	3.72e+00	2.01e+00	1.16e+00	7.06e-01	9.38e+00	5.34e+00	3.27e+00	2.00e+00	1.26e+00
R	ELL	2	1.11e+01	6.66e+00	3.45e+00	1.90e+00	1.07e+00	6.65e-01	8.73e+00	5.01e+00	3.05e+00	1.86e+00	1.17e+00
R	ELL	2	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
R	ELL	48	4.55e+00	2.29e+00	1.29e+00	7.78e-01	4.83e-01	2.96e-01	3.59e+00	2.25e+00	1.46e+00	9.16e-01	6.06e-01
R	ELL	48	4.58e+00	2.37e+00	1.34e+00	7.84e-01	4.92e-01	3.00e-01	3.64e+00	2.22e+00	1.42e+00	8.69e-01	5.58e-01
R	ELL	48	1.19e+01	6.26e+00	3.58e+00	1.91e+00	1.25e+00	7.69e-01	9.38e+00	5.63e+00	3.68e+00	2.27e+00	1.47e+00
R	ELL	48	1.10e+01	5.83e+00	3.30e+00	1.87e+00	1.16e+00	6.99e-01	8.81e+00	5.32e+00	3.41e+00	2.10e+00	1.37e+00
R	ELL	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
R	ELL	240	4.68e+00	3.03e-01	5.53e-01	9.61e-01	5.70e-01	3.38e-01	4.50e+00	3.94e+00	2.90e+00	2.30e+00	1.94e+00
R	ELL	240	4.62e+00	4.50e+00	4.72e-01	1.11e+00	6.35e-01	3.82e-01	3.72e+00	3.23e+00	2.05e+00	1.39e+00	9.88e-01
R	ELL	240	1.20e+01	7.56e+00	4.26e+00	2.34e+00	1.35e+00	8.71e-01	1.42e+01	9.75e+00	7.23e+00	5.80e+00	4.88e+00
R	ELL	240	1.12e+01	1.90e+00	6.61e-01	2.56e-01	1.20e-01	8.25e-02	2.57e+00	1.88e+00	1.61e+00	1.48e+00	1.40e+00
R	ELL	240	0.00e+00	NA	NA	0.00e+00	NA	NA	NA	NA	NA	NA	0.00e+00
R	ELL	720	4.64e+00	3.47e+00	1.84e+00	1.06e+00	5.82e-01	0.00e+00	3.70e+00	1.78e+00	6.13e-01	0.00e+00	0.00e+00
R	ELL	720	4.57e+00	3.26e+00	1.74e+00	1.02e+00	5.61e-01	0.00e+00	3.73e+00	1.93e+00	8.02e-01	2.11e-01	2.11e-01
R	ELL	720	1.19e+01	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
R	ELL	720	1.11e+01	9.84e-01	3.98e+00	2.42e+00	8.65e-02	0.00e+00	9.17e+00	5.00e+00	2.36e+00	2.27e+00	2.27e+00
R	ELL	720	0.00e+00	NA	NA	NA	NA	0.00e+00	NA	NA	NA	0.00e+00	0.00e+00

Table E.5 – continued from previous page

MC	S	t_{Ads}	C_{CTRL}	C_A	C_{D1}	C_{D2}	C_{D3}	C_{D4}	q_A	q_{D1}	q_{D2}	q_{D3}	q_{D4}
R	FT	2	4.59e+00	3.78e+00	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
R	FT	2	4.50e+00	3.89e+00	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
R	FT	2	1.20e+01	9.69e+00	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
R	FT	2	1.11e+01	8.99e+00	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
R	FT	2	0.00e+00	0.00e+00	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
R	FT	48	4.58e+00	3.75e+00	1.62e+00	6.89e-01	3.11e-01	1.43e-01	2.96e+00	1.25e+00	5.23e-01	2.03e-01	4.95e-02
R	FT	48	4.56e+00	3.69e+00	1.60e+00	6.96e-01	3.00e-01	1.42e-01	2.93e+00	1.27e+00	5.25e-01	2.14e-01	5.68e-02
R	FT	48	1.20e+01	9.83e+00	4.28e+00	1.78e+00	7.82e-01	0.00e+00	7.52e+00	3.08e+00	1.18e+00	3.83e-01	3.83e-01
R	FT	48	1.09e+01	8.99e+00	3.77e+00	1.62e+00	6.87e-01	3.00e-01	6.67e+00	2.85e+00	1.13e+00	4.19e-01	8.55e-02
R	FT	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
R	FT	240	4.55e+00	3.97e+00	1.49e+00	5.28e-01	2.41e-01	1.07e-01	3.02e+00	1.21e+00	4.88e-01	2.33e-01	1.19e-01
R	FT	240	4.56e+00	3.85e+00	1.49e+00	5.47e-01	2.53e-01	1.04e-01	3.02e+00	1.22e+00	4.81e-01	2.10e-01	1.01e-01
R	FT	240	1.20e+01	1.00e+01	3.91e+00	1.51e+00	6.67e-01	2.89e-01	7.99e+00	3.35e+00	1.29e+00	5.78e-01	2.75e-01
R	FT	240	1.10e+01	9.23e+00	3.46e+00	1.34e+00	5.91e-01	2.50e-01	6.98e+00	2.84e+00	1.05e+00	4.24e-01	1.50e-01
R	FT	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
R	FT	720	4.62e+00	3.91e+00	1.65e+00	7.21e-01	2.89e-01	1.07e-01	2.93e+00	1.21e+00	4.29e-01	1.14e-01	0.00e+00
R	FT	720	4.64e+00	4.42e+00	1.83e+00	6.62e-01	3.03e-01	1.18e-01	3.06e+00	1.17e+00	4.54e-01	1.24e-01	0.00e+00
R	FT	720	1.20e+01	1.13e+01	4.49e+00	1.65e+00	7.91e-01	3.14e-01	7.83e+00	3.14e+00	1.35e+00	4.90e-01	1.58e-01
R	FT	720	1.12e+01	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
R	FT	720	0.00e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
R	GAS	2	4.50e+00	6.19e-01	1.43e-01	NA	NA	NA	NA	NA	NA	NA	0.00e+00
R	GAS	2	4.47e+00	5.63e-01	1.40e-01	NA	NA	NA	NA	NA	NA	NA	0.00e+00
R	GAS	2	1.19e+01	1.18e+00	4.99e-01	NA	NA	NA	NA	NA	NA	NA	0.00e+00
R	GAS	2	1.09e+01	1.28e+00	4.19e-01	NA	NA	NA	NA	NA	NA	NA	0.00e+00
R	GAS	2	0.00e+00	0.00e+00	0.00e+00	NA	NA	NA	NA	NA	NA	NA	0.00e+00
R	GAS	48	4.54e+00	3.41e-01	1.14e-01	1.32e-01	1.30e-01	1.24e-01	3.27e+00	3.15e+00	3.02e+00	2.88e+00	2.75e+00
R	GAS	48	4.52e+00	2.66e-01	1.26e-01	1.33e-01	1.38e-01	1.19e-01	3.98e+00	3.85e+00	3.72e+00	3.57e+00	3.44e+00
R	GAS	48	1.19e+01	9.55e-01	4.30e-01	3.93e-01	3.77e-01	3.53e-01	1.40e+01	1.36e+01	1.32e+01	1.28e+01	1.24e+01
R	GAS	48	1.08e+01	1.86e-01	0.00e+00	6.87e-02	7.39e-02	6.28e-02	7.56e+00	7.56e+00	7.49e+00	7.41e+00	7.35e+00
R	GAS	48	0.00e+00	0.00e+00	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
R	GAS	240	4.47e+00	2.06e-01	1.95e-01	1.64e-01	1.54e-01	1.63e-01	2.69e+00	2.47e+00	2.26e+00	2.10e+00	1.93e+00
R	GAS	240	4.50e+00	7.74e-02	8.40e-02	6.73e-02	6.07e-02	9.17e-02	2.26e+00	2.18e+00	2.09e+00	2.03e+00	1.93e+00
R	GAS	240	1.17e+01	6.06e-01	5.25e-01	4.88e-01	4.25e-01	4.28e-01	1.10e+01	1.05e+01	9.84e+00	9.40e+00	8.95e+00
R	GAS	240	1.09e+01	2.55e-01	2.29e-01	3.31e-01	2.98e-01	2.92e-01	1.04e+01	1.02e+01	9.75e+00	9.44e+00	9.13e+00
R	GAS	240	0.00e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
R	GAS	720	4.54e+00	0.00e+00	0.00e+00	8.00e-01	0.00e+00	1.27e-01	3.81e+00	3.81e+00	2.94e+00	2.94e+00	2.80e+00
R	GAS	720	4.55e+00	0.00e+00	0.00e+00	8.49e-01	0.00e+00	1.53e-01	3.65e+00	3.65e+00	2.72e+00	2.72e+00	2.55e+00
R	GAS	720	1.19e+01	1.48e-01	2.07e-01	2.11e+00	2.91e-01	2.87e-01	1.23e+01	1.21e+01	9.75e+00	9.45e+00	9.13e+00
R	GAS	720	1.10e+01	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
R	GAS	720	0.00e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00

Table E.5 – continued from previous page

MC	S	t_{Ads}	C_{CTRL}	C_A	C_{D1}	C_{D2}	C_{D3}	C_{D4}	q_A	q_{D1}	q_{D2}	q_{D3}	q_{D4}
R	GUA	2	4.73e+00	3.50e+00	1.44e+00	6.03e-01	2.69e-01	1.24e-01	2.62e+00	1.12e+00	5.01e-01	2.13e-01	8.85e-02
R	GUA	2	4.74e+00	3.55e+00	1.38e+00	6.10e-01	2.71e-01	1.27e-01	2.56e+00	1.11e+00	4.97e-01	2.06e-01	8.98e-02
R	GUA	2	1.23e+01	9.11e+00	3.73e+00	1.58e+00	7.01e-01	3.17e-01	6.84e+00	2.88e+00	1.27e+00	5.42e-01	2.39e-01
R	GUA	2	1.13e+01	8.30e+00	3.44e+00	1.47e+00	6.58e-01	3.03e-01	6.30e+00	2.64e+00	1.15e+00	4.47e-01	1.87e-01
R	GUA	2	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
R	GUA	48	4.24e+00	2.92e+00	1.38e+00	6.22e-01	2.71e-01	1.26e-01	2.56e+00	1.22e+00	5.62e-01	2.73e-01	1.40e-01
R	GUA	48	4.25e+00	3.24e+00	1.42e+00	NA	2.44e-01	1.16e-01	NA	NA	4.74e-01	2.18e-01	9.44e-02
R	GUA	48	1.21e+01	8.49e+00	3.73e+00	1.62e+00	7.28e-01	3.34e-01	7.03e+00	3.12e+00	1.41e+00	6.29e-01	2.79e-01
R	GUA	48	1.14e+01	8.77e+00	3.66e+00	1.56e+00	6.93e-01	3.28e-01	6.98e+00	2.96e+00	1.34e+00	6.02e-01	2.59e-01
R	GUA	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
R	GUA	240	4.20e+00	3.01e+00	1.36e+00	5.96e-01	2.79e-01	1.23e-01	2.52e+00	1.12e+00	4.99e-01	2.01e-01	6.88e-02
R	GUA	240	4.24e+00	3.12e+00	1.53e+00	6.10e-01	2.83e-01	1.19e-01	2.70e+00	1.13e+00	4.92e-01	1.91e-01	6.39e-02
R	GUA	240	1.20e+01	8.92e+00	3.96e+00	1.68e+00	7.85e-01	3.58e-01	7.38e+00	3.28e+00	1.54e+00	7.12e-01	3.25e-01
R	GUA	240	1.13e+01	8.37e+00	3.71e+00	1.66e+00	7.38e-01	0.00e+00	6.45e+00	2.64e+00	8.79e-01	1.01e-01	1.01e-01
R	GUA	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	NA	NA	NA	NA	NA	0.00e+00
R	GUA	720	4.24e+00	1.96e+00	8.30e-01	3.40e-01	1.53e-01	4.92e-02	1.50e+00	6.30e-01	2.77e-01	1.16e-01	6.43e-02
R	GUA	720	4.24e+00	1.75e+00	7.64e-01	3.01e-01	1.43e-01	4.46e-02	1.39e+00	5.86e-01	2.73e-01	1.23e-01	7.52e-02
R	GUA	720	1.21e+01	7.78e+00	3.39e+00	1.45e+00	6.59e-01	2.01e-01	6.25e+00	2.71e+00	1.20e+00	5.17e-01	3.03e-01
R	GUA	720	1.13e+01	6.86e+00	2.99e+00	1.32e+00	5.67e-01	1.87e-01	5.58e+00	2.59e+00	1.15e+00	5.54e-01	3.58e-01
R	GUA	720	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
R	H	2	5.15e+00	3.20e+00	1.40e+00	6.38e-01	3.67e-01	1.65e-01	2.94e+00	1.46e+00	8.05e-01	4.17e-01	2.42e-01
R	H	2	5.10e+00	3.23e+00	1.38e+00	6.39e-01	3.61e-01	1.69e-01	2.89e+00	1.43e+00	7.65e-01	3.86e-01	2.09e-01
R	H	2	1.35e+01	8.35e+00	3.59e+00	1.60e+00	8.82e-01	4.32e-01	7.58e+00	3.71e+00	2.02e+00	1.08e+00	6.35e-01
R	H	2	1.24e+01	1.07e+00	3.16e+00	1.58e+00	9.53e-01	4.89e-01	7.26e+00	3.95e+00	2.29e+00	1.28e+00	7.69e-01
R	H	2	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
R	H	48	4.57e+00	2.58e+00	1.25e+00	6.62e-01	2.64e-01	1.46e-01	3.31e+00	2.00e+00	1.31e+00	1.04e+00	8.90e-01
R	H	48	4.57e+00	2.48e+00	1.30e+00	6.60e-01	3.45e-01	2.23e-01	3.75e+00	2.37e+00	1.68e+00	1.32e+00	1.09e+00
R	H	48	1.30e+01	6.83e+00	3.35e+00	1.70e+00	8.93e-01	5.64e-01	8.93e+00	5.37e+00	3.57e+00	2.63e+00	2.05e+00
R	H	48	1.23e+01	7.00e+00	3.29e+00	1.62e+00	8.27e-01	6.35e-01	7.91e+00	4.35e+00	2.65e+00	1.78e+00	1.10e+00
R	H	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	NA	0.00e+00	NA	NA	NA	0.00e+00	0.00e+00
R	H	240	4.58e+00	2.03e+00	1.23e+00	6.54e-01	3.41e-01	2.35e-01	2.89e+00	1.63e+00	9.61e-01	6.06e-01	3.58e-01
R	H	240	4.59e+00	2.09e+00	1.26e+00	6.29e-01	3.25e-01	2.25e-01	2.89e+00	1.59e+00	9.38e-01	6.05e-01	3.63e-01
R	H	240	1.30e+01	6.18e+00	3.56e+00	1.73e+00	9.19e-01	6.14e-01	7.91e+00	4.29e+00	2.48e+00	1.52e+00	8.79e-01
R	H	240	1.23e+01	5.72e+00	3.09e+00	1.93e+00	9.55e-01	5.87e-01	8.20e+00	5.00e+00	2.96e+00	1.97e+00	1.36e+00
R	H	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
R	H	720	4.55e+00	1.93e+00	1.11e+00	5.79e-01	2.65e-01	1.49e-01	3.21e+00	2.05e+00	1.45e+00	1.17e+00	1.02e+00
R	H	720	4.57e+00	1.88e+00	7.17e-01	7.68e-01	3.60e-01	1.73e-01	2.57e+00	1.83e+00	1.02e+00	6.53e-01	4.73e-01
R	H	720	1.30e+01	6.22e+00	3.04e+00	1.56e+00	7.22e-01	3.99e-01	8.12e+00	4.89e+00	3.26e+00	2.52e+00	2.10e+00
R	H	720	1.23e+01	5.38e+00	2.57e+00	2.70e+00	1.48e+00	7.16e-01	9.53e+00	6.90e+00	4.12e+00	2.57e+00	1.83e+00
R	H	720	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00

Table E.5 – continued from previous page

MC	S	t_{Ads}	C_{CTRL}	C_A	C_{D1}	C_{D2}	C_{D3}	C_{D4}	q_A	q_{D1}	q_{D2}	q_{D3}	q_{D4}
R	J	2	4.71e+00	1.86e+00	9.73e-01	6.11e-01	4.39e-01	2.58e-01	6.70e+00	4.87e+00	3.78e+00	3.02e+00	2.57e+00
R	J	2	4.72e+00	1.73e+00	8.31e-01	5.46e-01	4.19e-01	2.36e-01	6.24e+00	4.74e+00	3.78e+00	3.05e+00	2.63e+00
R	J	2	1.19e+01	5.52e+00	2.63e+00	1.62e+00	1.17e+00	7.40e-01	1.71e+01	1.23e+01	9.45e+00	7.43e+00	6.13e+00
R	J	2	1.13e+01	4.79e+00	2.41e+00	1.43e+00	1.06e+00	7.01e-01	1.40e+01	9.71e+00	7.21e+00	5.38e+00	4.14e+00
R	J	2	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
R	J	48	4.22e+00	1.08e+00	7.06e-01	5.16e-01	3.76e-01	2.81e-01	7.11e+00	5.85e+00	4.96e+00	4.29e+00	3.80e+00
R	J	48	4.23e+00	1.12e+00	7.65e-01	5.47e-01	3.64e-01	2.79e-01	6.47e+00	5.12e+00	4.15e+00	3.50e+00	3.02e+00
R	J	48	1.21e+01	3.70e+00	2.24e+00	1.62e+00	1.13e+00	8.53e-01	1.85e+01	1.44e+01	1.17e+01	9.72e+00	8.22e+00
R	J	48	1.15e+01	3.93e+00	2.28e+00	1.53e+00	1.05e+00	9.26e-01	1.77e+01	1.35e+01	1.08e+01	9.00e+00	7.36e+00
R	J	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
R	J	240	4.25e+00	8.67e-01	6.28e-01	4.29e-01	3.15e-01	2.88e-01	8.61e+00	7.56e+00	6.80e+00	6.27e+00	5.79e+00
R	J	240	4.25e+00	7.78e-01	5.64e-01	3.90e-01	2.94e-01	2.70e-01	7.08e+00	6.12e+00	5.44e+00	4.93e+00	4.49e+00
R	J	240	1.21e+01	3.18e+00	2.08e+00	1.36e+00	9.48e-01	8.34e-01	1.81e+01	1.46e+01	1.22e+01	1.06e+01	9.22e+00
R	J	240	1.14e+01	2.88e+00	1.82e+00	1.40e+00	1.07e+00	7.90e-01	1.97e+01	1.67e+01	1.43e+01	1.25e+01	1.11e+01
R	J	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
R	J	720	4.25e+00	6.80e-01	3.85e-01	4.13e-01	3.19e-01	1.90e-01	6.59e+00	5.91e+00	5.18e+00	4.66e+00	4.34e+00
R	J	720	4.23e+00	7.25e-01	5.39e-01	3.66e-01	2.09e-01	1.67e-01	6.52e+00	5.56e+00	4.91e+00	4.57e+00	4.28e+00
R	J	720	1.21e+01	2.27e+00	1.89e+00	1.28e+00	1.04e+00	6.33e-01	2.08e+01	1.75e+01	1.53e+01	1.35e+01	1.25e+01
R	J	720	1.13e+01	2.49e+00	1.82e+00	1.43e+00	1.00e+00	5.69e-01	1.83e+01	1.53e+01	1.28e+01	1.11e+01	1.01e+01
R	J	720	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
R	KA	2	5.01e+00	4.36e+00	1.41e+00	4.42e-01	1.32e-01	3.87e-02	3.65e+00	1.14e+00	3.64e-01	1.34e-01	6.49e-02
R	KA	2	5.01e+00	4.40e+00	1.36e+00	4.29e-01	1.28e-01	3.81e-02	3.55e+00	1.12e+00	3.61e-01	1.38e-01	6.97e-02
R	KA	2	1.27e+01	1.15e+01	3.61e+00	1.14e+00	3.52e-01	1.07e-01	9.27e+00	2.92e+00	8.78e-01	2.69e-01	7.59e-02
R	KA	2	1.20e+01	1.08e+01	3.25e+00	1.05e+00	3.17e-01	9.75e-02	8.40e+00	2.66e+00	7.73e-01	2.19e-01	4.43e-02
R	KA	2	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
R	KA	48	4.43e+00	3.80e+00	1.32e+00	3.87e-01	1.15e-01	3.67e-02	3.29e+00	9.49e-01	2.68e-01	6.36e-02	0.00e+00
R	KA	48	4.43e+00	4.15e+00	NA	3.97e-01	1.14e-01	3.57e-02	NA	9.68e-01	2.60e-01	6.25e-02	0.00e+00
R	KA	48	1.26e+01	1.09e+01	3.70e+00	1.20e+00	3.51e-01	1.12e-01	8.76e+00	2.94e+00	8.19e-01	1.97e-01	0.00e+00
R	KA	48	1.19e+01	1.10e+01	3.38e+00	1.07e+00	3.26e-01	1.36e-01	8.89e+00	2.82e+00	9.27e-01	3.57e-01	1.21e-01
R	KA	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
R	KA	240	4.43e+00	4.01e+00	1.25e+00	3.90e-01	1.25e-01	0.00e+00	3.12e+00	9.16e-01	2.20e-01	0.00e+00	0.00e+00
R	KA	240	4.43e+00	3.95e+00	1.25e+00	3.85e-01	1.17e-01	3.52e-02	3.11e+00	9.45e-01	2.65e-01	6.08e-02	0.00e+00
R	KA	240	1.26e+01	1.12e+01	3.60e+00	1.10e+00	3.42e-01	1.02e-01	9.03e+00	2.75e+00	7.80e-01	1.77e-01	0.00e+00
R	KA	240	1.20e+01	1.06e+01	3.27e+00	1.02e+00	2.58e-01	9.40e-02	8.10e+00	2.42e+00	6.22e-01	1.67e-01	0.00e+00
R	KA	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
R	KA	720	4.44e+00	3.88e+00	1.20e+00	3.68e-01	8.96e-02	0.00e+00	2.95e+00	7.94e-01	1.54e-01	0.00e+00	0.00e+00
R	KA	720	4.41e+00	4.00e+00	1.23e+00	3.59e-01	8.84e-02	0.00e+00	2.98e+00	7.89e-01	1.52e-01	0.00e+00	0.00e+00
R	KA	720	1.26e+01	1.10e+01	3.40e+00	1.06e+00	2.41e-01	5.41e-02	8.59e+00	2.45e+00	5.98e-01	1.81e-01	8.60e-02
R	KA	720	1.19e+01	NA	3.31e+00	1.01e+00	2.24e-01	5.56e-02	8.08e+00	2.40e+00	5.85e-01	1.81e-01	8.26e-02
R	KA	720	0.00e+00	0.00e+00	NA	0.00e+00	0.00e+00	0.00e+00	NA	0.00e+00	0.00e+00	0.00e+00	0.00e+00

Table E.5 – continued from previous page

MC	S	t_{Ads}	C_{CTRL}	C_A	C_{D1}	C_{D2}	C_{D3}	C_{D4}	q_A	q_{D1}	q_{D2}	q_{D3}	q_{D4}
R	LCL	2	4.23e+00	2.49e+00	1.16e+00	NA	NA	NA	NA	NA	NA	NA	0.00e+00
R	LCL	2	4.16e+00	2.56e+00	1.18e+00	NA	NA	NA	NA	NA	NA	NA	0.00e+00
R	LCL	2	1.12e+01	6.35e+00	3.19e+00	NA	NA	NA	NA	NA	NA	NA	0.00e+00
R	LCL	2	1.03e+01	5.92e+00	0.00e+00	NA	NA	NA	NA	NA	NA	NA	0.00e+00
R	LCL	2	0.00e+00	0.00e+00	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
R	LCL	48	4.21e+00	2.03e+00	1.06e+00	6.78e-01	4.73e-01	3.49e-01	3.74e+00	2.62e+00	1.89e+00	1.39e+00	1.02e+00
R	LCL	48	4.20e+00	1.99e+00	1.05e+00	6.76e-01	4.73e-01	3.60e-01	3.79e+00	2.68e+00	1.97e+00	1.46e+00	1.09e+00
R	LCL	48	1.11e+01	5.54e+00	2.97e+00	1.82e+00	1.22e+00	8.57e-01	9.83e+00	6.73e+00	4.78e+00	3.48e+00	2.56e+00
R	LCL	48	1.01e+01	4.92e+00	2.61e+00	1.60e+00	1.09e+00	7.84e-01	8.78e+00	6.06e+00	4.37e+00	3.20e+00	2.37e+00
R	LCL	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
R	LCL	240	4.25e+00	1.74e+00	1.01e+00	6.49e-01	4.51e-01	3.00e-01	3.81e+00	2.57e+00	1.90e+00	1.43e+00	1.11e+00
R	LCL	240	4.22e+00	1.76e+00	1.02e+00	6.48e-01	4.49e-01	3.04e-01	3.88e+00	2.61e+00	1.93e+00	1.46e+00	1.13e+00
R	LCL	240	1.11e+01	4.82e+00	2.74e+00	1.78e+00	1.19e+00	6.64e-01	1.04e+01	7.02e+00	5.18e+00	3.90e+00	3.19e+00
R	LCL	240	1.02e+01	4.34e+00	2.59e+00	1.64e+00	1.10e+00	7.10e-01	9.46e+00	6.26e+00	4.56e+00	3.42e+00	2.66e+00
R	LCL	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
R	LCL	720	4.24e+00	1.41e+00	9.72e-01	6.71e-01	4.44e-01	2.97e-01	3.92e+00	2.88e+00	2.15e+00	1.69e+00	1.38e+00
R	LCL	720	4.24e+00	1.42e+00	9.38e-01	6.66e-01	4.45e-01	NA	NA	NA	NA	NA	1.42e+00
R	LCL	720	1.11e+01	3.96e+00	2.66e+00	1.85e+00	1.21e+00	8.05e-01	1.06e+01	7.79e+00	5.74e+00	4.49e+00	3.63e+00
R	LCL	720	1.03e+01	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
R	LCL	720	0.00e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
R	LCO	2	4.61e+00	2.48e+00	8.88e-01	NA	NA	NA	NA	NA	NA	NA	0.00e+00
R	LCO	2	4.72e+00	2.67e+00	8.08e-01	NA	NA	NA	NA	NA	NA	NA	0.00e+00
R	LCO	2	1.22e+01	6.13e+00	2.77e+00	NA	NA	NA	NA	NA	NA	NA	0.00e+00
R	LCO	2	1.12e+01	4.93e+00	2.58e+00	NA	NA	NA	NA	NA	NA	NA	0.00e+00
R	LCO	2	0.00e+00	0.00e+00	0.00e+00	NA	NA	NA	NA	NA	NA	NA	0.00e+00
R	LCO	48	4.66e+00	1.42e+00	7.99e-01	5.88e-01	4.76e-01	4.62e-01	4.94e+00	4.12e+00	3.51e+00	2.98e+00	2.52e+00
R	LCO	48	4.66e+00	3.73e+00	7.90e-01	5.83e-01	4.75e-01	3.77e-01	4.97e+00	4.15e+00	3.55e+00	3.03e+00	2.63e+00
R	LCO	48	1.22e+01	3.79e+00	2.44e+00	1.71e+00	1.32e+00	1.02e+00	1.30e+01	1.06e+01	8.86e+00	7.42e+00	6.34e+00
R	LCO	48	1.13e+01	3.42e+00	2.05e+00	1.41e+00	1.14e+00	8.99e-01	1.12e+01	9.01e+00	7.53e+00	6.29e+00	5.34e+00
R	LCO	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
R	LCO	240	4.71e+00	1.15e+00	7.55e-01	5.25e-01	4.25e-01	3.17e-01	4.71e+00	3.83e+00	3.11e+00	2.68e+00	2.34e+00
R	LCO	240	4.73e+00	1.11e+00	7.22e-01	4.96e-01	3.91e-01	2.99e-01	4.54e+00	3.55e+00	2.86e+00	2.46e+00	2.14e+00
R	LCO	240	1.23e+01	3.43e+00	2.21e+00	1.50e+00	1.12e+00	8.22e-01	1.18e+01	9.19e+00	7.11e+00	5.98e+00	5.11e+00
R	LCO	240	1.13e+01	3.01e+00	2.01e+00	1.34e+00	1.03e+00	7.19e-01	1.04e+01	8.03e+00	6.17e+00	5.12e+00	4.36e+00
R	LCO	240	0.00e+00	NA	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
R	LCO	720	4.76e+00	8.32e-01	6.46e-01	5.09e-01	4.04e-01	2.88e-01	4.70e+00	4.04e+00	3.49e+00	3.06e+00	2.74e+00
R	LCO	720	4.74e+00	9.07e-01	7.15e-01	5.84e-01	3.99e-01	2.91e-01	4.69e+00	3.95e+00	3.31e+00	2.89e+00	2.57e+00
R	LCO	720	1.24e+01	2.51e+00	1.96e+00	1.48e+00	1.14e+00	7.90e-01	1.20e+01	1.01e+01	8.45e+00	7.23e+00	6.37e+00
R	LCO	720	1.15e+01	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
R	LCO	720	0.00e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00

Table E.5 – continued from previous page

MC	S	t_{Ads}	C_{CTRL}	C_A	C_{D1}	C_{D2}	C_{D3}	C_{D4}	q_A	q_{D1}	q_{D2}	q_{D3}	q_{D4}
R	M	2	4.95e+00	3.57e+00	1.52e+00	6.81e-01	3.24e-01	1.56e-01	2.97e+00	1.33e+00	6.56e-01	2.96e-01	1.31e-01
R	M	2	4.96e+00	3.67e+00	1.48e+00	6.68e-01	3.32e-01	1.57e-01	2.97e+00	1.34e+00	6.74e-01	3.05e-01	1.36e-01
R	M	2	1.28e+01	9.22e+00	3.87e+00	1.68e+00	8.22e-01	3.72e-01	7.50e+00	3.27e+00	1.59e+00	6.83e-01	2.87e-01
R	M	2	1.18e+01	8.63e+00	3.59e+00	1.58e+00	7.49e-01	3.44e-01	7.09e+00	3.25e+00	1.66e+00	8.42e-01	4.80e-01
R	M	2	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
R	M	48	4.24e+00	2.91e+00	1.26e+00	6.29e-01	2.95e-01	1.53e-01	2.91e+00	1.62e+00	9.68e-01	6.55e-01	5.01e-01
R	M	48	4.23e+00	2.96e+00	1.41e+00	6.28e-01	2.83e-01	1.47e-01	2.80e+00	1.36e+00	6.93e-01	3.93e-01	2.41e-01
R	M	48	1.20e+01	7.99e+00	3.52e+00	1.70e+00	7.73e-01	3.89e-01	7.37e+00	3.77e+00	1.97e+00	1.15e+00	7.50e-01
R	M	48	1.15e+01	8.27e+00	3.61e+00	1.73e+00	7.21e-01	4.19e-01	7.45e+00	3.49e+00	1.67e+00	9.11e-01	4.64e-01
R	M	48	0.00e+00	NA	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
R	M	240	4.26e+00	2.55e+00	1.19e+00	5.56e-01	2.66e-01	1.08e-01	2.32e+00	1.05e+00	4.61e-01	1.80e-01	7.36e-02
R	M	240	4.25e+00	2.82e+00	1.29e+00	6.82e-01	2.92e-01	1.40e-01	2.75e+00	1.34e+00	6.20e-01	3.08e-01	1.69e-01
R	M	240	1.20e+01	8.32e+00	3.97e+00	1.79e+00	8.20e-01	4.11e-01	7.91e+00	3.59e+00	1.71e+00	8.33e-01	4.23e-01
R	M	240	1.14e+01	7.71e+00	3.64e+00	1.73e+00	8.19e-01	3.70e-01	7.18e+00	3.52e+00	1.67e+00	8.16e-01	4.16e-01
R	M	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
R	M	720	4.24e+00	2.68e+00	1.44e+00	6.54e-01	2.50e-01	9.10e-02	2.83e+00	1.28e+00	5.75e-01	3.22e-01	2.27e-01
R	M	720	4.23e+00	2.71e+00	1.40e+00	NA	2.48e-01	9.23e-02	NA	NA	6.11e-01	3.63e-01	2.65e-01
R	M	720	1.21e+01	7.87e+00	3.73e+00	1.73e+00	6.94e-01	2.64e-01	7.72e+00	3.69e+00	1.85e+00	1.15e+00	8.74e-01
R	M	720	1.13e+01	0.00e+00	3.68e+00	1.83e+00	6.50e-01	NA	NA	NA	NA	NA	6.34e-01
R	M	720	0.00e+00	NA	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
R	N	2	4.88e+00	3.92e+00	1.37e+00	5.34e-01	2.41e-01	9.67e-02	2.40e+00	9.47e-01	3.90e-01	1.45e-01	4.18e-02
R	N	2	4.91e+00	3.84e+00	1.35e+00	5.21e-01	2.17e-01	8.56e-02	2.34e+00	9.00e-01	3.51e-01	1.26e-01	3.54e-02
R	N	2	1.30e+01	1.04e+01	3.58e+00	1.23e+00	4.85e-01	1.81e-01	5.95e+00	2.07e+00	7.53e-01	2.49e-01	6.09e-02
R	N	2	1.19e+01	9.56e+00	3.21e+00	1.13e+00	4.57e-01	1.72e-01	5.26e+00	1.88e+00	7.06e-01	2.35e-01	5.27e-02
R	N	2	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
R	N	48	4.36e+00	3.13e+00	1.22e+00	4.83e-01	1.87e-01	8.54e-02	2.25e+00	9.84e-01	4.57e-01	2.62e-01	1.72e-01
R	N	48	4.38e+00	3.52e+00	1.30e+00	4.97e-01	1.91e-01	8.32e-02	2.32e+00	9.69e-01	4.41e-01	2.37e-01	1.52e-01
R	N	48	1.25e+01	9.42e+00	3.43e+00	1.36e+00	5.23e-01	2.28e-01	6.10e+00	2.56e+00	1.08e+00	5.27e-01	2.87e-01
R	N	48	1.18e+01	9.41e+00	3.32e+00	1.31e+00	4.92e-01	2.43e-01	6.04e+00	2.39e+00	9.97e-01	4.85e-01	2.32e-01
R	N	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
R	N	240	4.35e+00	3.39e+00	1.32e+00	5.05e-01	2.04e-01	9.67e-02	2.34e+00	9.27e-01	3.99e-01	1.82e-01	7.86e-02
R	N	240	4.38e+00	3.34e+00	1.33e+00	5.07e-01	2.04e-01	9.83e-02	2.36e+00	9.39e-01	4.01e-01	1.86e-01	8.16e-02
R	N	240	1.24e+01	9.44e+00	3.67e+00	1.40e+00	5.63e-01	2.70e-01	6.47e+00	2.58e+00	1.09e+00	5.01e-01	2.17e-01
R	N	240	1.18e+01	8.98e+00	3.37e+00	1.41e+00	5.52e-01	2.37e-01	5.93e+00	2.44e+00	9.72e-01	3.88e-01	1.40e-01
R	N	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
R	N	720	4.37e+00	3.11e+00	1.18e+00	4.55e-01	1.60e-01	5.81e-02	1.96e+00	7.14e-01	2.30e-01	5.96e-02	0.00e+00
R	N	720	4.35e+00	2.98e+00	1.15e+00	4.46e-01	1.59e-01	7.21e-02	2.08e+00	8.74e-01	3.96e-01	2.31e-01	1.55e-01
R	N	720	1.25e+01	9.26e+00	3.46e+00	1.37e+00	4.89e-01	1.63e-01	6.25e+00	2.53e+00	1.06e+00	5.40e-01	3.70e-01
R	N	720	1.17e+01	0.00e+00	3.45e+00	1.46e+00	0.00e+00	1.61e-01	5.51e+00	1.99e+00	4.05e-01	4.05e-01	2.35e-01
R	N	720	0.00e+00	NA	0.00e+00	0.00e+00	NA	0.00e+00	NA	NA	NA	0.00e+00	0.00e+00

Table E.5 – continued from previous page

MC	S	t_{Ads}	C_{CTRL}	C_A	C_{D1}	C_{D2}	C_{D3}	C_{D4}	q_A	q_{D1}	q_{D2}	q_{D3}	q_{D4}
R	P	2	4.81e+00	5.94e-01	3.25e-01	2.97e-01	3.11e-01	2.80e-01	8.04e+00	7.49e+00	6.98e+00	6.42e+00	6.05e+00
R	P	2	4.80e+00	5.53e-01	3.20e-01	3.20e-01	2.99e-01	2.75e-01	9.15e+00	8.60e+00	8.05e+00	7.51e+00	7.25e+00
R	P	2	1.28e+01	1.69e+00	1.06e+00	9.13e-01	8.29e-01	7.53e-01	2.12e+01	1.94e+01	1.78e+01	1.63e+01	1.54e+01
R	P	2	1.17e+01	7.49e+00	7.22e-01	6.64e-01	6.19e-01	NA	NA	NA	NA	NA	0.00e+00
R	P	2	0.00e+00	0.00e+00	0.00e+00	NA	NA	NA	NA	NA	NA	NA	0.00e+00
R	P	48	4.31e+00	3.78e-01	3.37e-01	3.37e-01	2.57e-01	2.42e-01	7.27e+00	6.69e+00	6.11e+00	5.65e+00	5.25e+00
R	P	48	4.31e+00	3.79e-01	3.28e-01	3.09e-01	2.44e-01	2.43e-01	7.70e+00	7.16e+00	6.62e+00	6.19e+00	5.78e+00
R	P	48	1.22e+01	1.09e+00	9.79e-01	9.15e-01	7.40e-01	7.29e-01	1.98e+01	1.81e+01	1.66e+01	1.53e+01	1.40e+01
R	P	48	1.16e+01	7.02e-01	6.58e-01	6.69e-01	5.18e-01	4.94e-01	1.92e+01	1.81e+01	1.69e+01	1.61e+01	1.52e+01
R	P	48	0.00e+00	1.12e-01	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
R	P	240	4.29e+00	2.73e-01	2.19e-01	1.74e-01	1.61e-01	1.42e-01	5.74e+00	5.36e+00	5.06e+00	4.78e+00	4.54e+00
R	P	240	4.30e+00	2.11e-01	1.88e-01	1.69e-01	1.55e-01	1.44e-01	5.78e+00	5.47e+00	5.17e+00	4.91e+00	4.66e+00
R	P	240	1.23e+01	8.05e-01	7.14e-01	6.45e-01	5.77e-01	5.30e-01	1.64e+01	1.52e+01	1.41e+01	1.31e+01	1.22e+01
R	P	240	1.16e+01	5.75e-01	5.37e-01	0.00e+00	3.61e-01	3.97e-01	1.23e+01	1.15e+01	1.15e+01	1.08e+01	1.02e+01
R	P	240	0.00e+00	0.00e+00	0.00e+00	NA	0.00e+00	0.00e+00	NA	NA	0.00e+00	0.00e+00	0.00e+00
R	P	720	4.30e+00	2.06e-01	9.73e-02	0.00e+00	1.34e-01	0.00e+00	6.51e+00	6.34e+00	6.34e+00	6.11e+00	6.11e+00
R	P	720	4.30e+00	1.93e-01	1.25e-01	2.38e-01	1.16e-01	1.28e-01	7.89e+00	7.69e+00	7.30e+00	7.11e+00	6.90e+00
R	P	720	1.23e+01	3.88e-01	3.31e-01	3.79e-01	2.35e-01	2.15e-01	1.46e+01	1.40e+01	1.34e+01	1.30e+01	1.27e+01
R	P	720	1.16e+01	1.74e-01	1.28e-01	0.00e+00	1.22e-01	0.00e+00	8.18e+00	7.98e+00	7.98e+00	7.78e+00	7.78e+00
R	P	720	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
R	PO	2	4.54e+00	1.96e+00	1.04e+00	NA	NA	NA	NA	NA	NA	NA	0.00e+00
R	PO	2	4.44e+00	2.53e+00	1.16e+00	NA	NA	NA	NA	NA	NA	NA	0.00e+00
R	PO	2	1.19e+01	6.49e+00	2.76e+00	NA	NA	NA	NA	NA	NA	NA	0.00e+00
R	PO	2	1.09e+01	6.45e+00	2.61e+00	NA	NA	NA	NA	NA	NA	NA	0.00e+00
R	PO	2	0.00e+00	0.00e+00	0.00e+00	NA	NA	NA	NA	NA	NA	NA	0.00e+00
R	PO	48	4.62e+00	2.04e+00	1.13e+00	7.73e-01	6.01e-01	4.61e-01	3.12e+00	1.94e+00	1.12e+00	4.89e-01	0.00e+00
R	PO	48	4.52e+00	1.98e+00	1.12e+00	8.11e-01	5.98e-01	4.63e-01	5.14e+00	3.96e+00	3.11e+00	2.49e+00	2.00e+00
R	PO	48	1.19e+01	5.20e+00	2.78e+00	1.86e+00	1.42e+00	1.03e+00	1.17e+01	8.73e+00	6.78e+00	5.59e+00	4.49e+00
R	PO	48	1.07e+01	5.39e+00	2.66e+00	1.65e+00	1.15e+00	8.52e-01	9.82e+00	7.02e+00	5.28e+00	4.10e+00	3.19e+00
R	PO	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
R	PO	240	4.52e+00	1.74e+00	1.03e+00	6.97e-01	4.87e-01	3.21e-01	4.45e+00	3.16e+00	2.25e+00	1.75e+00	1.41e+00
R	PO	240	4.49e+00	1.43e+00	1.02e+00	6.23e-01	5.13e-01	3.31e-01	4.28e+00	3.01e+00	2.19e+00	1.67e+00	1.32e+00
R	PO	240	1.18e+01	4.66e+00	3.00e+00	1.63e+00	1.15e+00	7.49e-01	1.17e+01	8.01e+00	5.84e+00	4.66e+00	3.87e+00
R	PO	240	1.09e+01	3.55e+00	2.32e+00	NA	1.01e+00	6.73e-01	NA	NA	5.66e+00	4.63e+00	3.90e+00
R	PO	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
R	PO	720	4.55e+00	1.19e+00	8.40e-01	5.27e-01	4.95e-01	3.30e-01	3.90e+00	3.05e+00	2.50e+00	1.98e+00	1.63e+00
R	PO	720	4.53e+00	3.39e+00	1.17e+00	5.78e-01	4.05e-01	3.44e-01	5.09e+00	3.90e+00	3.29e+00	2.86e+00	2.50e+00
R	PO	720	1.19e+01	3.64e+00	2.79e+00	1.54e+00	1.27e+00	8.08e-01	1.19e+01	9.02e+00	7.41e+00	6.08e+00	5.22e+00
R	PO	720	1.09e+01	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
R	PO	720	0.00e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00

Table E.5 – continued from previous page

MC	S	t_{Ads}	C_{CTRL}	C_A	C_{D1}	C_{D2}	C_{D3}	C_{D4}	q_A	q_{D1}	q_{D2}	q_{D3}	q_{D4}
R	R	2	4.76e+00	1.41e+00	9.15e-01	6.93e-01	5.74e-01	4.46e-01	7.66e+00	6.10e+00	4.87e+00	3.87e+00	3.12e+00
R	R	2	4.80e+00	1.39e+00	8.31e-01	6.93e-01	5.73e-01	4.40e-01	7.34e+00	5.92e+00	4.69e+00	3.69e+00	2.95e+00
R	R	2	1.25e+01	3.72e+00	2.46e+00	1.86e+00	1.48e+00	1.12e+00	1.90e+01	1.47e+01	1.14e+01	8.83e+00	6.94e+00
R	R	2	1.15e+01	3.28e+00	2.25e+00	1.69e+00	1.34e+00	1.03e+00	1.75e+01	1.37e+01	1.07e+01	8.36e+00	6.57e+00
R	R	2	0.00e+00	0.00e+00	0.00e+00	0.00e+00	NA	0.00e+00	NA	NA	NA	0.00e+00	0.00e+00
R	R	48	4.22e+00	1.07e+00	7.67e-01	6.20e-01	4.94e-01	3.95e-01	7.80e+00	6.46e+00	5.39e+00	4.53e+00	3.84e+00
R	R	48	4.24e+00	1.06e+00	8.59e-01	6.52e-01	4.64e-01	3.76e-01	7.89e+00	6.45e+00	5.33e+00	4.54e+00	3.89e+00
R	R	48	1.21e+01	2.83e+00	2.14e+00	1.66e+00	1.32e+00	1.06e+00	2.01e+01	1.62e+01	1.35e+01	1.12e+01	9.40e+00
R	R	48	1.14e+01	2.87e+00	2.14e+00	1.65e+00	1.26e+00	1.06e+00	1.77e+01	1.39e+01	1.10e+01	8.89e+00	7.00e+00
R	R	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
R	R	240	4.25e+00	8.74e-01	6.40e-01	4.90e-01	3.91e-01	3.38e-01	5.42e+00	4.32e+00	3.49e+00	2.83e+00	2.27e+00
R	R	240	4.24e+00	7.29e-01	6.00e-01	4.25e-01	3.87e-01	3.27e-01	5.15e+00	4.13e+00	3.41e+00	2.73e+00	2.19e+00
R	R	240	1.20e+01	2.33e+00	1.91e+00	1.49e+00	1.18e+00	NA	NA	NA	NA	NA	7.64e+00
R	R	240	1.14e+01	2.25e+00	1.78e+00	1.49e+00	1.12e+00	9.24e-01	1.76e+01	1.45e+01	1.18e+01	9.96e+00	8.35e+00
R	R	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
R	R	720	4.24e+00	7.92e-01	6.17e-01	4.30e-01	3.58e-01	2.41e-01	6.98e+00	5.90e+00	5.15e+00	4.52e+00	4.12e+00
R	R	720	4.23e+00	6.02e-01	4.61e-01	4.08e-01	3.39e-01	2.32e-01	6.53e+00	5.72e+00	5.01e+00	4.42e+00	4.03e+00
R	R	720	1.21e+01	2.10e+00	1.71e+00	1.28e+00	1.08e+00	7.21e-01	1.93e+01	1.63e+01	1.40e+01	1.22e+01	1.10e+01
R	R	720	1.14e+01	1.96e+00	1.59e+00	1.30e+00	1.03e+00	7.20e-01	1.79e+01	1.52e+01	1.29e+01	1.12e+01	9.88e+00
R	R	720	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
R	SOU	2	4.63e+00	3.32e+00	1.47e+00	7.29e-01	3.60e-01	1.79e-01	2.87e+00	1.38e+00	6.37e-01	2.59e-01	6.85e-02
R	SOU	2	4.47e+00	3.32e+00	1.49e+00	7.24e-01	3.56e-01	1.72e-01	2.87e+00	1.35e+00	6.15e-01	2.39e-01	5.43e-02
R	SOU	2	1.21e+01	8.47e+00	0.00e+00	1.80e+00	8.68e-01	4.09e-01	3.40e+00	3.40e+00	1.54e+00	6.11e-01	1.70e-01
R	SOU	2	1.10e+01	8.00e+00	3.65e+00	1.63e+00	8.13e-01	3.79e-01	6.99e+00	3.36e+00	1.69e+00	8.21e-01	4.20e-01
R	SOU	2	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
R	SOU	48	4.12e+00	3.05e+00	1.33e+00	6.55e-01	2.95e-01	1.50e-01	2.56e+00	1.16e+00	4.73e-01	1.60e-01	0.00e+00
R	SOU	48	4.13e+00	3.04e+00	1.48e+00	7.11e-01	3.06e-01	1.55e-01	2.79e+00	1.24e+00	4.92e-01	1.65e-01	0.00e+00
R	SOU	48	1.17e+01	8.28e+00	3.86e+00	1.81e+00	8.59e-01	4.36e-01	7.96e+00	3.88e+00	1.95e+00	1.03e+00	5.64e-01
R	SOU	48	1.11e+01	7.67e+00	3.74e+00	1.84e+00	8.64e-01	4.75e-01	8.00e+00	4.00e+00	2.06e+00	1.14e+00	6.54e-01
R	SOU	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
R	SOU	240	4.13e+00	2.95e+00	1.50e+00	6.96e-01	3.42e-01	2.01e-01	3.33e+00	1.77e+00	1.05e+00	6.85e-01	4.82e-01
R	SOU	240	4.14e+00	2.97e+00	1.52e+00	7.10e-01	3.42e-01	NA	NA	NA	NA	NA	0.00e+00
R	SOU	240	1.17e+01	7.16e+00	4.16e+00	2.01e+00	9.86e-01	3.28e-02	8.04e+00	3.75e+00	1.64e+00	6.12e-01	5.78e-01
R	SOU	240	1.11e+01	7.87e+00	3.74e+00	1.98e+00	9.42e-01	4.90e-01	8.20e+00	4.28e+00	2.30e+00	1.30e+00	7.79e-01
R	SOU	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	NA	NA	NA	NA	NA	0.00e+00
R	SOU	720	4.12e+00	2.86e+00	1.33e+00	6.53e-01	2.15e-01	1.17e-01	2.62e+00	1.20e+00	5.06e-01	2.86e-01	1.60e-01
R	SOU	720	4.12e+00	2.95e+00	1.37e+00	6.49e-01	2.27e-01	1.32e-01	2.51e+00	1.05e+00	3.73e-01	1.44e-01	0.00e+00
R	SOU	720	1.17e+01	8.57e+00	3.87e+00	1.85e+00	1.10e+00	3.38e-01	7.77e+00	3.61e+00	1.65e+00	5.10e-01	1.45e-01
R	SOU	720	1.10e+01	7.74e+00	3.80e+00	2.19e+00	1.10e+00	0.00e+00	6.72e+00	2.87e+00	1.50e+00	3.88e-01	3.88e-01
R	SOU	720	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	NA	NA	NA	NA	NA	0.00e+00

Table E.5 – continued from previous page

MC	S	t_{Ads}	C_{CTRL}	C_A	C_{D1}	C_{D2}	C_{D3}	C_{D4}	q_A	q_{D1}	q_{D2}	q_{D3}	q_{D4}
R	SSL1	2	4.54e+00	3.46e+00	1.43e+00	6.53e-01	2.88e-01	1.37e-01	2.73e+00	1.19e+00	5.23e-01	2.23e-01	8.15e-02
R	SSL1	2	4.56e+00	3.45e+00	1.52e+00	6.39e-01	2.91e-01	3.58e-01	3.09e+00	1.45e+00	7.81e-01	4.71e-01	9.57e-02
R	SSL1	2	1.19e+01	8.96e+00	3.82e+00	1.62e+00	7.39e-01	NA	NA	NA	NA	NA	2.36e-01
R	SSL1	2	1.11e+01	8.29e+00	3.54e+00	1.53e+00	7.33e-01	3.31e-01	6.79e+00	2.96e+00	1.35e+00	5.76e-01	2.28e-01
R	SSL1	2	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
R	SSL1	48	4.51e+00	3.28e+00	0.00e+00	6.80e-01	3.13e-01	1.69e-01	1.33e+00	1.33e+00	6.10e-01	2.75e-01	9.80e-02
R	SSL1	48	4.55e+00	3.34e+00	3.56e+00	7.02e-01	3.11e-01	1.60e-01	5.18e+00	1.35e+00	5.96e-01	2.63e-01	9.50e-02
R	SSL1	48	1.18e+01	8.61e+00	3.99e+00	1.71e+00	7.93e-01	3.84e-01	7.52e+00	3.25e+00	1.47e+00	6.26e-01	2.29e-01
R	SSL1	48	1.09e+01	NA	NA	1.64e+00	7.47e-01	3.82e-01	NA	3.25e+00	1.53e+00	7.31e-01	3.32e-01
R	SSL1	48	0.00e+00	0.00e+00	NA	0.00e+00	0.00e+00	0.00e+00	NA	0.00e+00	0.00e+00	0.00e+00	0.00e+00
R	SSL1	240	4.53e+00	3.40e+00	1.63e+00	7.64e-01	3.75e-01	1.84e-01	3.36e+00	1.69e+00	8.36e-01	4.41e-01	2.44e-01
R	SSL1	240	4.56e+00	3.64e+00	1.66e+00	8.03e-01	4.02e-01	2.11e-01	3.50e+00	1.80e+00	9.10e-01	4.86e-01	2.60e-01
R	SSL1	240	1.18e+01	1.08e+01	3.92e+00	NA	9.33e-01	4.51e-01	NA	NA	2.21e+00	1.25e+00	7.67e-01
R	SSL1	240	1.09e+01	5.51e+00	3.64e+00	NA	NA	4.44e-01	NA	NA	NA	1.08e+00	6.03e-01
R	SSL1	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
R	SSL1	720	4.52e+00	3.23e+00	1.52e+00	7.20e-01	3.55e-01	1.77e-01	2.99e+00	1.33e+00	5.83e-01	1.90e-01	0.00e+00
R	SSL1	720	4.48e+00	3.20e+00	1.51e+00	7.03e-01	3.37e-01	1.68e-01	2.96e+00	1.30e+00	5.60e-01	1.81e-01	0.00e+00
R	SSL1	720	1.18e+01	8.62e+00	3.87e+00	1.86e+00	9.03e-01	4.81e-01	7.50e+00	3.42e+00	1.51e+00	5.18e-01	0.00e+00
R	SSL1	720	1.11e+01	NA	3.72e+00	1.76e+00	8.60e-01	4.23e-01	7.53e+00	3.55e+00	1.72e+00	7.65e-01	3.12e-01
R	SSL1	720	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
R	SSL2	2	4.73e+00	3.54e+00	1.51e+00	6.73e-01	3.07e-01	1.57e-01	2.89e+00	1.30e+00	5.93e-01	2.61e-01	9.90e-02
R	SSL2	2	4.75e+00	3.56e+00	1.62e+00	7.14e-01	3.37e-01	1.66e-01	3.09e+00	1.46e+00	7.12e-01	3.44e-01	1.68e-01
R	SSL2	2	1.24e+01	9.34e+00	4.00e+00	1.74e+00	8.08e-01	3.80e-01	7.65e+00	3.39e+00	1.58e+00	7.00e-01	3.07e-01
R	SSL2	2	1.15e+01	8.55e+00	3.63e+00	1.59e+00	7.35e-01	NA	NA	NA	NA	NA	2.34e-01
R	SSL2	2	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
R	SSL2	48	4.73e+00	3.50e+00	1.54e+00	7.10e-01	3.19e-01	1.59e-01	2.95e+00	1.37e+00	6.09e-01	2.72e-01	1.06e-01
R	SSL2	48	4.73e+00	3.31e+00	1.52e+00	6.97e-01	3.23e-01	1.65e-01	2.90e+00	1.34e+00	6.16e-01	2.64e-01	9.45e-02
R	SSL2	48	1.23e+01	8.94e+00	4.08e+00	1.84e+00	8.40e-01	4.02e-01	7.84e+00	3.60e+00	1.71e+00	7.98e-01	3.88e-01
R	SSL2	48	1.14e+01	8.17e+00	3.79e+00	1.72e+00	8.17e-01	4.03e-01	7.45e+00	3.45e+00	1.68e+00	7.93e-01	3.81e-01
R	SSL2	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
R	SSL2	240	4.75e+00	3.57e+00	1.65e+00	7.65e-01	3.88e-01	1.85e-01	3.47e+00	1.83e+00	9.60e-01	5.51e-01	3.58e-01
R	SSL2	240	4.71e+00	3.22e+00	1.72e+00	8.85e-01	4.79e-01	2.26e-01	3.38e+00	1.71e+00	7.34e-01	2.38e-01	0.00e+00
R	SSL2	240	1.24e+01	9.09e+00	4.11e+00	1.94e+00	9.15e-01	4.32e-01	7.79e+00	3.77e+00	1.57e+00	6.04e-01	1.46e-01
R	SSL2	240	1.14e+01	8.20e+00	3.77e+00	1.83e+00	8.64e-01	NA	NA	NA	NA	NA	1.52e-01
R	SSL2	240	0.00e+00	NA	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
R	SSL2	720	4.68e+00	3.30e+00	1.54e+00	7.62e-01	3.65e-01	0.00e+00	2.89e+00	1.20e+00	3.97e-01	0.00e+00	0.00e+00
R	SSL2	720	4.70e+00	3.35e+00	1.56e+00	7.37e-01	3.43e-01	0.00e+00	2.90e+00	1.17e+00	3.77e-01	0.00e+00	0.00e+00
R	SSL2	720	1.23e+01	8.96e+00	4.35e+00	2.06e+00	9.70e-01	0.00e+00	8.57e+00	3.83e+00	1.64e+00	5.91e-01	5.91e-01
R	SSL2	720	1.14e+01	8.08e+00	3.74e+00	1.81e+00	8.35e-01	0.00e+00	6.91e+00	2.71e+00	9.10e-01	0.00e+00	0.00e+00
R	SSL2	720	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00

Table E.5 – continued from previous page

MC	S	t_{Ads}	C_{CTRL}	C_A	C_{D1}	C_{D2}	C_{D3}	C_{D4}	q_A	q_{D1}	q_{D2}	q_{D3}	q_{D4}
R	SSL3	2	4.67e+00	3.37e+00	1.53e+00	6.71e-01	3.07e-01	1.54e-01	2.93e+00	1.31e+00	5.85e-01	2.61e-01	1.01e-01
R	SSL3	2	4.68e+00	3.39e+00	1.55e+00	6.80e-01	3.36e-01	1.41e-01	2.98e+00	1.33e+00	5.97e-01	2.43e-01	9.70e-02
R	SSL3	2	1.22e+01	9.04e+00	3.92e+00	1.75e+00	8.32e-01	4.36e-01	7.75e+00	3.56e+00	1.65e+00	7.72e-01	3.20e-01
R	SSL3	2	1.13e+01	8.44e+00	3.74e+00	1.65e+00	7.48e-01	NA	NA	NA	NA	NA	2.81e-01
R	SSL3	2	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
R	SSL3	48	4.66e+00	3.12e+00	1.50e+00	7.06e-01	2.93e-01	1.55e-01	2.90e+00	1.31e+00	5.71e-01	2.57e-01	9.78e-02
R	SSL3	48	4.65e+00	3.24e+00	1.51e+00	7.08e-01	3.27e-01	1.69e-01	2.98e+00	1.38e+00	6.44e-01	2.88e-01	1.12e-01
R	SSL3	48	1.22e+01	9.55e+00	3.90e+00	1.82e+00	8.35e-01	4.18e-01	7.74e+00	3.59e+00	1.68e+00	7.90e-01	3.59e-01
R	SSL3	48	1.13e+01	8.09e+00	3.69e+00	NA	NA	3.86e-01	NA	NA	NA	7.62e-01	3.66e-01
R	SSL3	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
R	SSL3	240	4.67e+00	3.40e+00	1.68e+00	7.97e-01	3.88e-01	1.99e-01	3.35e+00	1.67e+00	7.59e-01	3.50e-01	1.35e-01
R	SSL3	240	4.63e+00	3.54e+00	1.68e+00	8.29e-01	4.12e-01	2.05e-01	3.36e+00	1.69e+00	7.81e-01	3.52e-01	1.32e-01
R	SSL3	240	1.22e+01	8.85e+00	4.10e+00	2.10e+00	1.04e+00	6.54e-01	8.16e+00	4.14e+00	1.79e+00	6.98e-01	0.00e+00
R	SSL3	240	1.11e+01	8.06e+00	3.72e+00	1.81e+00	8.83e-01	4.37e-01	8.36e+00	4.63e+00	2.57e+00	1.63e+00	1.17e+00
R	SSL3	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
R	SSL3	720	4.66e+00	3.23e+00	1.54e+00	7.64e-01	3.65e-01	2.02e-01	3.11e+00	1.42e+00	6.16e-01	2.16e-01	0.00e+00
R	SSL3	720	4.67e+00	3.24e+00	1.59e+00	7.71e-01	3.77e-01	1.84e-01	3.11e+00	1.41e+00	6.12e-01	1.97e-01	0.00e+00
R	SSL3	720	1.23e+01	8.89e+00	3.95e+00	1.92e+00	9.33e-01	5.10e-01	7.85e+00	3.55e+00	1.57e+00	5.38e-01	0.00e+00
R	SSL3	720	1.14e+01	8.43e+00	3.80e+00	1.80e+00	8.53e-01	5.52e-01	7.57e+00	3.42e+00	1.51e+00	5.85e-01	0.00e+00
R	SSL3	720	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
R	ST	2	3.90e+00	1.88e+00	1.16e+00	6.60e-01	3.98e-01	3.21e-01	4.85e+00	2.88e+00	1.70e+00	9.95e-01	4.50e-01
R	ST	2	3.86e+00	1.92e+00	1.16e+00	6.83e-01	4.03e-01	2.68e-01	4.72e+00	2.75e+00	1.53e+00	8.31e-01	3.72e-01
R	ST	2	1.01e+01	5.54e+00	3.46e+00	2.06e+00	1.30e+00	9.03e-01	1.45e+01	8.61e+00	4.99e+00	2.77e+00	1.24e+00
R	ST	2	9.34e+00	5.30e+00	3.17e+00	1.95e+00	1.22e+00	8.08e-01	1.32e+01	7.69e+00	4.24e+00	2.12e+00	7.34e-01
R	ST	2	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
R	ST	48	3.85e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
R	ST	48	3.85e+00	1.92e+00	1.14e+00	7.87e-01	5.69e-01	4.14e-01	5.62e+00	3.70e+00	2.32e+00	1.32e+00	6.20e-01
R	ST	48	1.00e+01	6.37e+00	3.11e+00	1.86e+00	1.12e+00	9.70e-01	1.37e+01	8.49e+00	5.17e+00	3.16e+00	1.53e+00
R	ST	48	9.31e+00	4.69e+00	3.02e+00	1.77e+00	1.09e+00	9.38e-01	1.31e+01	7.99e+00	4.98e+00	3.05e+00	1.51e+00
R	ST	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
R	ST	240	3.90e+00	1.95e+00	1.15e+00	8.81e-01	5.95e-01	3.56e-01	5.70e+00	3.86e+00	2.34e+00	1.29e+00	6.44e-01
R	ST	240	3.87e+00	2.02e+00	1.11e+00	9.61e-01	5.79e-01	3.38e-01	5.97e+00	4.06e+00	2.39e+00	1.34e+00	7.28e-01
R	ST	240	1.08e+01	5.17e+00	3.16e+00	2.43e+00	1.68e+00	1.09e+00	1.63e+01	1.09e+01	6.62e+00	3.69e+00	1.74e+00
R	ST	240	9.32e+00	4.62e+00	2.34e+00	2.00e+00	1.34e+00	8.24e-01	1.30e+01	9.09e+00	5.57e+00	3.18e+00	1.71e+00
R	ST	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
R	ST	720	3.81e+00	1.95e+00	1.17e+00	7.63e-01	4.62e-01	2.38e-01	4.87e+00	2.91e+00	1.51e+00	6.96e-01	2.77e-01
R	ST	720	3.86e+00	2.00e+00	0.00e+00	7.73e-01	4.75e-01	2.70e-01	3.11e+00	3.11e+00	1.70e+00	8.61e-01	3.82e-01
R	ST	720	1.03e+01	5.07e+00	0.00e+00	1.97e+00	1.14e+00	8.00e-01	8.44e+00	8.44e+00	4.92e+00	2.87e+00	1.49e+00
R	ST	720	9.37e+00	4.70e+00	0.00e+00	1.86e+00	0.00e+00	6.40e-01	6.33e+00	6.33e+00	2.88e+00	2.88e+00	1.72e+00
R	ST	720	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00

Table E.5 – continued from previous page

MC	S	t_{Ads}	C_{CTRL}	C_A	C_{D1}	C_{D2}	C_{D3}	C_{D4}	q_A	q_{D1}	q_{D2}	q_{D3}	q_{D4}
R	W	2	4.60e+00	3.23e+00	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
R	W	2	4.50e+00	3.12e+00	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
R	W	2	1.21e+01	8.46e+00	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
R	W	2	1.10e+01	7.70e+00	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
R	W	2	0.00e+00	0.00e+00	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
R	W	48	4.52e+00	3.29e+00	1.46e+00	7.89e-01	4.67e-01	2.89e-01	3.48e+00	1.99e+00	1.16e+00	6.74e-01	3.55e-01
R	W	48	4.54e+00	2.98e+00	1.59e+00	2.05e+00	4.51e-01	2.91e-01	4.96e+00	3.32e+00	1.26e+00	7.81e-01	4.60e-01
R	W	48	1.20e+01	7.65e+00	3.74e+00	1.95e+00	1.12e+00	6.92e-01	9.01e+00	5.10e+00	3.15e+00	1.98e+00	1.22e+00
R	W	48	1.09e+01	7.02e+00	3.49e+00	1.76e+00	9.83e-01	5.73e-01	8.12e+00	4.45e+00	2.66e+00	1.63e+00	1.00e+00
R	W	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
R	W	240	4.57e+00	2.88e+00	1.39e+00	6.52e-01	2.99e-01	2.21e-01	3.52e+00	1.87e+00	9.87e-01	6.60e-01	4.33e-01
R	W	240	4.56e+00	2.88e+00	1.41e+00	6.71e-01	3.42e-01	2.23e-01	3.60e+00	1.92e+00	1.03e+00	6.53e-01	4.24e-01
R	W	240	1.20e+01	7.64e+00	3.79e+00	1.81e+00	1.04e+00	5.47e-01	9.90e+00	5.40e+00	3.05e+00	1.92e+00	1.33e+00
R	W	240	1.10e+01	6.74e+00	3.08e+00	1.50e+00	8.59e-01	4.58e-01	8.10e+00	4.42e+00	2.43e+00	1.50e+00	1.01e+00
R	W	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
R	W	720	4.61e+00	2.74e+00	1.52e+00	9.18e-01	5.00e-01	2.72e-01	3.88e+00	2.29e+00	1.28e+00	7.48e-01	4.47e-01
R	W	720	4.61e+00	2.80e+00	1.54e+00	9.06e-01	3.76e-01	2.35e-01	3.85e+00	2.25e+00	1.26e+00	8.63e-01	6.02e-01
R	W	720	1.21e+01	6.90e+00	3.73e+00	2.09e+00	1.31e+00	6.01e-01	9.14e+00	5.27e+00	3.02e+00	1.65e+00	9.82e-01
R	W	720	1.11e+01	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
R	W	720	0.00e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
R	W1	2	4.36e+00	3.21e+00	1.42e+00	6.68e-01	3.05e-01	1.43e-01	2.78e+00	1.29e+00	5.43e-01	2.32e-01	8.25e-02
R	W1	2	4.36e+00	3.24e+00	1.43e+00	6.78e-01	3.06e-01	1.57e-01	2.82e+00	1.31e+00	5.63e-01	2.49e-01	8.31e-02
R	W1	2	1.14e+01	8.46e+00	3.79e+00	1.77e+00	7.99e-01	3.91e-01	7.50e+00	3.53e+00	1.57e+00	7.42e-01	3.30e-01
R	W1	2	1.06e+01	7.78e+00	3.52e+00	1.66e+00	7.66e-01	3.61e-01	7.01e+00	3.32e+00	1.48e+00	6.90e-01	3.11e-01
R	W1	2	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
R	W1	48	4.33e+00	3.21e+00	1.44e+00	6.62e-01	3.20e-01	1.44e-01	2.84e+00	1.26e+00	5.88e-01	2.30e-01	7.80e-02
R	W1	48	4.36e+00	3.16e+00	1.46e+00	6.72e-01	3.16e-01	1.47e-01	2.88e+00	1.29e+00	5.98e-01	2.40e-01	8.42e-02
R	W1	48	1.14e+01	8.41e+00	3.84e+00	1.43e+00	8.18e-01	3.77e-01	7.25e+00	3.06e+00	1.61e+00	6.94e-01	2.99e-01
R	W1	48	1.05e+01	7.74e+00	3.60e+00	1.44e+00	7.64e-01	3.56e-01	6.89e+00	2.95e+00	1.50e+00	6.44e-01	2.70e-01
R	W1	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
R	W1	240	4.35e+00	3.18e+00	1.42e+00	6.61e-01	2.95e-01	1.35e-01	2.61e+00	1.21e+00	4.38e-01	1.43e-01	0.00e+00
R	W1	240	4.39e+00	3.23e+00	1.43e+00	6.74e-01	3.04e-01	1.48e-01	2.64e+00	1.25e+00	4.63e-01	1.55e-01	0.00e+00
R	W1	240	1.14e+01	8.65e+00	3.73e+00	1.72e+00	7.87e-01	3.62e-01	7.05e+00	3.43e+00	1.41e+00	6.06e-01	2.24e-01
R	W1	240	1.05e+01	7.83e+00	3.43e+00	1.60e+00	7.27e-01	3.33e-01	6.51e+00	3.17e+00	1.29e+00	5.56e-01	2.06e-01
R	W1	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
R	W1	720	4.40e+00	3.19e+00	1.46e+00	6.53e-01	3.09e-01	1.43e-01	2.85e+00	1.17e+00	4.80e-01	1.54e-01	0.00e+00
R	W1	720	4.34e+00	3.19e+00	1.45e+00	6.78e-01	3.05e-01	1.63e-01	2.83e+00	1.20e+00	4.98e-01	1.76e-01	0.00e+00
R	W1	720	1.14e+01	8.40e+00	3.87e+00	1.68e+00	7.72e-01	3.62e-01	7.65e+00	3.21e+00	1.42e+00	6.01e-01	2.10e-01
R	W1	720	1.06e+01	7.73e+00	3.56e+00	1.55e+00	7.51e-01	3.43e-01	7.01e+00	2.94e+00	1.29e+00	5.02e-01	1.31e-01
R	W1	720	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00

Table E.5 – continued from previous page

MC	S	t_{Ads}	C_{CTRL}	C_A	C_{D1}	C_{D2}	C_{D3}	C_{D4}	q_A	q_{D1}	q_{D2}	q_{D3}	q_{D4}
R	W2	2	4.42e+00	3.19e+00	1.43e+00	6.78e-01	3.18e-01	1.52e-01	2.87e+00	1.37e+00	6.20e-01	2.93e-01	1.34e-01
R	W2	2	4.41e+00	3.23e+00	1.46e+00	6.80e-01	3.19e-01	1.56e-01	2.92e+00	1.38e+00	6.26e-01	3.00e-01	1.32e-01
R	W2	2	1.16e+01	8.55e+00	3.80e+00	1.78e+00	8.34e-01	4.02e-01	7.58e+00	3.56e+00	1.58e+00	7.27e-01	2.90e-01
R	W2	2	1.07e+01	7.79e+00	3.59e+00	1.68e+00	7.85e-01	3.78e-01	7.13e+00	3.39e+00	1.52e+00	7.18e-01	3.10e-01
R	W2	2	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
R	W2	48	4.41e+00	3.14e+00	1.46e+00	6.96e-01	3.28e-01	1.51e-01	2.92e+00	1.32e+00	6.10e-01	2.37e-01	7.78e-02
R	W2	48	4.44e+00	3.22e+00	1.47e+00	6.97e-01	3.29e-01	1.50e-01	2.94e+00	1.29e+00	5.94e-01	2.21e-01	6.54e-02
R	W2	48	1.15e+01	8.34e+00	3.87e+00	1.80e+00	8.38e-01	3.90e-01	7.86e+00	3.51e+00	1.69e+00	7.40e-01	3.33e-01
R	W2	48	1.07e+01	7.68e+00	3.63e+00	1.66e+00	7.82e-01	3.73e-01	7.36e+00	3.27e+00	1.60e+00	7.14e-01	3.22e-01
R	W2	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
R	W2	240	4.40e+00	3.29e+00	1.48e+00	6.76e-01	3.05e-01	1.61e-01	3.22e+00	1.73e+00	1.00e+00	6.98e-01	5.26e-01
R	W2	240	4.44e+00	3.29e+00	1.48e+00	6.63e-01	3.06e-01	1.49e-01	2.99e+00	1.48e+00	7.55e-01	4.52e-01	2.90e-01
R	W2	240	1.11e+01	8.63e+00	3.78e+00	1.75e+00	7.88e-01	3.82e-01	7.48e+00	3.60e+00	1.71e+00	9.15e-01	5.14e-01
R	W2	240	1.06e+01	7.82e+00	3.53e+00	1.63e+00	7.46e-01	3.59e-01	7.25e+00	3.65e+00	1.86e+00	1.12e+00	7.31e-01
R	W2	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
R	W2	720	4.42e+00	3.34e+00	1.59e+00	7.36e-01	3.51e-01	1.68e-01	2.94e+00	1.29e+00	5.64e-01	1.80e-01	0.00e+00
R	W2	720	4.40e+00	3.21e+00	1.45e+00	6.86e-01	3.37e-01	1.62e-01	2.81e+00	1.24e+00	5.48e-01	1.76e-01	0.00e+00
R	W2	720	1.16e+01	8.26e+00	3.76e+00	1.72e+00	8.23e-01	4.08e-01	7.30e+00	3.22e+00	1.49e+00	5.82e-01	1.38e-01
R	W2	720	1.07e+01	7.84e+00	3.57e+00	1.63e+00	7.75e-01	3.82e-01	6.98e+00	3.06e+00	1.42e+00	5.60e-01	1.48e-01
R	W2	720	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
R	Z	2	4.82e+00	1.21e+00	NA	NA	6.33e-01	NA	NA	NA	NA	NA	0.00e+00
R	Z	2	4.88e+00	1.19e+00	8.72e-01	5.53e-01	NA	5.26e-01	NA	NA	NA	4.15e+00	3.37e+00
R	Z	2	1.30e+01	3.05e+00	1.89e+00	1.83e+00	1.56e+00	1.23e+00	2.07e+01	1.74e+01	1.42e+01	1.14e+01	9.36e+00
R	Z	2	1.18e+01	2.69e+00	1.77e+00	1.38e+00	9.81e-01	1.12e+00	1.74e+01	1.44e+01	1.21e+01	1.03e+01	8.37e+00
R	Z	2	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
R	Z	48	4.25e+00	9.25e-01	8.09e-01	6.52e-01	5.17e-01	4.64e-01	8.37e+00	6.98e+00	5.83e+00	4.93e+00	4.11e+00
R	Z	48	4.23e+00	1.07e+00	8.93e-01	7.28e-01	5.23e-01	4.65e-01	8.88e+00	7.40e+00	6.11e+00	5.19e+00	4.39e+00
R	Z	48	1.21e+01	2.33e+00	2.12e+00	1.75e+00	1.30e+00	1.19e+00	2.14e+01	1.78e+01	1.48e+01	1.24e+01	1.04e+01
R	Z	48	1.15e+01	2.34e+00	1.93e+00	1.66e+00	1.25e+00	1.08e+00	2.00e+01	1.66e+01	1.38e+01	1.16e+01	9.67e+00
R	Z	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
R	Z	240	4.24e+00	6.95e-01	5.85e-01	4.98e-01	4.10e-01	3.63e-01	7.24e+00	6.43e+00	5.55e+00	4.84e+00	4.20e+00
R	Z	240	4.23e+00	6.11e-01	5.36e-01	4.29e-01	3.27e-01	3.20e-01	6.98e+00	6.06e+00	5.33e+00	4.75e+00	4.18e+00
R	Z	240	1.21e+01	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
R	Z	240	1.13e+01	1.84e+00	1.58e+00	1.36e+00	7.99e-01	9.50e-01	1.79e+01	1.53e+01	1.29e+01	1.15e+01	9.87e+00
R	Z	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
R	Z	720	4.23e+00	6.73e-01	4.43e-01	5.79e-01	2.14e-01	1.96e-01	6.31e+00	5.51e+00	4.50e+00	4.14e+00	3.79e+00
R	Z	720	4.23e+00	6.24e-01	4.21e-01	3.51e-01	1.93e-01	1.89e-01	6.20e+00	5.47e+00	4.86e+00	4.53e+00	4.20e+00
R	Z	720	1.21e+01	1.83e+00	1.59e+00	1.27e+00	8.89e-01	6.75e-01	1.91e+01	1.64e+01	1.41e+01	1.27e+01	1.15e+01
R	Z	720	1.13e+01	1.72e+00	1.47e+00	1.23e+00	8.20e-01	6.07e-01	1.73e+01	1.48e+01	1.26e+01	1.11e+01	1.00e+01
R	Z	720	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00

Table E.5 – continued from previous page

MC	S	t_{Ads}	C_{CTRL}	C_A	C_{D1}	C_{D2}	C_{D3}	C_{D4}	q_A	q_{D1}	q_{D2}	q_{D3}	q_{D4}
T	AM	2	3.49e+00	1.02e+00	4.21e-01	3.04e-01	2.34e-01	1.58e-01	2.46e+00	1.99e+00	1.67e+00	1.42e+00	1.25e+00
T	AM	2	3.53e+00	9.27e-01	3.91e-01	2.85e-01	2.21e-01	1.57e-01	2.65e+00	2.22e+00	1.93e+00	1.69e+00	1.52e+00
T	AM	2	9.32e+00	3.14e+00	1.43e+00	9.60e-01	7.19e-01	4.97e-01	7.15e+00	5.60e+00	4.60e+00	3.82e+00	3.30e+00
T	AM	2	0.00e+00	0.00e+00	0.00e+00	0.00e+00	NA	0.00e+00	NA	NA	NA	0.00e+00	0.00e+00
T	AM	2	6.17e+00	1.67e+00	7.31e-01	5.30e-01	4.09e-01	2.80e-01	4.58e+00	3.78e+00	3.23e+00	2.78e+00	2.49e+00
T	AM	48	3.54e+00	1.35e-01	1.92e-01	1.31e-01	1.43e-01	5.50e-02	1.05e+00	8.41e-01	7.03e-01	5.53e-01	4.95e-01
T	AM	48	3.58e+00	5.89e-02	1.70e-01	1.21e-01	0.00e+00	5.10e-02	8.24e-01	6.44e-01	5.18e-01	5.18e-01	4.65e-01
T	AM	48	9.50e+00	5.11e-01	7.40e-01	5.05e-01	3.72e-01	2.36e-01	4.08e+00	3.29e+00	2.76e+00	2.37e+00	2.13e+00
T	AM	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	NA	0.00e+00	NA	NA	NA	0.00e+00	0.00e+00
T	AM	48	6.24e+00	3.74e-01	2.48e-01	1.77e-01	NA	8.78e-02	NA	NA	NA	1.24e+00	1.15e+00
T	AM	240	3.77e+00	0.00e+00	0.00e+00	3.88e-02	3.60e-02	0.00e+00	3.64e-01	3.64e-01	3.23e-01	2.86e-01	2.86e-01
T	AM	240	3.76e+00	0.00e+00	0.00e+00	4.58e-02	4.20e-02	3.62e-02	3.99e-01	3.99e-01	3.51e-01	3.08e-01	2.70e-01
T	AM	240	1.02e+01	0.00e+00	0.00e+00	7.02e-02	6.27e-02	5.68e-02	4.50e-01	4.50e-01	3.76e-01	3.12e-01	2.52e-01
T	AM	240	0.00e+00	0.00e+00	0.00e+00	NA	2.84e-02	0.00e+00	NA	NA	2.94e-02	0.00e+00	0.00e+00
T	AM	240	6.24e+00	NA	0.00e+00	2.79e-02	NA	NA	NA	NA	NA	NA	2.07e-01
T	AM	720	3.54e+00	6.65e-02	7.48e-02	0.00e+00	0.00e+00	0.00e+00	8.21e-02	0.00e+00	0.00e+00	0.00e+00	0.00e+00
T	AM	720	3.53e+00	5.99e-02	6.97e-02	0.00e+00	0.00e+00	0.00e+00	7.64e-02	0.00e+00	0.00e+00	0.00e+00	0.00e+00
T	AM	720	9.12e+00	1.54e-01	1.20e-01	0.00e+00	0.00e+00	1.14e-01	2.50e-01	1.21e-01	1.21e-01	1.21e-01	0.00e+00
T	AM	720	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
T	AM	720	6.21e+00	4.83e-02	5.95e-02	NA	NA	0.00e+00	NA	NA	NA	0.00e+00	0.00e+00
T	B	2	3.38e+00	2.85e+00	9.30e-01	NA	NA	NA	NA	NA	NA	NA	0.00e+00
T	B	2	3.55e+00	2.78e+00	8.90e-01	NA	NA	NA	NA	NA	NA	NA	0.00e+00
T	B	2	8.76e+00	6.87e+00	2.49e+00	NA	NA	NA	NA	NA	NA	NA	0.00e+00
T	B	2	0.00e+00	0.00e+00	0.00e+00	NA	NA	NA	NA	NA	NA	NA	0.00e+00
T	B	2	6.54e+00	4.23e+00	1.66e+00	NA	NA	NA	NA	NA	NA	NA	0.00e+00
T	B	48	3.46e+00	3.59e+00	9.76e-01	3.79e-01	1.59e-01	1.05e-01	1.94e+00	9.34e-01	5.35e-01	3.72e-01	2.62e-01
T	B	48	3.58e+00	3.31e+00	1.01e+00	3.84e-01	1.52e-01	1.07e-01	2.09e+00	1.05e+00	6.42e-01	4.87e-01	3.74e-01
T	B	48	8.38e+00	6.39e+00	2.50e+00	1.02e+00	4.45e-01	2.75e-01	5.00e+00	2.38e+00	1.30e+00	8.52e-01	5.57e-01
T	B	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
T	B	48	6.61e+00	3.44e+00	1.70e+00	6.99e-01	3.96e-01	2.28e-01	3.59e+00	1.82e+00	1.11e+00	6.93e-01	4.51e-01
T	B	240	3.88e+00	2.37e+00	8.85e-01	3.47e-01	1.87e-01	8.08e-02	2.15e+00	1.08e+00	6.49e-01	4.49e-01	3.64e-01
T	B	240	3.85e+00	2.35e+00	9.08e-01	3.52e-01	1.68e-01	8.97e-02	2.15e+00	1.09e+00	6.49e-01	4.71e-01	3.76e-01
T	B	240	8.90e+00	5.80e+00	2.18e+00	8.74e-01	4.62e-01	2.12e-01	5.29e+00	2.70e+00	1.61e+00	1.11e+00	8.84e-01
T	B	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
T	B	240	6.34e+00	3.70e+00	1.43e+00	6.88e-01	NA	1.33e-01	NA	NA	NA	1.44e-01	0.00e+00
T	B	720	3.90e+00	2.13e+00	9.36e-01	4.43e-01	1.85e-01	1.12e-01	2.16e+00	1.18e+00	7.05e-01	5.15e-01	3.90e-01
T	B	720	3.91e+00	2.26e+00	9.79e-01	4.37e-01	1.55e-01	9.49e-02	2.04e+00	1.06e+00	5.81e-01	4.22e-01	3.18e-01
T	B	720	1.07e+01	7.41e+00	2.73e+00	1.10e+00	4.13e-01	1.83e-01	5.01e+00	2.17e+00	9.93e-01	5.57e-01	3.57e-01
T	B	720	0.00e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
T	B	720	6.85e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00

Table E.5 – continued from previous page

MC	S	t_{Ads}	C_{CTRL}	C_A	C_{D1}	C_{D2}	C_{D3}	C_{D4}	q_A	q_{D1}	q_{D2}	q_{D3}	q_{D4}
T	BA	2	3.85e+00	2.72e+00	9.43e-01	4.06e-01	2.18e-01	1.55e-01	2.22e+00	1.25e+00	8.13e-01	5.84e-01	4.29e-01
T	BA	2	3.89e+00	2.69e+00	9.35e-01	4.00e-01	2.12e-01	1.48e-01	2.17e+00	1.22e+00	7.88e-01	5.65e-01	4.21e-01
T	BA	2	1.04e+01	7.41e+00	2.51e+00	1.04e+00	5.29e-01	3.47e-01	5.40e+00	2.83e+00	1.72e+00	1.16e+00	8.03e-01
T	BA	2	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
T	BA	2	6.83e+00	4.54e+00	1.62e+00	7.26e-01	3.69e-01	2.62e-01	3.82e+00	2.13e+00	1.35e+00	9.63e-01	6.97e-01
T	BA	48	3.94e+00	2.42e+00	1.03e+00	5.01e-01	2.56e-01	1.82e-01	2.55e+00	1.50e+00	9.77e-01	7.05e-01	5.14e-01
T	BA	48	3.95e+00	2.31e+00	1.03e+00	4.93e-01	2.55e-01	1.77e-01	2.35e+00	1.28e+00	7.66e-01	4.98e-01	3.13e-01
T	BA	48	1.07e+01	6.80e+00	2.74e+00	1.25e+00	6.10e-01	4.18e-01	6.47e+00	3.64e+00	2.32e+00	1.67e+00	1.23e+00
T	BA	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
T	BA	48	6.91e+00	4.02e+00	1.75e+00	8.48e-01	4.40e-01	3.10e-01	4.44e+00	2.62e+00	1.74e+00	1.27e+00	9.47e-01
T	BA	240	4.17e+00	2.03e+00	9.16e-01	NA	2.77e-01	1.51e-01	NA	NA	1.28e+00	1.00e+00	8.38e-01
T	BA	240	4.18e+00	1.95e+00	9.13e-01	5.16e-01	2.83e-01	1.66e-01	2.85e+00	1.91e+00	1.36e+00	1.07e+00	8.93e-01
T	BA	240	1.17e+01	6.58e+00	2.76e+00	1.39e+00	7.14e-01	3.85e-01	7.66e+00	4.79e+00	3.31e+00	2.58e+00	2.16e+00
T	BA	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
T	BA	240	6.92e+00	3.15e+00	1.50e+00	8.62e-01	4.85e-01	2.86e-01	4.73e+00	3.18e+00	2.26e+00	1.75e+00	1.45e+00
T	BA	720	3.77e+00	2.18e+00	9.25e-01	4.66e-01	2.30e-01	1.32e-01	2.33e+00	1.36e+00	8.63e-01	6.12e-01	4.73e-01
T	BA	720	3.78e+00	2.23e+00	9.34e-01	4.65e-01	2.27e-01	1.32e-01	2.35e+00	1.37e+00	8.72e-01	6.24e-01	4.84e-01
T	BA	720	9.69e+00	6.23e+00	2.50e+00	1.23e+00	5.65e-01	3.08e-01	5.92e+00	3.23e+00	2.01e+00	1.40e+00	1.07e+00
T	BA	720	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
T	BA	720	6.70e+00	3.74e+00	1.65e+00	7.95e-01	4.14e-01	2.39e-01	4.07e+00	2.28e+00	1.45e+00	1.01e+00	7.51e-01
T	BOX	2	3.08e+00	1.08e+00	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
T	BOX	2	3.37e+00	1.01e+00	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
T	BOX	2	8.37e+00	2.90e+00	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
T	BOX	2	0.00e+00	0.00e+00	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
T	BOX	2	6.04e+00	1.75e+00	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
T	BOX	48	3.21e+00	NA	4.80e-01	3.30e-01	2.57e-01	2.04e-01	3.09e+00	2.58e+00	2.22e+00	1.95e+00	1.73e+00
T	BOX	48	3.27e+00	9.59e-01	4.76e-01	3.38e-01	2.55e-01	2.13e-01	3.04e+00	2.53e+00	2.17e+00	1.90e+00	1.67e+00
T	BOX	48	7.87e+00	2.03e+00	1.31e+00	9.39e-01	7.15e-01	4.14e-01	7.29e+00	5.94e+00	4.95e+00	4.19e+00	3.75e+00
T	BOX	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
T	BOX	48	5.99e+00	NA	8.30e-01	5.95e-01	4.77e-01	NA	NA	NA	NA	NA	2.15e+00
T	BOX	240	3.52e+00	6.31e-01	4.54e-01	0.00e+00	2.58e-01	1.74e-01	2.69e+00	2.12e+00	2.12e+00	1.85e+00	1.66e+00
T	BOX	240	3.50e+00	6.65e-01	4.53e-01	5.51e-01	2.45e-01	1.76e-01	3.47e+00	2.90e+00	2.17e+00	1.91e+00	1.72e+00
T	BOX	240	8.08e+00	1.74e+00	1.18e+00	8.46e-01	6.15e-01	4.68e-01	7.43e+00	5.97e+00	4.83e+00	4.19e+00	3.69e+00
T	BOX	240	0.00e+00	0.00e+00	0.00e+00	NA	0.00e+00	0.00e+00	NA	NA	0.00e+00	0.00e+00	0.00e+00
T	BOX	240	5.70e+00	8.97e-01	6.34e-01	NA	3.48e-01	2.73e-01	NA	NA	3.04e+00	2.68e+00	2.39e+00
T	BOX	720	3.54e+00	5.17e-01	4.15e-01	3.25e-01	2.16e-01	1.82e-01	2.53e+00	2.10e+00	1.75e+00	1.53e+00	1.33e+00
T	BOX	720	3.53e+00	5.20e-01	4.04e-01	3.35e-01	2.21e-01	1.82e-01	2.49e+00	2.07e+00	1.71e+00	1.48e+00	1.28e+00
T	BOX	720	9.61e+00	1.65e+00	1.24e+00	9.51e-01	7.40e-01	5.29e-01	7.43e+00	6.15e+00	5.11e+00	4.35e+00	3.76e+00
T	BOX	720	0.00e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
T	BOX	720	6.22e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00

Table E.5 – continued from previous page

MC	S	t_{Ads}	C_{CTRL}	C_A	C_{D1}	C_{D2}	C_{D3}	C_{D4}	q_A	q_{D1}	q_{D2}	q_{D3}	q_{D4}
T	BT	2	3.89e+00	2.87e+00	9.34e-01	3.70e-01	1.82e-01	1.29e-01	1.96e+00	9.69e-01	5.75e-01	3.82e-01	2.48e-01
T	BT	2	3.88e+00	2.85e+00	9.30e-01	3.77e-01	1.88e-01	1.30e-01	2.06e+00	1.08e+00	6.83e-01	4.83e-01	3.47e-01
T	BT	2	1.04e+01	7.81e+00	2.47e+00	9.37e-01	4.33e-01	2.84e-01	4.94e+00	2.38e+00	1.39e+00	9.30e-01	6.38e-01
T	BT	2	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
T	BT	2	6.80e+00	4.86e+00	1.62e+00	6.66e-01	3.27e-01	2.25e-01	3.59e+00	1.86e+00	1.15e+00	8.06e-01	5.70e-01
T	BT	48	3.92e+00	2.55e+00	9.90e-01	4.49e-01	2.19e-01	1.61e-01	2.30e+00	1.29e+00	8.22e-01	5.93e-01	4.21e-01
T	BT	48	3.92e+00	2.71e+00	9.90e-01	4.51e-01	2.11e-01	1.59e-01	2.30e+00	1.32e+00	8.50e-01	6.31e-01	4.67e-01
T	BT	48	1.05e+01	7.56e+00	2.64e+00	1.14e+00	5.14e-01	3.45e-01	5.46e+00	2.81e+00	1.61e+00	1.07e+00	7.13e-01
T	BT	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
T	BT	48	6.95e+00	4.40e+00	1.72e+00	7.77e-01	3.66e-01	NA	NA	NA	NA	NA	6.18e-01
T	BT	240	4.19e+00	2.24e+00	9.08e-01	4.85e-01	2.44e-01	1.23e-01	2.33e+00	1.39e+00	8.78e-01	6.24e-01	4.97e-01
T	BT	240	4.20e+00	2.27e+00	9.07e-01	4.81e-01	2.46e-01	1.25e-01	2.34e+00	1.40e+00	8.90e-01	6.49e-01	5.17e-01
T	BT	240	1.16e+01	7.36e+00	2.58e+00	1.22e+00	5.66e-01	2.79e-01	5.98e+00	3.33e+00	2.05e+00	1.48e+00	1.18e+00
T	BT	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
T	BT	240	6.95e+00	3.68e+00	1.56e+00	8.36e-01	4.22e-01	2.22e-01	4.12e+00	2.53e+00	1.66e+00	1.23e+00	1.00e+00
T	BT	720	3.76e+00	2.34e+00	8.92e-01	4.16e-01	2.00e-01	1.05e-01	2.11e+00	1.17e+00	7.60e-01	5.35e-01	4.26e-01
T	BT	720	3.75e+00	2.41e+00	9.05e-01	4.29e-01	2.01e-01	NA	NA	NA	NA	NA	2.27e-01
T	BT	720	9.77e+00	6.63e+00	2.42e+00	1.05e+00	4.82e-01	2.41e-01	4.92e+00	2.56e+00	1.47e+00	9.48e-01	7.02e-01
T	BT	720	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
T	BT	720	6.77e+00	4.17e+00	1.71e+00	7.68e-01	3.73e-01	1.99e-01	3.57e+00	1.81e+00	1.05e+00	6.46e-01	4.40e-01
T	BU	2	3.27e+00	5.98e-01	2.54e-01	NA	NA	NA	NA	NA	NA	NA	0.00e+00
T	BU	2	3.53e+00	5.74e-01	2.08e-01	NA	NA	NA	NA	NA	NA	NA	0.00e+00
T	BU	2	8.90e+00	1.74e+00	7.21e-01	NA	NA	NA	NA	NA	NA	NA	0.00e+00
T	BU	2	0.00e+00	0.00e+00	0.00e+00	NA	NA	NA	NA	NA	NA	NA	0.00e+00
T	BU	2	6.38e+00	9.19e-01	4.00e-01	NA	NA	NA	NA	NA	NA	NA	0.00e+00
T	BU	48	3.54e+00	2.89e-01	1.49e-01	9.39e-02	8.56e-02	1.06e-01	3.42e+00	3.25e+00	3.15e+00	3.06e+00	2.95e+00
T	BU	48	3.56e+00	2.62e-01	1.19e-01	8.20e-02	7.21e-02	1.02e-01	3.39e+00	3.26e+00	3.18e+00	3.10e+00	2.99e+00
T	BU	48	8.49e+00	7.89e-01	4.41e-01	3.44e-01	3.19e-01	3.34e-01	8.62e+00	8.13e+00	7.77e+00	7.44e+00	7.07e+00
T	BU	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
T	BU	48	6.39e+00	4.45e-01	2.48e-01	2.01e-01	1.89e-01	2.01e-01	5.87e+00	5.60e+00	5.39e+00	5.19e+00	4.98e+00
T	BU	240	3.70e+00	1.60e-01	1.32e-01	1.19e-01	9.84e-02	8.50e-02	3.33e+00	3.16e+00	3.01e+00	2.90e+00	2.81e+00
T	BU	240	3.71e+00	1.66e-01	1.34e-01	1.19e-01	1.03e-01	8.91e-02	3.42e+00	3.28e+00	3.12e+00	3.01e+00	2.92e+00
T	BU	240	8.55e+00	5.07e-01	4.03e-01	3.70e-01	0.00e+00	2.68e-01	7.70e+00	7.21e+00	6.83e+00	6.83e+00	6.55e+00
T	BU	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
T	BU	240	6.00e+00	2.03e-01	NA	1.50e-01	1.37e-01	9.76e-02	NA	5.09e+00	4.94e+00	4.80e+00	4.70e+00
T	BU	720	3.73e+00	1.19e-01	1.03e-01	NA	7.14e-02	7.21e-02	NA	NA	2.72e+00	2.64e+00	2.56e+00
T	BU	720	3.69e+00	1.03e-01	9.94e-02	NA	6.07e-02	6.31e-02	NA	NA	2.55e+00	2.49e+00	2.42e+00
T	BU	720	1.01e+01	3.73e-01	3.07e-01	NA	2.86e-01	2.59e-01	NA	NA	8.16e+00	7.87e+00	7.58e+00
T	BU	720	0.00e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
T	BU	720	6.45e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00

Table E.5 – continued from previous page

MC	S	t_{Ads}	C_{CTRL}	C_A	C_{D1}	C_{D2}	C_{D3}	C_{D4}	q_A	q_{D1}	q_{D2}	q_{D3}	q_{D4}
T	CM	2	2.94e+00	1.33e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA
T	CM	2	2.93e+00	1.37e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA
T	CM	2	7.01e+00	3.42e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA
T	CM	2	0.00e+00	0.00e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA
T	CM	2	5.57e+00	2.33e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA
T	CM	48	3.05e+00	9.90e-01	5.13e-01	3.26e-01	2.32e-01	1.69e-01	NA	NA	NA	NA	NA
T	CM	48	3.09e+00	9.44e-01	5.10e-01	3.23e-01	2.25e-01	1.63e-01	NA	NA	NA	NA	NA
T	CM	48	7.30e+00	2.59e+00	1.35e+00	9.16e-01	6.55e-01	5.15e-01	NA	NA	NA	NA	NA
T	CM	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	NA	NA	NA	NA	NA
T	CM	48	5.75e+00	1.15e+00	8.05e-01	5.44e-01	4.26e-01	3.81e-01	NA	NA	NA	NA	NA
T	CM	240	3.37e+00	7.69e-01	4.71e-01	3.38e-01	2.44e-01	1.68e-01	NA	NA	NA	NA	NA
T	CM	240	3.41e+00	7.69e-01	4.75e-01	3.44e-01	2.45e-01	1.67e-01	NA	NA	NA	NA	NA
T	CM	240	7.90e+00	2.13e+00	1.28e+00	9.14e-01	6.32e-01	4.31e-01	NA	NA	NA	NA	NA
T	CM	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	NA	NA	NA	NA	NA
T	CM	240	5.49e+00	1.05e+00	6.56e-01	4.85e-01	3.48e-01	2.52e-01	NA	NA	NA	NA	NA
T	CM	720	3.40e+00	4.70e-01	3.47e-01	1.97e-01	1.23e-01	1.28e-01	NA	NA	NA	NA	NA
T	CM	720	3.37e+00	4.91e-01	3.62e-01	1.98e-01	1.37e-01	1.40e-01	NA	NA	NA	NA	NA
T	CM	720	9.27e+00	1.63e+00	1.10e+00	6.05e-01	4.92e-01	3.97e-01	NA	NA	NA	NA	NA
T	CM	720	0.00e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
T	CM	720	5.95e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
T	ELL	2	3.56e+00	8.77e-01	3.78e-01	2.82e-01	2.22e-01	1.77e-01	2.67e+00	2.26e+00	1.97e+00	1.72e+00	1.54e+00
T	ELL	2	3.56e+00	8.45e-01	3.58e-01	2.64e-01	2.18e-01	1.71e-01	2.58e+00	2.20e+00	1.93e+00	1.69e+00	1.51e+00
T	ELL	2	9.39e+00	2.84e+00	1.32e+00	9.29e-01	7.42e-01	5.52e-01	7.95e+00	6.52e+00	5.56e+00	4.75e+00	4.17e+00
T	ELL	2	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
T	ELL	2	6.23e+00	1.28e+00	5.76e-01	4.70e-01	3.62e-01	2.99e-01	4.93e+00	4.30e+00	3.82e+00	3.41e+00	3.10e+00
T	ELL	48	3.58e+00	2.19e-01	1.34e-01	1.07e-01	8.88e-02	6.84e-02	1.24e+00	1.10e+00	9.88e-01	8.88e-01	8.17e-01
T	ELL	48	3.59e+00	1.66e-01	1.31e-01	9.97e-02	8.23e-02	6.01e-02	1.19e+00	1.05e+00	9.53e-01	8.60e-01	7.98e-01
T	ELL	48	9.51e+00	1.30e+00	9.31e-01	6.18e-01	5.38e-01	4.07e-01	6.27e+00	5.29e+00	4.66e+00	4.06e+00	3.63e+00
T	ELL	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
T	ELL	48	6.33e+00	2.34e-01	1.82e-01	1.50e-01	1.22e-01	9.49e-02	2.20e+00	2.01e+00	1.85e+00	1.72e+00	1.62e+00
T	ELL	240	3.90e+00	0.00e+00	0.00e+00	1.71e-02	0.00e+00	0.00e+00	7.12e-01	7.12e-01	6.93e-01	6.93e-01	6.93e-01
T	ELL	240	3.86e+00	0.00e+00	0.00e+00	1.93e-02	0.00e+00	0.00e+00	2.43e-01	2.43e-01	2.22e-01	2.22e-01	2.22e-01
T	ELL	240	1.07e+01	0.00e+00	0.00e+00	2.81e-02	2.63e-02	0.00e+00	1.08e+00	1.08e+00	1.05e+00	1.03e+00	1.03e+00
T	ELL	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	2.07e-01	2.07e-01	2.07e-01	2.07e-01	2.07e-01
T	ELL	240	6.36e+00	NA	NA	1.44e-02	NA	NA	NA	NA	NA	NA	0.00e+00
T	ELL	720	3.50e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
T	ELL	720	3.47e+00	2.68e-02	0.00e+00	0.00e+00	0.00e+00	0.00e+00	5.04e-01	5.04e-01	5.04e-01	5.04e-01	5.04e-01
T	ELL	720	8.82e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
T	ELL	720	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
T	ELL	720	6.25e+00	NA	NA	NA	NA	0.00e+00	NA	NA	NA	0.00e+00	0.00e+00

Table E.5 – continued from previous page

MC	S	t_{Ads}	C_{CTRL}	C_A	C_{D1}	C_{D2}	C_{D3}	C_{D4}	q_A	q_{D1}	q_{D2}	q_{D3}	q_{D4}
T	FT	2	3.30e+00	2.72e+00	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
T	FT	2	3.61e+00	2.59e+00	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
T	FT	2	8.46e+00	6.70e+00	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
T	FT	2	0.00e+00	0.00e+00	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
T	FT	2	6.27e+00	4.69e+00	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
T	FT	48	3.46e+00	2.50e+00	1.16e+00	5.01e-01	2.41e-01	1.02e-01	2.38e+00	1.16e+00	6.32e-01	3.84e-01	2.75e-01
T	FT	48	3.46e+00	2.49e+00	1.14e+00	5.11e-01	2.36e-01	1.03e-01	2.35e+00	1.16e+00	6.12e-01	3.67e-01	2.53e-01
T	FT	48	8.24e+00	6.07e+00	2.79e+00	1.26e+00	6.10e-01	2.76e-01	5.85e+00	2.96e+00	1.62e+00	9.96e-01	6.95e-01
T	FT	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
T	FT	48	6.11e+00	4.24e+00	1.90e+00	8.59e-01	4.63e-01	2.81e-01	3.96e+00	2.05e+00	1.14e+00	6.63e-01	3.52e-01
T	FT	240	3.54e+00	2.41e+00	1.01e+00	4.02e-01	2.14e-01	1.05e-01	2.46e+00	1.23e+00	6.84e-01	4.58e-01	3.47e-01
T	FT	240	3.54e+00	2.35e+00	1.00e+00	4.20e-01	2.26e-01	1.04e-01	2.51e+00	1.30e+00	7.31e-01	4.88e-01	3.79e-01
T	FT	240	8.13e+00	5.75e+00	2.46e+00	1.02e+00	5.45e-01	2.55e-01	5.85e+00	2.94e+00	1.54e+00	9.62e-01	6.95e-01
T	FT	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
T	FT	240	5.82e+00	3.84e+00	1.59e+00	6.25e-01	3.31e-01	1.46e-01	3.52e+00	1.60e+00	7.75e-01	4.25e-01	2.70e-01
T	FT	720	3.59e+00	2.29e+00	1.04e+00	5.32e-01	2.49e-01	1.10e-01	2.21e+00	1.13e+00	5.50e-01	2.78e-01	1.61e-01
T	FT	720	3.65e+00	2.29e+00	1.06e+00	4.41e-01	2.61e-01	1.30e-01	2.13e+00	1.04e+00	5.67e-01	2.82e-01	1.45e-01
T	FT	720	9.87e+00	6.78e+00	2.88e+00	1.16e+00	6.83e-01	3.30e-01	5.97e+00	2.95e+00	1.70e+00	9.57e-01	6.08e-01
T	FT	720	0.00e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
T	FT	720	6.24e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
T	GAS	2	3.13e+00	6.44e-02	2.02e-02	NA	NA	NA	NA	NA	NA	NA	0.00e+00
T	GAS	2	3.24e+00	6.91e-02	1.60e-02	NA	NA	NA	NA	NA	NA	NA	0.00e+00
T	GAS	2	7.58e+00	1.01e-01	4.75e-02	NA	NA	NA	NA	NA	NA	NA	0.00e+00
T	GAS	2	0.00e+00	0.00e+00	0.00e+00	NA	NA	NA	NA	NA	NA	NA	0.00e+00
T	GAS	2	5.96e+00	1.19e-01	4.08e-02	NA	NA	NA	NA	NA	NA	NA	0.00e+00
T	GAS	48	3.22e+00	5.03e-02	0.00e+00	0.00e+00	0.00e+00	1.65e-02	3.84e+00	3.84e+00	3.84e+00	3.84e+00	3.82e+00
T	GAS	48	3.22e+00	3.97e-02	0.00e+00	0.00e+00	0.00e+00	1.80e-02	3.07e+00	3.07e+00	3.07e+00	3.07e+00	3.05e+00
T	GAS	48	7.54e+00	1.10e-01	4.85e-02	3.67e-02	4.23e-02	3.79e-02	8.03e+00	7.99e+00	7.95e+00	7.90e+00	7.86e+00
T	GAS	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
T	GAS	48	5.91e+00	3.30e-02	NA	NA	NA	NA	NA	NA	NA	NA	5.69e+00
T	GAS	240	3.44e+00	2.15e-02	1.94e-02	1.67e-02	1.50e-02	1.47e-02	3.38e+00	3.36e+00	3.34e+00	3.32e+00	3.31e+00
T	GAS	240	3.47e+00	1.86e-02	1.51e-02	1.40e-02	1.04e-02	1.31e-02	2.71e+00	2.70e+00	2.68e+00	2.67e+00	2.65e+00
T	GAS	240	7.95e+00	5.25e-02	3.95e-02	3.94e-02	3.04e-02	3.63e-02	7.17e+00	7.13e+00	7.08e+00	7.05e+00	7.01e+00
T	GAS	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
T	GAS	240	5.69e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA	4.54e+00
T	GAS	720	3.58e+00	0.00e+00	0.00e+00	2.56e-01	1.42e-02	0.00e+00	3.17e+00	3.17e+00	2.89e+00	2.88e+00	2.88e+00
T	GAS	720	3.58e+00	0.00e+00	0.00e+00	2.70e-01	1.59e-02	0.00e+00	3.03e+00	3.03e+00	2.74e+00	2.72e+00	2.72e+00
T	GAS	720	9.72e+00	3.22e-02	2.44e-02	7.96e-01	3.91e-02	4.58e-02	8.89e+00	8.86e+00	7.99e+00	7.95e+00	7.90e+00
T	GAS	720	0.00e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
T	GAS	720	6.18e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00

Table E.5 – continued from previous page

MC	S	t_{Ads}	C_{CTRL}	C_A	C_{D1}	C_{D2}	C_{D3}	C_{D4}	q_A	q_{D1}	q_{D2}	q_{D3}	q_{D4}
T	GUA	2	3.83e+00	2.28e+00	6.70e-01	3.20e-01	1.22e-01	7.13e-02	1.41e+00	7.10e-01	3.85e-01	2.54e-01	1.82e-01
T	GUA	2	3.85e+00	2.28e+00	6.47e-01	3.38e-01	1.41e-01	8.12e-02	1.46e+00	7.86e-01	4.46e-01	2.95e-01	2.20e-01
T	GUA	2	1.09e+01	6.77e+00	2.25e+00	1.09e+00	4.79e-01	2.63e-01	4.70e+00	2.32e+00	1.21e+00	7.18e-01	4.67e-01
T	GUA	2	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
T	GUA	2	6.50e+00	3.55e+00	1.15e+00	5.87e-01	2.91e-01	1.67e-01	2.70e+00	1.45e+00	8.50e-01	5.40e-01	3.84e-01
T	GUA	48	3.58e+00	6.38e-02	6.21e-02	2.50e-01	1.95e-02	1.10e-02	4.79e-01	4.18e-01	1.54e-01	1.33e-01	1.21e-01
T	GUA	48	3.58e+00	6.85e-01	4.83e-01	NA	1.20e-01	7.34e-02	NA	NA	3.93e-01	2.67e-01	1.89e-01
T	GUA	48	1.06e+01	1.60e+00	1.89e+00	9.53e-01	4.99e-01	2.85e-01	4.33e+00	2.34e+00	1.33e+00	8.00e-01	5.01e-01
T	GUA	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
T	GUA	48	6.68e+00	1.59e+00	9.19e-01	5.08e-01	2.77e-01	1.70e-01	2.38e+00	1.42e+00	8.79e-01	5.83e-01	4.04e-01
T	GUA	240	3.53e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
T	GUA	240	3.56e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
T	GUA	240	1.04e+01	5.73e-01	1.76e-01	9.02e-02	5.02e-02	3.07e-02	4.78e-01	2.95e-01	2.02e-01	1.49e-01	1.16e-01
T	GUA	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
T	GUA	240	6.67e+00	2.93e-02	2.16e-02	1.45e-02	1.25e-02	NA	NA	NA	NA	NA	2.38e-02
T	GUA	720	3.57e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
T	GUA	720	3.57e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
T	GUA	720	1.05e+01	0.00e+00	0.00e+00	0.00e+00	5.00e-02	0.00e+00	5.18e-02	5.18e-02	5.18e-02	0.00e+00	0.00e+00
T	GUA	720	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
T	GUA	720	6.68e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
T	H	2	4.16e+00	1.48e+00	8.38e-01	5.49e-01	4.10e-01	2.68e-01	3.10e+00	2.22e+00	1.65e+00	1.22e+00	9.36e-01
T	H	2	4.17e+00	1.50e+00	8.40e-01	5.54e-01	4.13e-01	2.77e-01	3.12e+00	2.23e+00	1.65e+00	1.22e+00	9.28e-01
T	H	2	1.19e+01	4.22e+00	2.38e+00	1.52e+00	1.11e+00	7.60e-01	8.56e+00	5.99e+00	4.38e+00	3.20e+00	2.42e+00
T	H	2	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
T	H	2	7.12e+00	1.69e-01	1.30e+00	8.81e-01	6.83e-01	4.68e-01	5.25e+00	3.87e+00	2.95e+00	2.24e+00	1.76e+00
T	H	48	3.86e+00	9.45e-01	6.71e-01	5.00e-01	3.24e-01	2.73e-01	3.03e+00	2.33e+00	1.81e+00	1.47e+00	1.19e+00
T	H	48	3.85e+00	9.89e-01	7.18e-01	4.99e-01	3.31e-01	2.64e-01	3.05e+00	2.29e+00	1.76e+00	1.42e+00	1.15e+00
T	H	48	1.14e+01	2.94e+00	2.08e+00	1.46e+00	1.01e+00	7.75e-01	8.58e+00	6.36e+00	4.82e+00	3.76e+00	2.96e+00
T	H	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
T	H	48	7.19e+00	1.69e+00	1.24e+00	9.33e-01	NA	4.84e-01	NA	NA	NA	2.64e+00	2.15e+00
T	H	240	3.83e+00	7.00e-01	5.68e-01	4.24e-01	3.27e-01	2.78e-01	2.82e+00	2.24e+00	1.80e+00	1.46e+00	1.17e+00
T	H	240	3.84e+00	7.46e-01	5.91e-01	4.34e-01	3.20e-01	2.72e-01	2.84e+00	2.23e+00	1.78e+00	1.45e+00	1.16e+00
T	H	240	1.13e+01	2.41e+00	1.88e+00	1.34e+00	1.00e+00	8.35e-01	8.56e+00	6.64e+00	5.24e+00	4.20e+00	3.33e+00
T	H	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
T	H	240	7.14e+00	1.18e+00	1.05e+00	7.85e-01	5.84e-01	5.05e-01	5.94e+00	4.85e+00	4.02e+00	3.41e+00	2.88e+00
T	H	720	3.84e+00	6.76e-01	4.79e-01	1.48e-01	8.36e-02	1.24e-01	2.63e+00	2.13e+00	1.97e+00	1.89e+00	1.76e+00
T	H	720	3.85e+00	7.49e-01	5.23e-01	1.56e-01	9.33e-02	1.19e-01	2.47e+00	1.93e+00	1.77e+00	1.67e+00	1.55e+00
T	H	720	1.14e+01	2.45e+00	1.60e+00	5.24e-01	4.45e-01	3.60e-01	7.64e+00	5.94e+00	5.39e+00	4.93e+00	4.56e+00
T	H	720	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
T	H	720	7.18e+00	1.46e+00	1.01e+00	3.26e-01	2.45e-01	2.45e-01	4.84e+00	3.77e+00	3.43e+00	3.18e+00	2.93e+00

Table E.5 – continued from previous page

MC	S	t_{Ads}	C_{CTRL}	C_A	C_{D1}	C_{D2}	C_{D3}	C_{D4}	q_A	q_{D1}	q_{D2}	q_{D3}	q_{D4}
T	J	2	3.84e+00	4.54e-01	1.66e-01	1.26e-01	9.40e-02	6.96e-02	6.10e+00	5.79e+00	5.56e+00	5.40e+00	5.28e+00
T	J	2	3.83e+00	3.99e-01	1.33e-01	1.05e-01	8.25e-02	5.64e-02	5.46e+00	5.22e+00	5.03e+00	4.89e+00	4.79e+00
T	J	2	1.05e+01	1.62e+00	5.89e-01	4.59e-01	3.65e-01	2.88e-01	1.50e+01	1.39e+01	1.31e+01	1.25e+01	1.20e+01
T	J	2	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
T	J	2	6.48e+00	6.53e-01	2.09e-01	1.99e-01	1.55e-01	1.25e-01	8.35e+00	7.98e+00	7.63e+00	7.36e+00	7.15e+00
T	J	48	3.56e+00	1.39e-01	1.08e-01	9.35e-02	7.16e-02	7.70e-02	5.14e+00	4.94e+00	4.78e+00	4.65e+00	4.52e+00
T	J	48	3.57e+00	1.10e-01	9.87e-02	8.92e-02	6.34e-02	6.78e-02	4.28e+00	4.11e+00	3.95e+00	3.84e+00	3.72e+00
T	J	48	1.05e+01	4.79e-01	3.83e-01	3.65e-01	2.90e-01	2.85e-01	1.47e+01	1.40e+01	1.34e+01	1.29e+01	1.24e+01
T	J	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
T	J	48	6.62e+00	1.98e-01	1.67e-01	1.53e-01	1.29e-01	1.30e-01	9.18e+00	8.88e+00	8.62e+00	8.39e+00	8.16e+00
T	J	240	3.57e+00	0.00e+00	1.88e-02	1.25e-02	1.26e-02	1.33e-02	1.16e+00	1.13e+00	1.11e+00	1.09e+00	1.06e+00
T	J	240	3.57e+00	1.97e-02	2.16e-02	2.09e-02	2.03e-02	2.01e-02	2.07e+00	2.04e+00	2.00e+00	1.96e+00	1.93e+00
T	J	240	1.06e+01	8.66e-02	1.27e-01	1.05e-01	9.54e-02	9.65e-02	8.57e+00	8.36e+00	8.17e+00	8.01e+00	7.85e+00
T	J	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
T	J	240	6.66e+00	2.19e-02	2.29e-02	1.93e-02	2.00e-02	1.64e-02	1.07e+00	1.03e+00	9.96e-01	9.62e-01	9.35e-01
T	J	720	3.58e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	2.24e-01	2.24e-01	2.24e-01	2.24e-01	2.24e-01
T	J	720	3.57e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	1.77e-01	1.77e-01	1.77e-01	1.77e-01	1.77e-01
T	J	720	1.05e+01	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	1.74e+00	1.74e+00	1.74e+00	1.74e+00	1.74e+00
T	J	720	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
T	J	720	6.69e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	1.46e+00	1.46e+00	1.46e+00	1.46e+00	1.46e+00
T	KA	2	4.06e+00	3.52e+00	1.05e+00	3.32e-01	9.55e-02	2.89e-02	2.77e+00	8.95e-01	3.08e-01	1.42e-01	8.98e-02
T	KA	2	4.06e+00	3.56e+00	1.03e+00	3.29e-01	9.68e-02	2.94e-02	2.70e+00	8.63e-01	2.78e-01	1.10e-01	5.75e-02
T	KA	2	1.12e+01	9.94e+00	2.94e+00	9.18e-01	2.77e-01	8.22e-02	7.50e+00	2.34e+00	6.93e-01	2.14e-01	6.57e-02
T	KA	2	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
T	KA	2	6.90e+00	5.79e+00	1.69e+00	5.50e-01	1.68e-01	4.93e-02	4.44e+00	1.42e+00	4.32e-01	1.40e-01	5.21e-02
T	KA	48	3.73e+00	3.19e+00	1.07e+00	3.02e-01	8.96e-02	3.05e-02	2.65e+00	7.44e-01	2.12e-01	5.28e-02	0.00e+00
T	KA	48	3.73e+00	3.45e+00	NA	3.09e-01	8.70e-02	2.97e-02	NA	7.55e-01	2.03e-01	5.19e-02	0.00e+00
T	KA	48	1.10e+01	9.45e+00	3.06e+00	9.61e-01	2.61e-01	8.51e-02	7.13e+00	2.31e+00	6.11e-01	1.49e-01	0.00e+00
T	KA	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
T	KA	48	6.97e+00	6.00e+00	1.84e+00	5.65e-01	1.63e-01	5.30e-02	4.66e+00	1.39e+00	3.83e-01	9.36e-02	0.00e+00
T	KA	240	3.71e+00	3.29e+00	9.93e-01	2.88e-01	8.81e-02	1.59e-01	2.70e+00	9.45e-01	4.31e-01	2.75e-01	0.00e+00
T	KA	240	3.72e+00	3.32e+00	9.99e-01	2.98e-01	9.08e-02	2.91e-02	2.47e+00	7.36e-01	2.09e-01	5.04e-02	0.00e+00
T	KA	240	1.10e+01	9.60e+00	2.97e+00	8.80e-01	2.59e-01	8.26e-02	7.36e+00	2.17e+00	6.01e-01	1.43e-01	0.00e+00
T	KA	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
T	KA	240	7.00e+00	6.27e+00	1.91e+00	5.58e-01	1.67e-01	5.25e-02	4.75e+00	1.38e+00	3.88e-01	9.05e-02	0.00e+00
T	KA	720	3.73e+00	3.20e+00	9.32e-01	1.71e-01	4.34e-02	0.00e+00	2.04e+00	3.73e-01	7.47e-02	0.00e+00	0.00e+00
T	KA	720	3.72e+00	3.31e+00	9.59e-01	1.50e-01	4.40e-02	0.00e+00	2.19e+00	4.79e-01	2.14e-01	1.38e-01	1.38e-01
T	KA	720	1.10e+01	9.44e+00	2.78e+00	5.09e-01	7.85e-02	3.49e-02	6.22e+00	1.21e+00	3.18e-01	1.82e-01	1.21e-01
T	KA	720	0.00e+00	NA	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
T	KA	720	6.98e+00	6.18e+00	NA	5.86e-01	1.22e-01	4.07e-02	NA	1.40e+00	3.75e-01	1.68e-01	9.58e-02

Table E.5 – continued from previous page

MC	S	t_{Ads}	C_{CTRL}	C_A	C_{D1}	C_{D2}	C_{D3}	C_{D4}	q_A	q_{D1}	q_{D2}	q_{D3}	q_{D4}
T	LCL	2	3.03e+00	1.05e+00	3.97e-01	NA	NA	NA	NA	NA	NA	NA	0.00e+00
T	LCL	2	3.22e+00	1.02e+00	4.34e-01	NA	NA	NA	NA	NA	NA	NA	0.00e+00
T	LCL	2	7.81e+00	2.62e+00	1.10e+00	NA	NA	NA	NA	NA	NA	NA	0.00e+00
T	LCL	2	0.00e+00	0.00e+00	0.00e+00	NA	NA	NA	NA	NA	NA	NA	0.00e+00
T	LCL	2	5.77e+00	1.60e+00	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
T	LCL	48	3.18e+00	5.73e-01	2.63e-01	1.85e-01	1.58e-01	1.64e-01	3.03e+00	2.76e+00	2.56e+00	2.39e+00	2.21e+00
T	LCL	48	3.17e+00	5.60e-01	2.50e-01	1.90e-01	1.53e-01	1.68e-01	3.01e+00	2.74e+00	2.55e+00	2.38e+00	2.21e+00
T	LCL	48	7.59e+00	1.58e+00	8.24e-01	6.41e-01	5.42e-01	4.88e-01	7.70e+00	6.84e+00	6.15e+00	5.58e+00	5.06e+00
T	LCL	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
T	LCL	48	5.64e+00	8.56e-01	4.39e-01	3.36e-01	3.24e-01	2.87e-01	5.66e+00	5.22e+00	4.87e+00	4.52e+00	4.22e+00
T	LCL	240	3.30e+00	3.45e-01	2.57e-01	2.20e-01	1.82e-01	1.48e-01	2.91e+00	2.60e+00	2.37e+00	2.18e+00	2.02e+00
T	LCL	240	3.29e+00	3.51e-01	2.62e-01	2.21e-01	1.88e-01	1.51e-01	2.84e+00	2.52e+00	2.28e+00	2.09e+00	1.92e+00
T	LCL	240	7.58e+00	9.92e-01	7.23e-01	6.03e-01	4.96e-01	3.39e-01	7.50e+00	6.62e+00	6.00e+00	5.47e+00	5.10e+00
T	LCL	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
T	LCL	240	5.26e+00	4.65e-01	4.25e-01	2.81e-01	2.42e-01	2.03e-01	4.30e+00	3.77e+00	3.48e+00	3.23e+00	3.01e+00
T	LCL	720	3.34e+00	1.82e-01	1.64e-01	1.45e-01	8.71e-02	1.29e-01	2.50e+00	2.33e+00	2.17e+00	2.08e+00	1.95e+00
T	LCL	720	3.28e+00	1.83e-01	1.57e-01	1.42e-01	8.44e-02	NA	NA	NA	NA	NA	1.88e+00
T	LCL	720	9.10e+00	6.78e-01	5.68e-01	4.86e-01	3.49e-01	3.52e-01	7.23e+00	6.62e+00	6.09e+00	5.73e+00	5.35e+00
T	LCL	720	0.00e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
T	LCL	720	5.77e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
T	LCO	2	3.28e+00	7.99e-01	2.00e-01	NA	NA	NA	NA	NA	NA	NA	0.00e+00
T	LCO	2	3.48e+00	1.03e+00	2.02e-01	NA	NA	NA	NA	NA	NA	NA	0.00e+00
T	LCO	2	8.82e+00	1.94e+00	6.70e-01	NA	NA	NA	NA	NA	NA	NA	0.00e+00
T	LCO	2	0.00e+00	0.00e+00	0.00e+00	NA	NA	NA	NA	NA	NA	NA	0.00e+00
T	LCO	2	6.34e+00	1.12e+00	3.80e-01	NA	NA	NA	NA	NA	NA	NA	0.00e+00
T	LCO	48	3.54e+00	2.74e-01	1.29e-01	8.07e-02	1.04e-01	6.44e-02	2.94e+00	2.80e+00	2.72e+00	2.60e+00	2.54e+00
T	LCO	48	3.52e+00	7.56e-01	1.43e-01	7.96e-02	1.03e-01	9.06e-02	3.01e+00	2.86e+00	2.78e+00	2.66e+00	2.57e+00
T	LCO	48	8.32e+00	8.06e-01	5.07e-01	3.65e-01	3.27e-01	2.82e-01	8.49e+00	7.99e+00	7.61e+00	7.26e+00	6.96e+00
T	LCO	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
T	LCO	48	6.31e+00	4.13e-01	2.08e-01	1.67e-01	1.73e-01	1.73e-01	5.02e+00	4.81e+00	4.63e+00	4.44e+00	4.26e+00
T	LCO	240	3.65e+00	1.57e-01	1.27e-01	1.08e-01	9.55e-02	8.42e-02	2.98e+00	2.83e+00	2.68e+00	2.59e+00	2.50e+00
T	LCO	240	3.65e+00	1.54e-01	1.29e-01	1.11e-01	9.58e-02	8.65e-02	2.98e+00	2.80e+00	2.65e+00	2.55e+00	2.46e+00
T	LCO	240	8.41e+00	5.23e-01	4.23e-01	3.63e-01	3.12e-01	2.68e-01	7.12e+00	6.63e+00	6.13e+00	5.81e+00	5.53e+00
T	LCO	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
T	LCO	240	5.97e+00	NA	1.42e-01	1.13e-01	1.11e-01	9.16e-02	1.52e+00	1.35e+00	1.20e+00	1.08e+00	9.88e-01
T	LCO	720	3.71e+00	1.01e-01	7.59e-02	7.29e-02	6.88e-02	5.20e-02	2.30e+00	2.23e+00	2.15e+00	2.07e+00	2.02e+00
T	LCO	720	3.73e+00	9.62e-02	8.79e-02	8.84e-02	7.24e-02	5.83e-02	2.51e+00	2.42e+00	2.33e+00	2.25e+00	2.19e+00
T	LCO	720	1.01e+01	3.25e-01	2.97e-01	2.70e-01	2.49e-01	2.03e-01	6.73e+00	6.43e+00	6.13e+00	5.87e+00	5.65e+00
T	LCO	720	0.00e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
T	LCO	720	6.42e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00

Table E.5 – continued from previous page

MC	S	t_{Ads}	C_{CTRL}	C_A	C_{D1}	C_{D2}	C_{D3}	C_{D4}	q_A	q_{D1}	q_{D2}	q_{D3}	q_{D4}
T	M	2	4.01e+00	1.72e+00	7.22e-01	4.67e-01	3.02e-01	2.13e-01	2.54e+00	1.75e+00	1.29e+00	9.58e-01	7.33e-01
T	M	2	4.03e+00	1.78e+00	7.44e-01	4.72e-01	3.18e-01	2.15e-01	2.66e+00	1.84e+00	1.37e+00	1.02e+00	7.87e-01
T	M	2	1.13e+01	5.30e+00	2.31e+00	1.37e+00	8.93e-01	5.68e-01	7.10e+00	4.58e+00	3.20e+00	2.22e+00	1.61e+00
T	M	2	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
T	M	2	6.85e+00	2.57e+00	1.20e+00	7.80e-01	5.33e-01	3.44e-01	4.37e+00	3.02e+00	2.24e+00	1.65e+00	1.29e+00
T	M	48	3.58e+00	9.15e-01	5.63e-01	3.91e-01	2.58e-01	1.95e-01	2.34e+00	1.76e+00	1.36e+00	1.08e+00	8.88e-01
T	M	48	3.57e+00	9.35e-01	6.22e-01	3.97e-01	2.58e-01	1.93e-01	2.51e+00	1.87e+00	1.45e+00	1.18e+00	9.80e-01
T	M	48	1.05e+01	3.25e+00	1.89e+00	1.25e+00	7.81e-01	5.56e-01	6.96e+00	5.02e+00	3.69e+00	2.86e+00	2.29e+00
T	M	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
T	M	48	6.62e+00	NA	1.01e+00	7.13e-01	4.73e-01	3.64e-01	4.38e+00	3.35e+00	2.61e+00	2.11e+00	1.74e+00
T	M	240	3.58e+00	4.22e-01	2.70e-01	1.70e-01	1.14e-01	1.05e-01	1.26e+00	9.66e-01	7.87e-01	6.67e-01	5.64e-01
T	M	240	3.57e+00	4.64e-01	2.67e-01	1.71e-01	1.18e-01	1.01e-01	1.31e+00	1.02e+00	8.42e-01	7.17e-01	6.16e-01
T	M	240	1.04e+01	2.01e+00	1.10e+00	6.68e-01	4.23e-01	3.53e-01	4.35e+00	3.16e+00	2.46e+00	2.01e+00	1.65e+00
T	M	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
T	M	240	6.69e+00	7.84e-01	4.83e-01	3.13e-01	2.16e-01	1.93e-01	2.35e+00	1.83e+00	1.50e+00	1.27e+00	1.08e+00
T	M	720	3.56e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	5.09e-02	5.09e-02	5.09e-02	5.09e-02	5.09e-02
T	M	720	3.57e+00	0.00e+00	0.00e+00	NA	0.00e+00	0.00e+00	NA	NA	5.19e-02	5.19e-02	5.19e-02
T	M	720	1.05e+01	2.76e-01	1.44e-01	7.50e-02	3.86e-02	0.00e+00	1.29e+00	1.14e+00	1.06e+00	1.02e+00	1.02e+00
T	M	720	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	NA	NA	NA	NA	NA	0.00e+00
T	M	720	6.67e+00	NA	0.00e+00	0.00e+00	0.00e+00	0.00e+00	5.43e-01	5.43e-01	5.43e-01	5.43e-01	5.43e-01
T	N	2	3.97e+00	2.18e+00	5.81e-01	3.13e-01	1.56e-01	8.93e-02	1.41e+00	7.93e-01	4.67e-01	3.08e-01	2.12e-01
T	N	2	4.01e+00	2.16e+00	6.24e-01	3.30e-01	1.69e-01	1.02e-01	1.56e+00	8.95e-01	5.47e-01	3.73e-01	2.64e-01
T	N	2	1.15e+01	6.80e+00	2.14e+00	1.01e+00	5.16e-01	2.68e-01	4.76e+00	2.44e+00	1.35e+00	8.18e-01	5.38e-01
T	N	2	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
T	N	2	6.84e+00	3.33e+00	1.13e+00	5.96e-01	3.33e-01	1.94e-01	2.87e+00	1.65e+00	1.02e+00	6.74e-01	4.66e-01
T	N	48	3.68e+00	8.93e-01	4.86e-01	2.92e-01	1.63e-01	1.09e-01	1.80e+00	1.29e+00	9.74e-01	8.04e-01	6.89e-01
T	N	48	3.68e+00	9.48e-01	4.96e-01	2.68e-01	1.53e-01	1.02e-01	1.62e+00	1.11e+00	8.21e-01	6.57e-01	5.53e-01
T	N	48	1.09e+01	3.70e+00	1.80e+00	9.79e-01	5.27e-01	3.48e-01	5.12e+00	3.27e+00	2.20e+00	1.65e+00	1.28e+00
T	N	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
T	N	48	6.87e+00	1.71e+00	9.50e-01	5.47e-01	3.31e-01	2.20e-01	3.24e+00	2.25e+00	1.66e+00	1.31e+00	1.08e+00
T	N	240	3.66e+00	8.14e-02	3.86e-02	2.41e-02	0.00e+00	2.48e-02	1.63e-01	1.22e-01	9.69e-02	9.69e-02	7.03e-02
T	N	240	3.67e+00	4.80e-02	3.28e-02	2.77e-02	0.00e+00	1.46e-02	1.51e-01	1.16e-01	8.65e-02	8.65e-02	7.10e-02
T	N	240	1.08e+01	6.43e-01	3.23e-01	1.76e-01	1.04e-01	8.61e-02	1.12e+00	7.75e-01	5.87e-01	4.78e-01	3.87e-01
T	N	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
T	N	240	6.85e+00	3.20e-02	3.00e-02	2.51e-02	1.51e-02	1.79e-02	2.16e-01	1.84e-01	1.57e-01	1.41e-01	1.22e-01
T	N	720	3.68e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
T	N	720	3.65e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
T	N	720	1.10e+01	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	9.32e-02	9.32e-02	9.32e-02	9.32e-02	9.32e-02
T	N	720	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
T	N	720	6.89e+00	NA	0.00e+00	0.00e+00	NA	0.00e+00	NA	NA	NA	2.81e-02	2.81e-02

Table E.5 – continued from previous page

MC	S	t_{Ads}	C_{CTRL}	C_A	C_{D1}	C_{D2}	C_{D3}	C_{D4}	q_A	q_{D1}	q_{D2}	q_{D3}	q_{D4}
T	P	2	3.90e+00	1.73e-01	6.43e-02	6.41e-02	5.58e-02	5.16e-02	5.23e+00	5.12e+00	5.01e+00	4.91e+00	4.84e+00
T	P	2	3.89e+00	1.55e-01	6.79e-02	6.59e-02	5.47e-02	7.40e-02	5.49e+00	5.38e+00	5.26e+00	5.16e+00	5.09e+00
T	P	2	1.13e+01	6.21e-01	2.49e-01	2.30e-01	2.09e-01	1.96e-01	1.57e+01	1.53e+01	1.49e+01	1.45e+01	1.43e+01
T	P	2	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	NA	NA	NA	NA	NA	0.00e+00
T	P	2	6.71e+00	2.03e+00	8.63e-02	NA	NA	NA	NA	NA	NA	NA	0.00e+00
T	P	48	3.64e+00	1.89e-01	5.97e-02	6.12e-02	5.97e-02	6.47e-02	5.13e+00	5.02e+00	4.92e+00	4.81e+00	4.70e+00
T	P	48	3.64e+00	6.31e-02	5.79e-02	5.44e-02	4.95e-02	5.43e-02	5.13e+00	5.03e+00	4.94e+00	4.85e+00	4.76e+00
T	P	48	1.07e+01	2.22e-01	2.24e-01	2.10e-01	1.85e-01	1.94e-01	1.45e+01	1.41e+01	1.37e+01	1.34e+01	1.31e+01
T	P	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
T	P	48	6.76e+00	9.13e-02	8.66e-02	9.22e-02	8.03e-02	8.46e-02	9.99e+00	9.84e+00	9.68e+00	9.54e+00	9.40e+00
T	P	240	3.60e+00	1.40e-02	9.86e-03	0.00e+00	0.00e+00	1.28e-02	6.35e-01	6.18e-01	6.18e-01	6.18e-01	5.96e-01
T	P	240	3.62e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	1.04e-02	5.82e-01	5.82e-01	5.82e-01	5.82e-01	5.65e-01
T	P	240	1.08e+01	0.00e+00	0.00e+00	0.00e+00	1.24e-02	1.40e-02	1.09e+00	1.09e+00	1.09e+00	1.07e+00	1.05e+00
T	P	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
T	P	240	6.76e+00	0.00e+00	0.00e+00	NA	0.00e+00	0.00e+00	NA	NA	1.22e+00	1.22e+00	1.22e+00
T	P	720	3.62e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	2.00e-01	2.00e-01	2.00e-01	2.00e-01	2.00e-01
T	P	720	3.62e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
T	P	720	1.07e+01	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	2.97e-01	2.97e-01	2.97e-01	2.97e-01	2.97e-01
T	P	720	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
T	P	720	6.78e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	4.67e-01	4.67e-01	4.67e-01	4.67e-01	4.67e-01
T	PO	2	3.25e+00	5.42e-01	2.36e-01	NA	NA	NA	NA	NA	NA	NA	0.00e+00
T	PO	2	3.39e+00	8.30e-01	3.87e-01	NA	NA	NA	NA	NA	NA	NA	0.00e+00
T	PO	2	8.06e+00	2.13e+00	1.04e+00	NA	NA	NA	NA	NA	NA	NA	0.00e+00
T	PO	2	0.00e+00	0.00e+00	0.00e+00	NA	NA	NA	NA	NA	NA	NA	0.00e+00
T	PO	2	6.08e+00	1.46e+00	6.76e-01	NA	NA	NA	NA	NA	NA	NA	0.00e+00
T	PO	48	3.27e+00	4.26e-01	3.04e-01	1.93e-01	1.79e-01	1.85e-01	9.08e-01	5.89e-01	3.84e-01	1.97e-01	0.00e+00
T	PO	48	3.26e+00	4.94e-01	2.61e-01	1.96e-01	1.71e-01	1.90e-01	3.49e+00	3.21e+00	3.01e+00	2.83e+00	2.63e+00
T	PO	48	7.86e+00	1.25e+00	7.46e-01	5.94e-01	5.51e-01	5.19e-01	9.50e+00	8.71e+00	8.09e+00	7.63e+00	7.08e+00
T	PO	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
T	PO	48	5.96e+00	7.70e-01	5.53e-01	3.71e-01	3.58e-01	3.62e-01	6.08e+00	5.51e+00	5.12e+00	4.75e+00	4.38e+00
T	PO	240	3.51e+00	3.26e-01	3.07e-01	2.30e-01	1.80e-01	1.52e-01	3.65e+00	3.27e+00	2.97e+00	2.78e+00	2.62e+00
T	PO	240	3.48e+00	3.25e-01	3.01e-01	2.34e-01	1.77e-01	1.56e-01	3.58e+00	3.21e+00	2.90e+00	2.72e+00	2.56e+00
T	PO	240	8.07e+00	9.52e-01	7.52e-01	5.63e-01	4.70e-01	3.98e-01	8.42e+00	7.49e+00	6.74e+00	6.26e+00	5.84e+00
T	PO	240	0.00e+00	0.00e+00	0.00e+00	NA	0.00e+00	0.00e+00	NA	NA	0.00e+00	0.00e+00	0.00e+00
T	PO	240	5.68e+00	5.08e-01	3.85e-01	2.89e-01	2.52e-01	2.14e-01	5.62e+00	5.14e+00	4.76e+00	4.50e+00	4.27e+00
T	PO	720	3.56e+00	2.57e-01	2.24e-01	9.48e-02	1.46e-01	1.43e-01	3.11e+00	2.88e+00	2.78e+00	2.63e+00	2.48e+00
T	PO	720	3.54e+00	0.00e+00	2.23e-01	9.65e-02	1.56e-01	1.39e-01	3.22e+00	2.99e+00	2.89e+00	2.72e+00	2.57e+00
T	PO	720	9.67e+00	7.57e-01	7.04e-01	3.40e-01	5.37e-01	4.51e-01	8.75e+00	8.03e+00	7.67e+00	7.11e+00	6.63e+00
T	PO	720	0.00e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
T	PO	720	6.15e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00

Table E.5 – continued from previous page

MC	S	t_{Ads}	C_{CTRL}	C_A	C_{D1}	C_{D2}	C_{D3}	C_{D4}	q_A	q_{D1}	q_{D2}	q_{D3}	q_{D4}
T	R	2	3.86e+00	4.63e-01	2.57e-01	2.38e-01	2.15e-01	1.96e-01	5.78e+00	5.34e+00	4.92e+00	4.54e+00	4.21e+00
T	R	2	3.91e+00	4.15e-01	2.52e-01	2.38e-01	2.18e-01	1.93e-01	5.95e+00	5.52e+00	5.10e+00	4.72e+00	4.40e+00
T	R	2	1.10e+01	1.38e+00	8.29e-01	7.58e-01	6.64e-01	6.03e-01	1.65e+01	1.50e+01	1.37e+01	1.25e+01	1.15e+01
T	R	2	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
T	R	2	6.61e+00	6.31e-01	4.12e-01	3.85e-01	NA	3.31e-01	NA	NA	NA	7.61e+00	7.05e+00
T	R	48	3.56e+00	2.38e-01	2.11e-01	2.01e-01	1.80e-01	1.68e-01	5.39e+00	5.03e+00	4.68e+00	4.36e+00	4.07e+00
T	R	48	3.58e+00	2.51e-01	2.15e-01	2.18e-01	1.74e-01	1.66e-01	5.38e+00	5.02e+00	4.64e+00	4.34e+00	4.06e+00
T	R	48	1.06e+01	7.64e-01	6.51e-01	6.29e-01	5.49e-01	5.10e-01	1.58e+01	1.46e+01	1.36e+01	1.26e+01	1.18e+01
T	R	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
T	R	48	6.66e+00	4.24e-01	3.78e-01	3.62e-01	3.22e-01	3.08e-01	1.07e+01	1.01e+01	9.45e+00	8.89e+00	8.37e+00
T	R	240	3.57e+00	1.91e-01	1.79e-01	1.64e-01	1.48e-01	1.44e-01	4.50e+00	4.19e+00	3.91e+00	3.66e+00	3.42e+00
T	R	240	3.56e+00	1.90e-01	1.73e-01	1.38e-01	1.43e-01	1.36e-01	4.45e+00	4.16e+00	3.93e+00	3.68e+00	3.45e+00
T	R	240	1.04e+01	5.96e-01	5.62e-01	5.11e-01	4.65e-01	NA	NA	NA	NA	NA	1.02e+01
T	R	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
T	R	240	6.67e+00	3.25e-01	3.00e-01	9.08e-02	2.46e-01	2.31e-01	7.71e+00	7.22e+00	7.06e+00	6.63e+00	6.24e+00
T	R	720	3.57e+00	1.54e-01	1.40e-01	6.71e-02	4.40e-02	5.63e-02	5.84e+00	5.59e+00	5.48e+00	5.40e+00	5.31e+00
T	R	720	3.56e+00	1.27e-01	1.13e-01	5.30e-02	4.05e-02	5.68e-02	5.42e+00	5.23e+00	5.13e+00	5.06e+00	4.97e+00
T	R	720	1.06e+01	4.90e-01	4.40e-01	1.92e-01	2.08e-01	1.49e-01	1.60e+01	1.53e+01	1.49e+01	1.46e+01	1.43e+01
T	R	720	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
T	R	720	6.67e+00	2.42e-01	2.24e-01	1.12e-01	9.60e-02	1.19e-01	9.90e+00	9.50e+00	9.30e+00	9.14e+00	8.94e+00
T	SOU	2	3.75e+00	2.25e+00	8.75e-01	4.97e-01	2.80e-01	1.66e-01	2.08e+00	1.20e+00	6.91e-01	3.96e-01	2.19e-01
T	SOU	2	3.62e+00	2.24e+00	9.08e-01	5.02e-01	2.80e-01	1.63e-01	2.20e+00	1.27e+00	7.62e-01	4.67e-01	2.93e-01
T	SOU	2	1.07e+01	6.53e+00	0.00e+00	1.40e+00	7.50e-01	4.13e-01	3.37e+00	3.37e+00	1.92e+00	1.12e+00	6.77e-01
T	SOU	2	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
T	SOU	2	6.26e+00	3.68e+00	1.53e+00	8.13e-01	4.74e-01	2.73e-01	3.82e+00	2.22e+00	1.38e+00	8.72e-01	5.86e-01
T	SOU	48	3.48e+00	1.60e+00	7.68e-01	4.49e-01	2.46e-01	1.88e-01	2.43e+00	1.62e+00	1.15e+00	8.88e-01	6.88e-01
T	SOU	48	3.48e+00	1.53e+00	8.24e-01	4.66e-01	2.44e-01	1.57e-01	2.30e+00	1.44e+00	9.45e-01	6.84e-01	5.19e-01
T	SOU	48	1.03e+01	4.97e+00	2.51e+00	1.33e+00	7.02e-01	4.39e-01	6.85e+00	4.20e+00	2.79e+00	2.03e+00	1.57e+00
T	SOU	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
T	SOU	48	6.48e+00	2.62e+00	1.42e+00	8.28e-01	4.73e-01	3.07e-01	4.23e+00	2.75e+00	1.88e+00	1.37e+00	1.04e+00
T	SOU	240	3.47e+00	6.23e-01	3.25e-01	1.78e-01	1.05e-01	8.36e-02	9.79e-01	6.43e-01	4.57e-01	3.45e-01	2.61e-01
T	SOU	240	3.47e+00	5.81e-01	3.06e-01	1.70e-01	9.77e-02	NA	NA	NA	NA	NA	0.00e+00
T	SOU	240	1.02e+01	2.43e+00	1.38e+00	7.44e-01	4.17e-01	2.98e-02	3.58e+00	2.16e+00	1.38e+00	9.39e-01	9.09e-01
T	SOU	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
T	SOU	240	6.49e+00	1.03e+00	5.27e-01	3.10e-01	1.86e-01	NA	NA	NA	NA	NA	6.53e-01
T	SOU	720	3.47e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	4.07e-02	4.07e-02	4.07e-02	4.07e-02	4.07e-02
T	SOU	720	3.47e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
T	SOU	720	1.02e+01	2.39e-01	1.22e-01	0.00e+00	0.00e+00	9.39e-03	5.61e-01	4.30e-01	4.30e-01	4.30e-01	4.20e-01
T	SOU	720	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
T	SOU	720	6.49e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	NA	NA	NA	NA	NA	6.85e-02

Table E.5 – continued from previous page

MC	S	t_{Ads}	C_{CTRL}	C_A	C_{D1}	C_{D2}	C_{D3}	C_{D4}	q_A	q_{D1}	q_{D2}	q_{D3}	q_{D4}
T	SSL1	2	3.50e+00	1.88e+00	9.30e-01	5.24e-01	3.28e-01	2.31e-01	2.68e+00	1.68e+00	1.14e+00	7.99e-01	5.62e-01
T	SSL1	2	3.55e+00	1.86e+00	9.38e-01	5.14e-01	3.28e-01	5.77e-01	3.08e+00	2.06e+00	1.52e+00	1.17e+00	5.69e-01
T	SSL1	2	9.37e+00	5.33e+00	2.53e+00	1.37e+00	8.47e-01	NA	NA	NA	NA	NA	1.28e+00
T	SSL1	2	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
T	SSL1	2	6.17e+00	3.12e+00	1.60e+00	9.65e-01	5.91e-01	4.07e-01	4.90e+00	3.22e+00	2.13e+00	1.50e+00	1.07e+00
T	SSL1	48	3.54e+00	1.60e+00	1.52e+00	6.10e-01	3.57e-01	2.51e-01	3.62e+00	1.97e+00	1.33e+00	9.46e-01	6.83e-01
T	SSL1	48	3.56e+00	1.62e+00	0.00e+00	5.87e-01	3.50e-01	2.45e-01	1.94e+00	1.94e+00	1.31e+00	9.38e-01	6.79e-01
T	SSL1	48	9.47e+00	4.58e+00	2.58e+00	1.51e+00	9.35e-01	6.28e-01	7.50e+00	4.75e+00	3.18e+00	2.18e+00	1.53e+00
T	SSL1	48	0.00e+00	NA	NA	0.00e+00	0.00e+00	0.00e+00	NA	0.00e+00	0.00e+00	0.00e+00	0.00e+00
T	SSL1	48	6.25e+00	2.59e+00	NA	9.60e-01	6.08e-01	4.21e-01	NA	3.24e+00	2.24e+00	1.60e+00	1.18e+00
T	SSL1	240	3.77e+00	1.09e+00	7.07e-01	5.58e-01	3.68e-01	2.53e-01	3.18e+00	2.46e+00	1.83e+00	1.45e+00	1.18e+00
T	SSL1	240	3.79e+00	1.15e+00	7.16e-01	5.66e-01	3.77e-01	2.58e-01	3.15e+00	2.42e+00	1.79e+00	1.40e+00	1.12e+00
T	SSL1	240	1.05e+01	4.52e+00	2.12e+00	NA	9.27e-01	6.26e-01	NA	NA	3.88e+00	2.92e+00	2.26e+00
T	SSL1	240	0.00e+00	0.00e+00	0.00e+00	NA	NA	0.00e+00	NA	NA	NA	0.00e+00	0.00e+00
T	SSL1	240	6.28e+00	2.43e+00	1.08e+00	7.94e-01	5.49e-01	3.75e-01	4.65e+00	3.51e+00	2.65e+00	2.08e+00	1.68e+00
T	SSL1	720	3.55e+00	1.45e+00	8.80e-01	5.66e-01	3.89e-01	2.60e-01	3.12e+00	2.16e+00	1.57e+00	1.14e+00	8.59e-01
T	SSL1	720	3.50e+00	1.47e+00	9.06e-01	5.81e-01	3.85e-01	2.47e-01	3.16e+00	2.16e+00	1.55e+00	1.12e+00	8.51e-01
T	SSL1	720	9.17e+00	3.91e+00	2.19e+00	1.37e+00	8.77e-01	5.43e-01	6.78e+00	4.46e+00	3.05e+00	2.09e+00	1.51e+00
T	SSL1	720	0.00e+00	NA	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
T	SSL1	720	6.16e+00	2.32e+00	1.39e+00	8.98e-01	6.01e-01	0.00e+00	4.41e+00	2.88e+00	1.93e+00	1.26e+00	1.26e+00
T	SSL2	2	3.64e+00	1.90e+00	9.37e-01	5.34e-01	3.36e-01	2.35e-01	2.80e+00	1.82e+00	1.26e+00	8.97e-01	6.54e-01
T	SSL2	2	3.65e+00	1.84e+00	9.37e-01	5.45e-01	3.60e-01	2.55e-01	2.88e+00	1.93e+00	1.36e+00	9.72e-01	7.02e-01
T	SSL2	2	9.81e+00	5.45e+00	2.58e+00	1.45e+00	9.15e-01	6.02e-01	7.36e+00	4.60e+00	3.09e+00	2.10e+00	1.48e+00
T	SSL2	2	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	NA	NA	NA	NA	NA	0.00e+00
T	SSL2	2	6.48e+00	3.14e+00	1.58e+00	9.33e-01	5.88e-01	4.12e-01	4.79e+00	3.11e+00	2.13e+00	1.49e+00	1.07e+00
T	SSL2	48	3.73e+00	1.61e+00	9.46e-01	5.83e-01	3.64e-01	2.51e-01	3.02e+00	2.05e+00	1.43e+00	1.04e+00	7.78e-01
T	SSL2	48	3.72e+00	1.61e+00	9.47e-01	5.87e-01	3.66e-01	2.57e-01	2.95e+00	1.98e+00	1.37e+00	9.72e-01	7.09e-01
T	SSL2	48	9.97e+00	4.72e+00	2.61e+00	1.62e+00	9.77e-01	6.49e-01	7.77e+00	5.06e+00	3.40e+00	2.34e+00	1.67e+00
T	SSL2	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
T	SSL2	48	6.51e+00	2.60e+00	1.58e+00	9.76e-01	6.09e-01	4.40e-01	4.96e+00	3.33e+00	2.33e+00	1.66e+00	1.21e+00
T	SSL2	240	3.96e+00	1.04e+00	7.02e-01	5.51e-01	3.73e-01	2.49e-01	2.42e+00	1.72e+00	1.10e+00	7.04e-01	4.43e-01
T	SSL2	240	3.92e+00	1.06e+00	6.98e-01	5.44e-01	3.79e-01	2.54e-01	2.36e+00	1.68e+00	1.08e+00	6.85e-01	4.17e-01
T	SSL2	240	1.10e+01	3.64e+00	2.22e+00	1.50e+00	9.45e-01	6.07e-01	6.38e+00	4.21e+00	2.51e+00	1.51e+00	8.67e-01
T	SSL2	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	NA	NA	NA	NA	NA	0.00e+00
T	SSL2	240	6.54e+00	NA	1.13e+00	8.22e-01	5.53e-01	3.90e-01	3.65e+00	2.50e+00	1.59e+00	1.02e+00	6.09e-01
T	SSL2	720	3.68e+00	1.42e+00	8.98e-01	5.82e-01	3.81e-01	0.00e+00	2.81e+00	1.82e+00	1.21e+00	7.99e-01	7.99e-01
T	SSL2	720	3.70e+00	1.50e+00	9.21e-01	5.83e-01	3.73e-01	0.00e+00	3.02e+00	1.99e+00	1.37e+00	9.57e-01	9.57e-01
T	SSL2	720	9.51e+00	3.99e+00	2.30e+00	1.40e+00	8.57e-01	0.00e+00	6.35e+00	3.85e+00	2.37e+00	1.44e+00	1.44e+00
T	SSL2	720	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
T	SSL2	720	6.47e+00	2.32e+00	1.40e+00	9.18e-01	6.04e-01	4.03e-01	5.01e+00	3.42e+00	2.45e+00	1.80e+00	1.37e+00

Table E.5 – continued from previous page

MC	S	t_{Ads}	C_{CTRL}	C_A	C_{D1}	C_{D2}	C_{D3}	C_{D4}	q_A	q_{D1}	q_{D2}	q_{D3}	q_{D4}
T	SSL3	2	3.60e+00	1.86e+00	9.34e-01	5.51e-01	3.43e-01	2.42e-01	2.83e+00	1.84e+00	1.25e+00	8.88e-01	6.37e-01
T	SSL3	2	3.62e+00	1.87e+00	9.43e-01	5.37e-01	3.40e-01	2.42e-01	2.78e+00	1.77e+00	1.20e+00	8.37e-01	5.87e-01
T	SSL3	2	9.57e+00	5.25e+00	2.59e+00	1.47e+00	9.04e-01	6.18e-01	7.44e+00	4.68e+00	3.08e+00	2.13e+00	1.49e+00
T	SSL3	2	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	NA	NA	NA	NA	NA	0.00e+00
T	SSL3	2	6.37e+00	3.07e+00	1.63e+00	9.49e-01	5.75e-01	4.19e-01	4.82e+00	3.11e+00	2.09e+00	1.49e+00	1.05e+00
T	SSL3	48	3.66e+00	1.58e+00	9.42e-01	5.98e-01	3.75e-01	2.58e-01	3.01e+00	2.01e+00	1.39e+00	9.86e-01	7.22e-01
T	SSL3	48	3.71e+00	1.58e+00	9.32e-01	5.82e-01	3.68e-01	2.57e-01	3.00e+00	2.00e+00	1.40e+00	1.00e+00	7.35e-01
T	SSL3	48	9.83e+00	4.72e+00	2.59e+00	1.57e+00	9.73e-01	6.63e-01	7.78e+00	5.03e+00	3.37e+00	2.34e+00	1.66e+00
T	SSL3	48	0.00e+00	0.00e+00	0.00e+00	NA	NA	0.00e+00	NA	NA	NA	0.00e+00	0.00e+00
T	SSL3	48	6.38e+00	2.69e+00	1.57e+00	9.90e-01	6.01e-01	3.75e-01	4.80e+00	3.13e+00	2.08e+00	1.43e+00	1.05e+00
T	SSL3	240	3.88e+00	1.08e+00	7.12e-01	5.55e-01	3.81e-01	2.68e-01	3.25e+00	2.54e+00	1.91e+00	1.51e+00	1.22e+00
T	SSL3	240	3.84e+00	1.10e+00	6.92e-01	5.65e-01	3.81e-01	2.58e-01	3.12e+00	2.43e+00	1.81e+00	1.41e+00	1.14e+00
T	SSL3	240	1.09e+01	3.47e+00	2.13e+00	1.48e+00	9.58e-01	6.16e-01	7.80e+00	5.71e+00	4.05e+00	3.05e+00	2.39e+00
T	SSL3	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
T	SSL3	240	6.36e+00	1.74e+00	1.13e+00	8.45e-01	5.73e-01	3.90e-01	4.92e+00	3.79e+00	2.87e+00	2.26e+00	1.85e+00
T	SSL3	720	3.46e+00	1.42e+00	8.86e-01	5.94e-01	3.95e-01	2.59e-01	3.06e+00	2.09e+00	1.47e+00	1.03e+00	7.57e-01
T	SSL3	720	3.47e+00	1.41e+00	9.02e-01	6.01e-01	3.97e-01	2.64e-01	3.08e+00	2.11e+00	1.49e+00	1.05e+00	7.71e-01
T	SSL3	720	8.96e+00	4.05e+00	2.25e+00	1.44e+00	9.07e-01	5.66e-01	6.85e+00	4.41e+00	2.92e+00	1.92e+00	1.32e+00
T	SSL3	720	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
T	SSL3	720	6.33e+00	2.34e+00	1.42e+00	9.28e-01	6.12e-01	4.09e-01	4.61e+00	3.07e+00	2.10e+00	1.43e+00	9.99e-01
T	ST	2	3.02e+00	1.09e+00	7.37e-01	4.78e-01	3.39e-01	2.80e-01	4.00e+00	2.75e+00	1.89e+00	1.29e+00	8.14e-01
T	ST	2	3.00e+00	1.10e+00	7.31e-01	4.83e-01	3.39e-01	2.42e-01	3.88e+00	2.64e+00	1.77e+00	1.18e+00	7.67e-01
T	ST	2	7.93e+00	3.31e+00	2.27e+00	1.50e+00	1.11e+00	8.20e-01	1.11e+01	7.28e+00	4.65e+00	2.76e+00	1.37e+00
T	ST	2	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
T	ST	2	5.27e+00	2.35e+00	1.50e+00	1.07e+00	7.42e-01	5.35e-01	8.18e+00	5.65e+00	3.72e+00	2.45e+00	1.54e+00
T	ST	48	3.01e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
T	ST	48	3.01e+00	1.16e+00	7.75e-01	5.71e-01	4.35e-01	3.31e-01	4.54e+00	3.24e+00	2.24e+00	1.48e+00	9.14e-01
T	ST	48	7.97e+00	3.62e+00	2.12e+00	1.38e+00	8.85e-01	7.64e-01	1.13e+01	7.79e+00	5.33e+00	3.75e+00	2.47e+00
T	ST	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
T	ST	48	5.34e+00	1.95e+00	1.53e+00	1.16e+00	8.49e-01	5.97e-01	8.65e+00	6.02e+00	4.06e+00	2.54e+00	1.53e+00
T	ST	240	3.26e+00	1.05e+00	6.96e-01	5.37e-01	3.82e-01	2.47e-01	4.34e+00	3.23e+00	2.30e+00	1.63e+00	1.18e+00
T	ST	240	3.24e+00	1.07e+00	6.68e-01	5.88e-01	3.75e-01	2.37e-01	4.53e+00	3.38e+00	2.36e+00	1.69e+00	1.25e+00
T	ST	240	9.61e+00	3.09e+00	2.11e+00	1.66e+00	1.22e+00	8.63e-01	1.35e+01	9.91e+00	6.96e+00	4.83e+00	3.28e+00
T	ST	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
T	ST	240	5.35e+00	1.78e+00	1.07e+00	8.47e-01	5.90e-01	4.05e-01	7.04e+00	5.24e+00	3.72e+00	2.66e+00	1.99e+00
T	ST	720	2.86e+00	1.19e+00	7.09e-01	4.85e-01	3.02e-01	1.61e-01	3.66e+00	2.47e+00	1.58e+00	1.05e+00	7.64e-01
T	ST	720	2.91e+00	1.17e+00	7.45e-01	4.84e-01	3.05e-01	1.77e-01	3.72e+00	2.51e+00	1.63e+00	1.09e+00	7.75e-01
T	ST	720	7.72e+00	2.99e+00	1.89e+00	1.21e+00	6.99e-01	5.02e-01	9.70e+00	6.53e+00	4.36e+00	3.09e+00	2.23e+00
T	ST	720	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
T	ST	720	5.24e+00	1.96e+00	1.31e+00	8.80e-01	5.34e-01	3.14e-01	6.97e+00	4.82e+00	3.19e+00	2.24e+00	1.67e+00

Table E.5 – continued from previous page

MC	S	t_{Ads}	C_{CTRL}	C_A	C_{D1}	C_{D2}	C_{D3}	C_{D4}	q_A	q_{D1}	q_{D2}	q_{D3}	q_{D4}
T	W	2	3.31e+00	1.42e+00	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
T	W	2	3.51e+00	1.44e+00	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
T	W	2	8.40e+00	3.60e+00	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
T	W	2	0.00e+00	0.00e+00	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
T	W	2	6.24e+00	2.52e+00	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
T	W	48	3.31e+00	9.85e-01	5.37e-01	3.58e-01	2.72e-01	1.98e-01	2.87e+00	2.32e+00	1.94e+00	1.66e+00	1.44e+00
T	W	48	3.40e+00	9.93e-01	4.56e-01	7.17e-01	2.78e-01	2.13e-01	3.28e+00	2.81e+00	2.09e+00	1.80e+00	1.56e+00
T	W	48	8.11e+00	2.54e+00	1.47e+00	1.02e+00	7.62e-01	6.51e-01	7.70e+00	6.17e+00	5.15e+00	4.36e+00	3.64e+00
T	W	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
T	W	48	6.12e+00	1.61e+00	9.23e-01	5.48e-01	5.32e-01	4.76e-01	5.17e+00	4.20e+00	3.64e+00	3.09e+00	2.55e+00
T	W	240	3.56e+00	8.23e-01	5.45e-01	3.69e-01	2.89e-01	1.83e-01	3.04e+00	2.39e+00	1.89e+00	1.57e+00	1.39e+00
T	W	240	3.53e+00	8.00e-01	5.38e-01	3.59e-01	2.28e-01	1.83e-01	2.93e+00	2.29e+00	1.82e+00	1.57e+00	1.38e+00
T	W	240	8.20e+00	2.07e+00	1.37e+00	9.18e-01	6.72e-01	4.53e-01	7.15e+00	5.52e+00	4.33e+00	3.60e+00	3.12e+00
T	W	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
T	W	240	5.75e+00	1.18e+00	7.40e-01	4.97e-01	3.81e-01	2.69e-01	4.12e+00	3.23e+00	2.56e+00	2.15e+00	1.87e+00
T	W	720	3.62e+00	5.81e-01	4.51e-01	3.56e-01	2.43e-01	1.74e-01	2.42e+00	1.95e+00	1.56e+00	1.30e+00	1.11e+00
T	W	720	3.62e+00	5.94e-01	4.59e-01	3.53e-01	1.53e-01	1.74e-01	2.27e+00	1.80e+00	1.41e+00	1.25e+00	1.06e+00
T	W	720	9.84e+00	1.92e+00	1.38e+00	1.02e+00	7.91e-01	4.92e-01	7.41e+00	5.98e+00	4.88e+00	4.04e+00	3.50e+00
T	W	720	0.00e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
T	W	720	6.26e+00	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
T	W1	2	3.35e+00	1.66e+00	7.55e-01	4.58e-01	3.07e-01	2.33e-01	2.90e+00	2.11e+00	1.59e+00	1.28e+00	1.04e+00
T	W1	2	3.37e+00	1.65e+00	7.41e-01	4.56e-01	3.08e-01	2.30e-01	2.89e+00	2.10e+00	1.60e+00	1.29e+00	1.04e+00
T	W1	2	8.94e+00	4.97e+00	2.20e+00	1.25e+00	7.83e-01	5.57e-01	7.23e+00	4.93e+00	3.54e+00	2.73e+00	2.15e+00
T	W1	2	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
T	W1	2	5.93e+00	2.67e+00	1.25e+00	7.98e-01	5.54e-01	4.10e-01	5.02e+00	3.70e+00	2.82e+00	2.25e+00	1.82e+00
T	W1	48	3.40e+00	1.36e+00	7.81e-01	4.84e-01	3.29e-01	2.45e-01	3.22e+00	2.35e+00	1.86e+00	1.50e+00	1.24e+00
T	W1	48	3.42e+00	1.32e+00	7.71e-01	4.89e-01	3.25e-01	2.44e-01	3.27e+00	2.43e+00	1.93e+00	1.56e+00	1.30e+00
T	W1	48	9.17e+00	4.29e+00	2.29e+00	1.06e+00	8.23e-01	6.04e-01	7.58e+00	5.08e+00	4.01e+00	3.08e+00	2.45e+00
T	W1	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
T	W1	48	5.99e+00	2.05e+00	1.25e+00	8.43e-01	5.64e-01	4.23e-01	5.59e+00	4.23e+00	3.38e+00	2.74e+00	2.30e+00
T	W1	240	3.62e+00	9.06e-01	5.61e-01	3.88e-01	2.61e-01	1.83e-01	2.81e+00	2.26e+00	1.81e+00	1.54e+00	1.35e+00
T	W1	240	3.64e+00	9.07e-01	5.62e-01	3.93e-01	2.60e-01	1.88e-01	2.79e+00	2.24e+00	1.79e+00	1.52e+00	1.33e+00
T	W1	240	1.01e+01	3.57e+00	1.93e+00	1.21e+00	7.75e-01	5.17e-01	7.66e+00	5.79e+00	4.36e+00	3.57e+00	3.02e+00
T	W1	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
T	W1	240	6.05e+00	1.41e+00	9.24e-01	6.49e-01	4.59e-01	3.42e-01	4.91e+00	4.01e+00	3.25e+00	2.78e+00	2.43e+00
T	W1	720	3.30e+00	1.14e+00	6.24e-01	3.90e-01	2.60e-01	1.81e-01	2.50e+00	1.78e+00	1.37e+00	1.09e+00	8.97e-01
T	W1	720	3.25e+00	1.13e+00	6.07e-01	4.03e-01	2.60e-01	1.75e-01	2.34e+00	1.66e+00	1.24e+00	9.69e-01	7.81e-01
T	W1	720	8.42e+00	3.63e+00	1.86e+00	1.06e+00	6.71e-01	4.36e-01	6.12e+00	3.99e+00	2.86e+00	2.14e+00	1.67e+00
T	W1	720	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
T	W1	720	5.88e+00	1.80e+00	1.01e+00	7.01e-01	4.14e-01	2.96e-01	4.42e+00	3.30e+00	2.61e+00	1.90e+00	1.57e+00

Table E.5 – continued from previous page

MC	S	t_{Ads}	C_{CTRL}	C_A	C_{D1}	C_{D2}	C_{D3}	C_{D4}	q_A	q_{D1}	q_{D2}	q_{D3}	q_{D4}
T	W2	2	3.41e+00	1.63e+00	7.70e-01	4.72e-01	3.19e-01	2.34e-01	2.96e+00	2.14e+00	1.62e+00	1.30e+00	1.05e+00
T	W2	2	3.42e+00	1.66e+00	7.71e-01	4.65e-01	3.09e-01	2.32e-01	2.90e+00	2.09e+00	1.57e+00	1.25e+00	1.00e+00
T	W2	2	9.20e+00	5.10e+00	2.18e+00	1.27e+00	8.09e-01	5.64e-01	7.14e+00	4.83e+00	3.42e+00	2.59e+00	1.98e+00
T	W2	2	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
T	W2	2	5.99e+00	2.72e+00	1.29e+00	8.36e-01	5.59e-01	4.13e-01	5.08e+00	3.72e+00	2.79e+00	2.21e+00	1.77e+00
T	W2	48	3.46e+00	1.35e+00	7.93e-01	5.17e-01	3.36e-01	2.46e-01	2.91e+00	2.04e+00	1.51e+00	1.13e+00	8.68e-01
T	W2	48	3.50e+00	1.37e+00	7.92e-01	5.15e-01	3.35e-01	2.47e-01	3.18e+00	2.29e+00	1.78e+00	1.40e+00	1.15e+00
T	W2	48	9.25e+00	4.33e+00	2.34e+00	1.39e+00	8.45e-01	5.93e-01	7.92e+00	5.30e+00	3.89e+00	2.93e+00	2.31e+00
T	W2	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
T	W2	48	6.11e+00	2.11e+00	1.32e+00	8.70e-01	5.82e-01	4.29e-01	5.63e+00	4.13e+00	3.25e+00	2.60e+00	2.15e+00
T	W2	240	3.65e+00	9.14e-01	5.96e-01	3.93e-01	2.59e-01	1.88e-01	2.84e+00	2.23e+00	1.81e+00	1.55e+00	1.35e+00
T	W2	240	3.69e+00	9.13e-01	5.95e-01	3.97e-01	2.73e-01	1.97e-01	2.87e+00	2.26e+00	1.83e+00	1.56e+00	1.34e+00
T	W2	240	9.82e+00	3.51e+00	1.97e+00	1.24e+00	7.65e-01	5.13e-01	7.33e+00	5.31e+00	3.96e+00	3.20e+00	2.66e+00
T	W2	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
T	W2	240	6.14e+00	1.48e+00	9.76e-01	6.77e-01	4.76e-01	3.50e-01	5.05e+00	4.05e+00	3.31e+00	2.83e+00	2.45e+00
T	W2	720	3.30e+00	1.18e+00	6.38e-01	4.04e-01	2.74e-01	1.81e-01	2.38e+00	1.72e+00	1.31e+00	1.01e+00	8.20e-01
T	W2	720	3.28e+00	1.18e+00	6.50e-01	4.07e-01	2.71e-01	1.82e-01	2.45e+00	1.74e+00	1.33e+00	1.03e+00	8.37e-01
T	W2	720	8.46e+00	3.63e+00	1.84e+00	1.07e+00	6.69e-01	4.30e-01	5.85e+00	3.85e+00	2.77e+00	2.04e+00	1.57e+00
T	W2	720	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
T	W2	720	5.98e+00	1.78e+00	1.04e+00	6.92e-01	4.80e-01	3.41e-01	4.14e+00	2.98e+00	2.29e+00	1.77e+00	1.39e+00
T	Z	2	3.91e+00	3.08e-01	NA	NA	1.88e-01	NA	NA	NA	NA	NA	0.00e+00
T	Z	2	4.01e+00	3.19e-01	1.97e-01	1.91e-01	NA	1.79e-01	NA	NA	NA	4.98e+00	4.71e+00
T	Z	2	1.14e+01	1.06e+00	6.62e-01	6.07e-01	5.99e-01	5.40e-01	1.69e+01	1.57e+01	1.47e+01	1.36e+01	1.27e+01
T	Z	2	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
T	Z	2	6.78e+00	5.95e-01	3.87e-01	3.33e-01	3.38e-01	3.02e-01	9.89e+00	9.20e+00	8.63e+00	8.02e+00	7.50e+00
T	Z	48	3.58e+00	1.94e-01	1.89e-01	1.72e-01	1.39e-01	1.49e-01	5.64e+00	5.32e+00	5.01e+00	4.77e+00	4.51e+00
T	Z	48	3.58e+00	2.25e-01	2.11e-01	1.94e-01	1.48e-01	1.64e-01	6.08e+00	5.73e+00	5.39e+00	5.13e+00	4.85e+00
T	Z	48	1.06e+01	6.05e-01	6.33e-01	5.85e-01	4.60e-01	4.96e-01	1.65e+01	1.54e+01	1.44e+01	1.36e+01	1.27e+01
T	Z	48	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
T	Z	48	6.67e+00	3.36e-01	3.50e-01	3.06e-01	2.79e-01	2.83e-01	1.08e+01	1.02e+01	9.62e+00	9.13e+00	8.66e+00
T	Z	240	3.56e+00	2.00e-01	1.77e-01	1.76e-01	1.45e-01	1.51e-01	6.13e+00	5.89e+00	5.58e+00	5.32e+00	5.06e+00
T	Z	240	3.56e+00	1.80e-01	1.70e-01	1.62e-01	1.15e-01	1.41e-01	5.81e+00	5.51e+00	5.24e+00	5.04e+00	4.79e+00
T	Z	240	1.05e+01	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00e+00
T	Z	240	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
T	Z	240	6.68e+00	3.72e-01	3.60e-01	3.26e-01	2.17e-01	2.89e-01	1.11e+01	1.04e+01	9.89e+00	9.50e+00	9.00e+00
T	Z	720	3.57e+00	1.60e-01	1.53e-01	1.20e-01	7.70e-02	0.00e+00	5.66e+00	5.38e+00	5.17e+00	5.05e+00	5.05e+00
T	Z	720	3.57e+00	1.57e-01	1.49e-01	1.04e-01	6.96e-02	0.00e+00	5.49e+00	5.23e+00	5.05e+00	4.93e+00	4.93e+00
T	Z	720	1.05e+01	5.05e-01	4.89e-01	5.92e-02	1.43e-01	1.58e-01	1.59e+01	1.51e+01	1.50e+01	1.47e+01	1.45e+01
T	Z	720	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00	0.00e+00
T	Z	720	6.67e+00	2.64e-01	2.50e-01	1.86e-01	6.17e-02	1.26e-01	9.85e+00	9.41e+00	9.09e+00	8.99e+00	8.77e+00