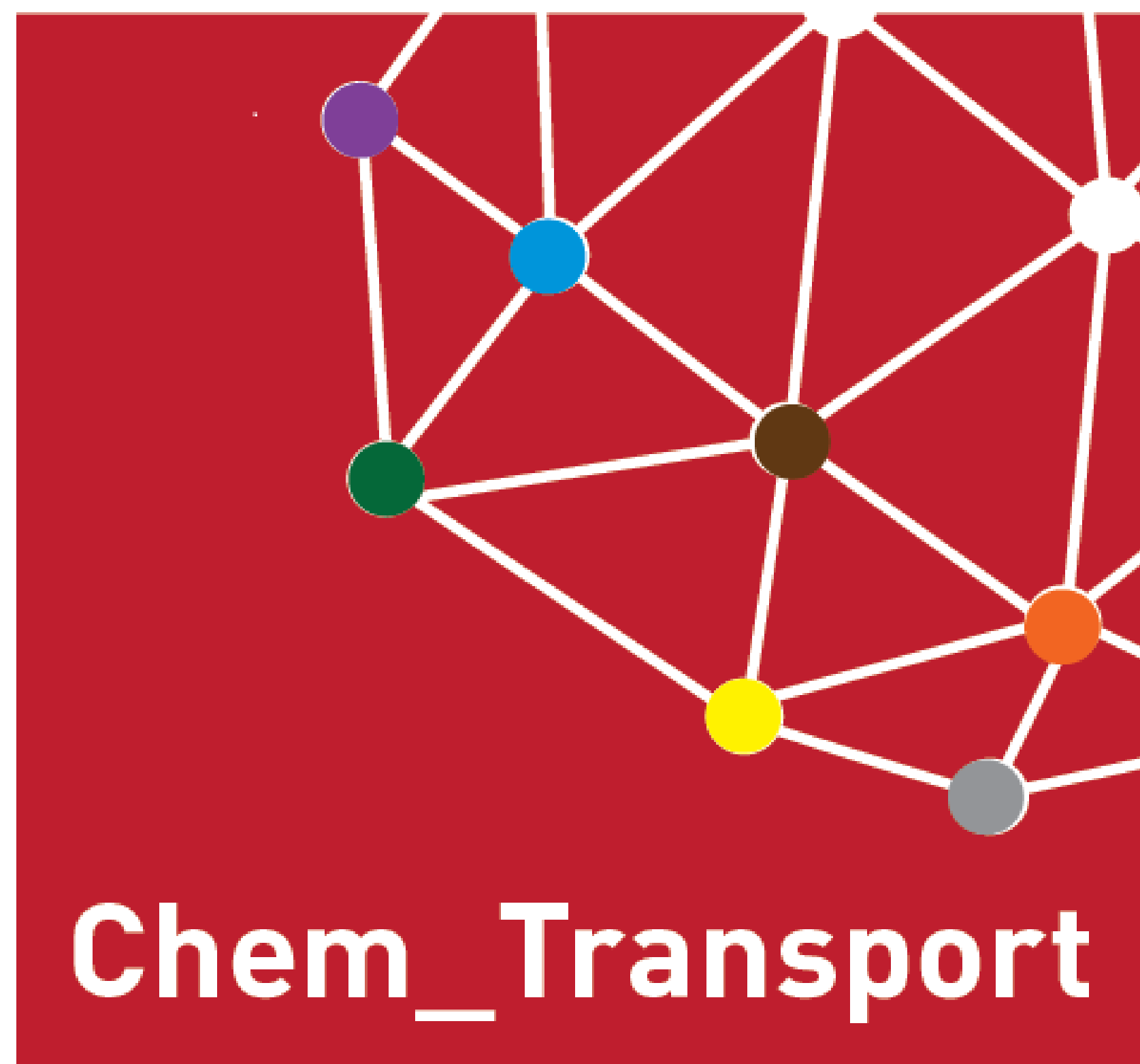


Software Models for Chemical Kinetic Retention and Transport in Soils

Magdi Selim (mselectim@agcenter.lsu.edu)

School of Plant, Environmental and Soil Sciences



Background

Chem_Transport is a software package of several models that describe the transport and sorption of chemicals in soils and other porous media. These models are characterized by two main features; they are nonlinear and kinetic in nature. The models are broad in nature and address various physical and chemical processes that influence the behavior of solutes in porous media.

Chem_Transport models are applicable for variety of chemicals in field settings as well as controlled laboratory and greenhouse environments. The models represent transport conditions and batch type reactors under no-flow conditions. Two types of models are presented; simulation type models where the user provides all physical and chemical parameters. This class of models is most suitable for classroom teaching and risk assessment. The second class of models is that where the user provides an experimentally measured data set and a selected model will provide best-fit description of measured results.

Users

Teaching - Can be incorporated in classroom teaching for undergraduate and graduate students in chemical and civil engineering, hydrology, geology, soil physics and chemistry, environmental sciences and environmental engineering.

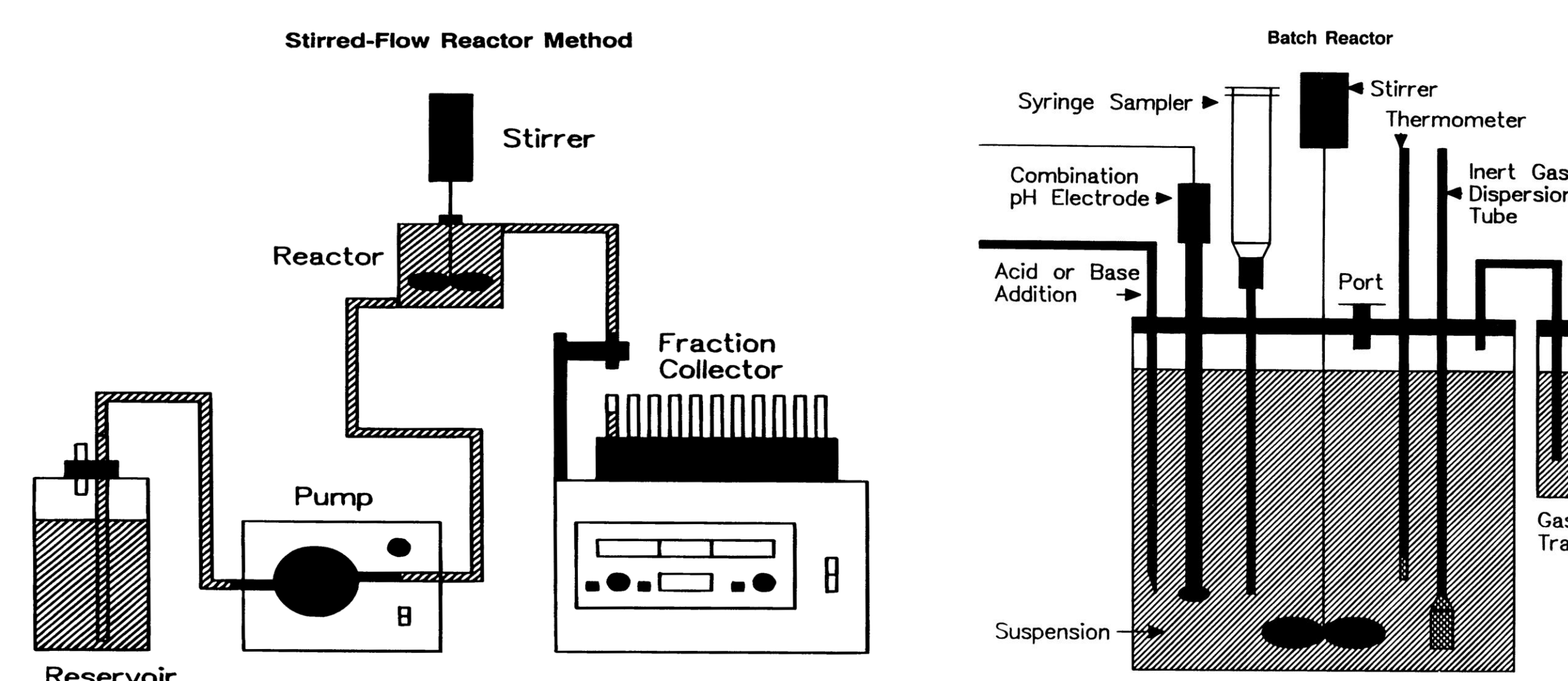
Simulations based on various scenarios provide information on system parameters (sensitivity analysis) and risk assessment.

Research - This software should be useful to environmental scientists, engineers, and geologists whose desire is to describe laboratory or field observations under various constraints such as batch reactors, miscible displacements, and transport in saturated and unsaturated soils. It should also be useful for federal and state agencies, researchers, consulting engineers, and decision makers in the management and restoration of contaminated sites.

List of Models

BATCH KINETIC	TRANSPORT
Simulations Models:	Simulations Models:
Nonlinear Kinetic (NKM)	Multireaction and Transport Model (MRTML)
Langmuir Kinetic (LKM)	Second Order Two-Site (SOTSL)
Multireaction Model (MRM)	SOTS Mobile-Immobile (SOMIM)
Second Order Two-Site (SOTS)	Competitive-MRTM (CMRM)
Stir-Flow with MRM (STIRFLOW-MRM)	MRTM Mobile Immobile (MRTM_MIM)
Thin-Disk Flow with MRM (THINDISK-MRM)	Ion-Exchange Transport Model (ION-EXCH)
Competitive-MRM	Model for Mixed Media (MRTM-MIXED)
	Tracer Transport (TRACER)
Fitting Models:	Fitting Models:
Multireaction Model (MRM-FIT)	Multireaction Model (MRTM-FIT)
Second Order Two-Site (SO-FIT)	Second Order Two-Site (SOT-FIT)
Competitive MRM (CMRM-FIT)	Second Order Mobile-Immobile (SOMIM-FIT)
	Multireaction-Immobile Model (MRTM-MIM-FIT)
	Competitive-Multireaction (CMRTM-FIT)

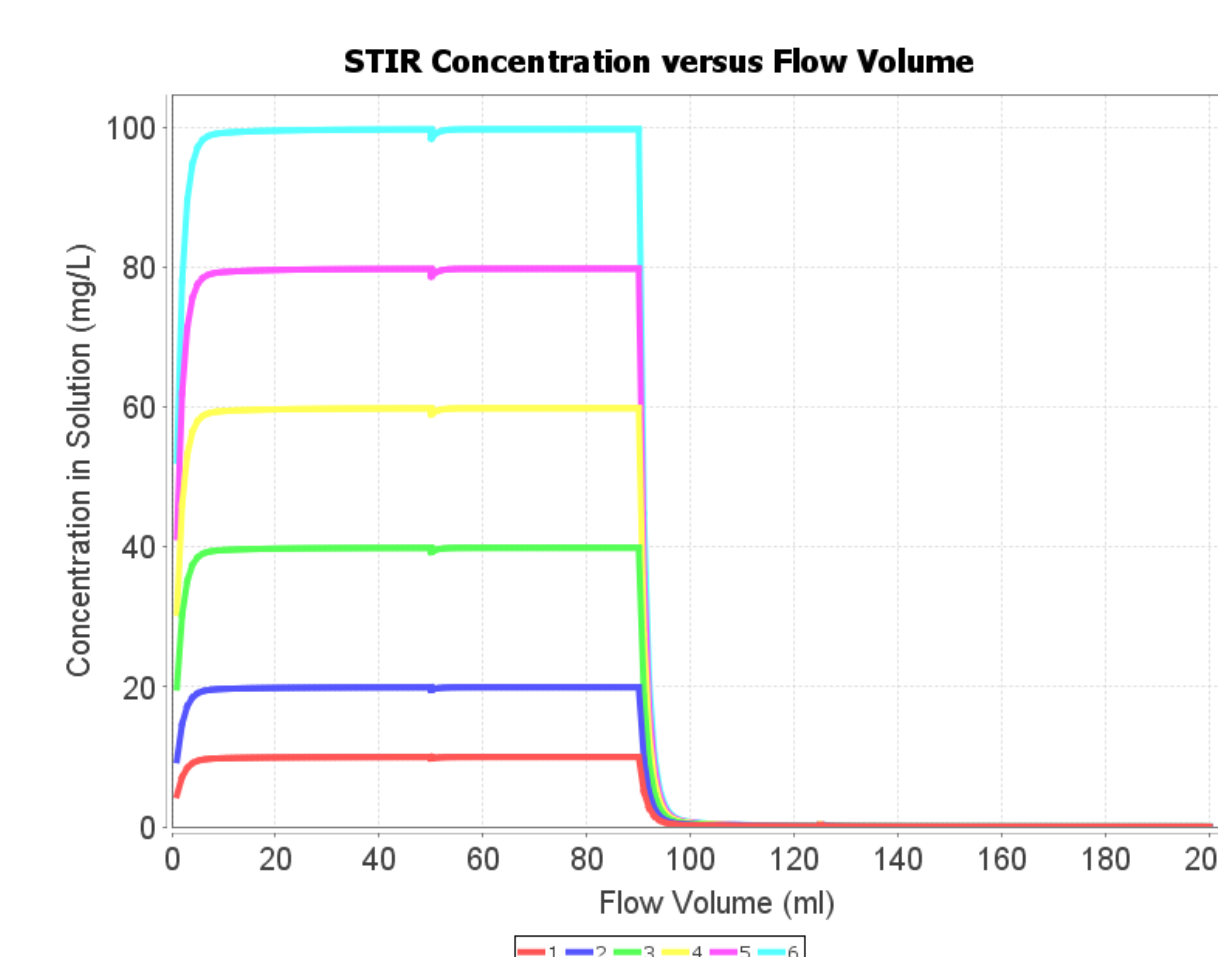
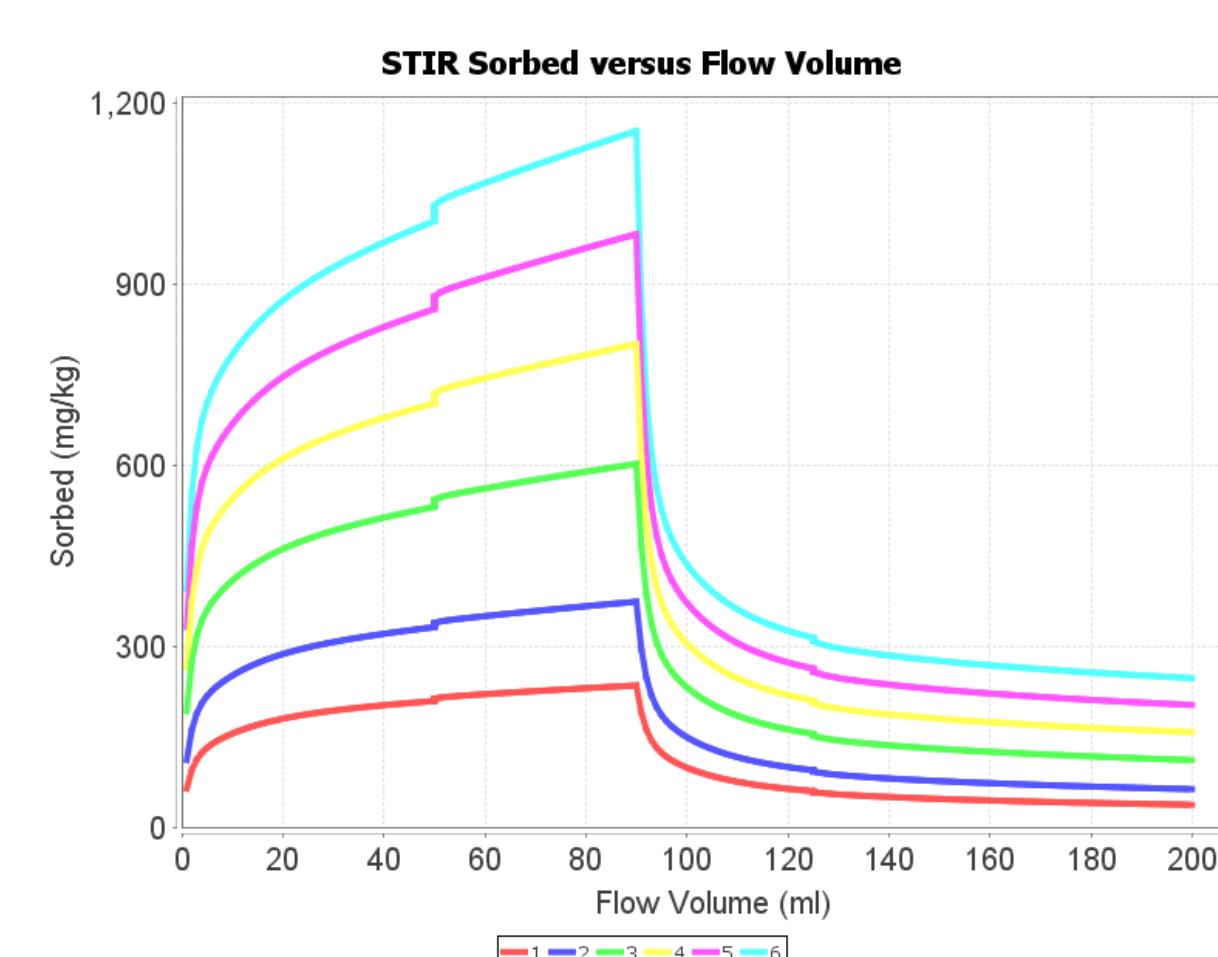
Batch Kinetic



Template for the STIRFLOW-MRM model

Model selected is STIRFLOW-MRM
Title: STIR FLOW USING MRM - TEST CASE - SENSITIVITY ANALYSIS

NUMBER OF ISOTHERMS DESIRED	Case 1	Case 2	Case 3
Moisture Content, CM3/CM3 (TH)	20.000E00	20.000E00	20.000E00
Bulk Density, G/CM3 (ROU)	1.000E00	1.000E00	1.000E00
Volume of Vessel (ML) (+VOLUME)	30	30	30
Flow Rate (ML/HR) (QFLOW)	1	1	1
Initial Concentration, MG/L (CO)	0.000E00	0.000E00	0.000E00
Applied Concentration, MG/L (CS)	10.000E00	20.000E00	40.000E00
Distribution Coefficient, KD CM3/G (KD)	20.000E00	20.000E00	20.000E00
Nonlinear Freundlich Parameter (N) (NEQ)	0.7500E00	0.7500E00	0.7500E00
Forward Rate Reaction, K1, min-1 (K1)	0.1	0.1	0.1
Forward Rate Reaction, K2, min-1 (K2)	0.1	0.1	0.1
Nonlinear Kinetic Parameter, U, (U)	0.500E00	0.500E00	0.500E00
Forward Rate Reaction, K3, min-1 (K3)	0.010E00	0.010E00	0.010E00
Forward Rate Reaction, K4, min-1 (K4)	0.010E00	0.010E00	0.010E00
Nonlinear Kinetic Parameter, U, (U)	0.500E00	0.500E00	0.500E00
Forward Rate Reaction, K5, min-1 (K5)	0.0	0	0
Backward Rate Reaction, K6, min-1 (K6)	0.000E00	0.000E00	0.000E00
Irreversible Reaction Rate, KS, min-1 (KS)	0.0010E00	0.0010E00	0.0010E00
Duration of Input Pulse Application (TP)	100	100	100
Concent of Leaching Solution, MG/L (CSL)	0.0	0.0	0.0
Total Simulation Time, minutes (TOTAL)	200.0E00	200.0E00	200.0E00
Printout Time Desired, minutes (TPRINT)	1.00E00	1.00E00	1.00E00
Number of Stop Flow or Interruptions (NSF)	2	2	2
Starting Time for Stop Flow # 1 (MIN)	50	50	50
Duration of Stop Flow # 1 (MIN)	10	10	10
Starting Time for Stop Flow # 2 (MIN)	125	125	125
Duration of Stop Flow # 2 (MIN)	10	10	10

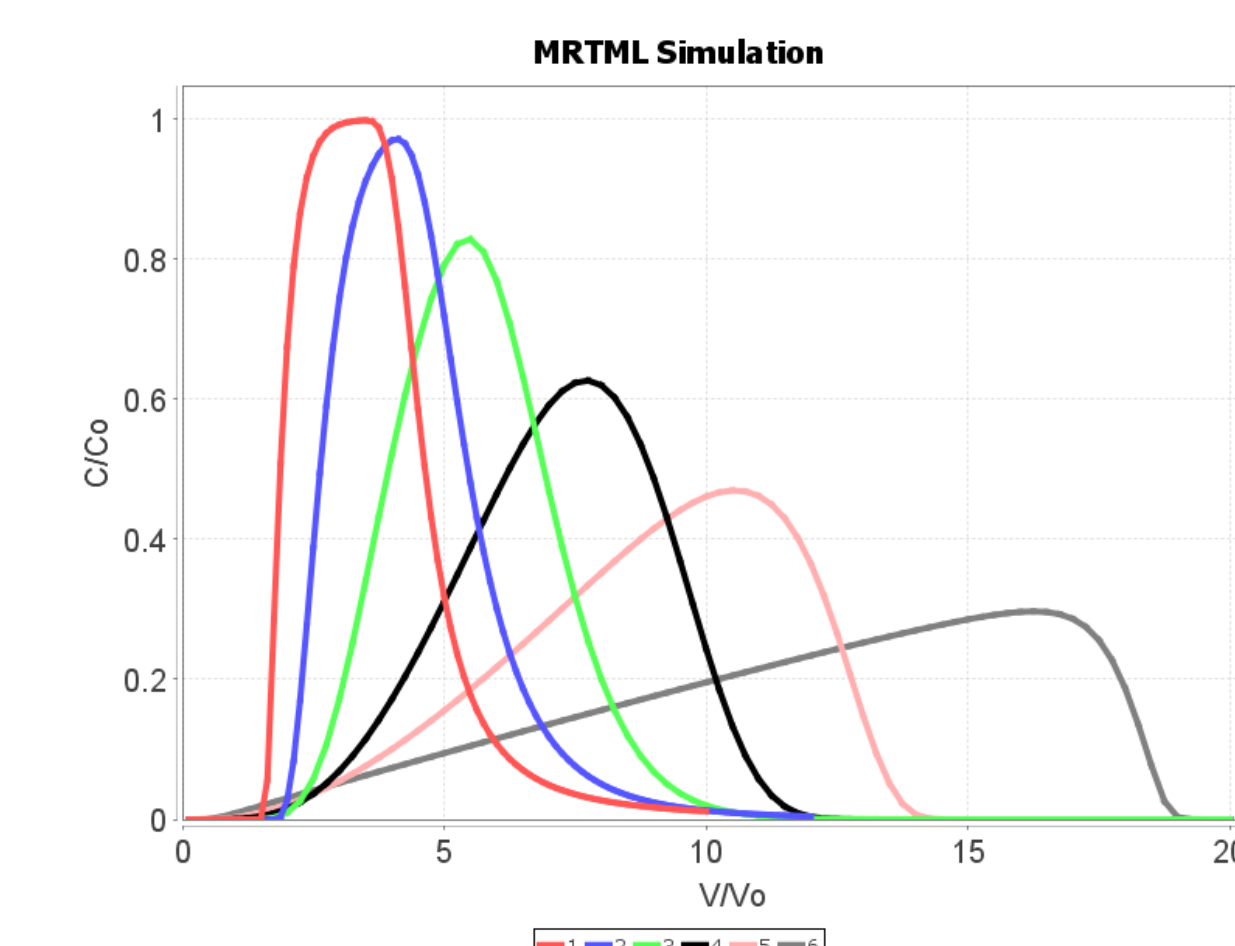


Transport

Template for the MRTML model

Model selected is MRTML
Title: MULTIREACTION TRANSPORT MODEL - SENSITIVITY ANALYSIS

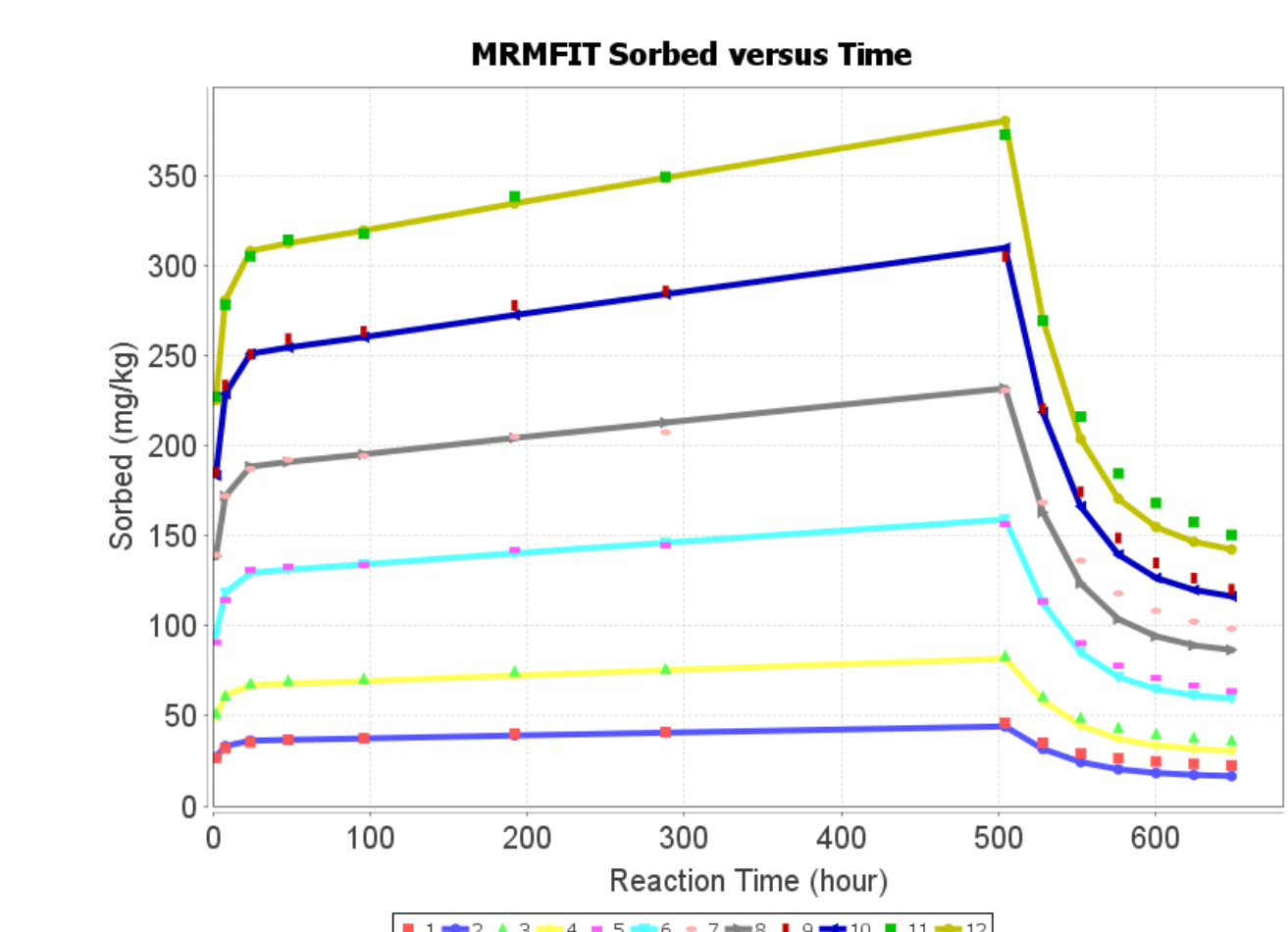
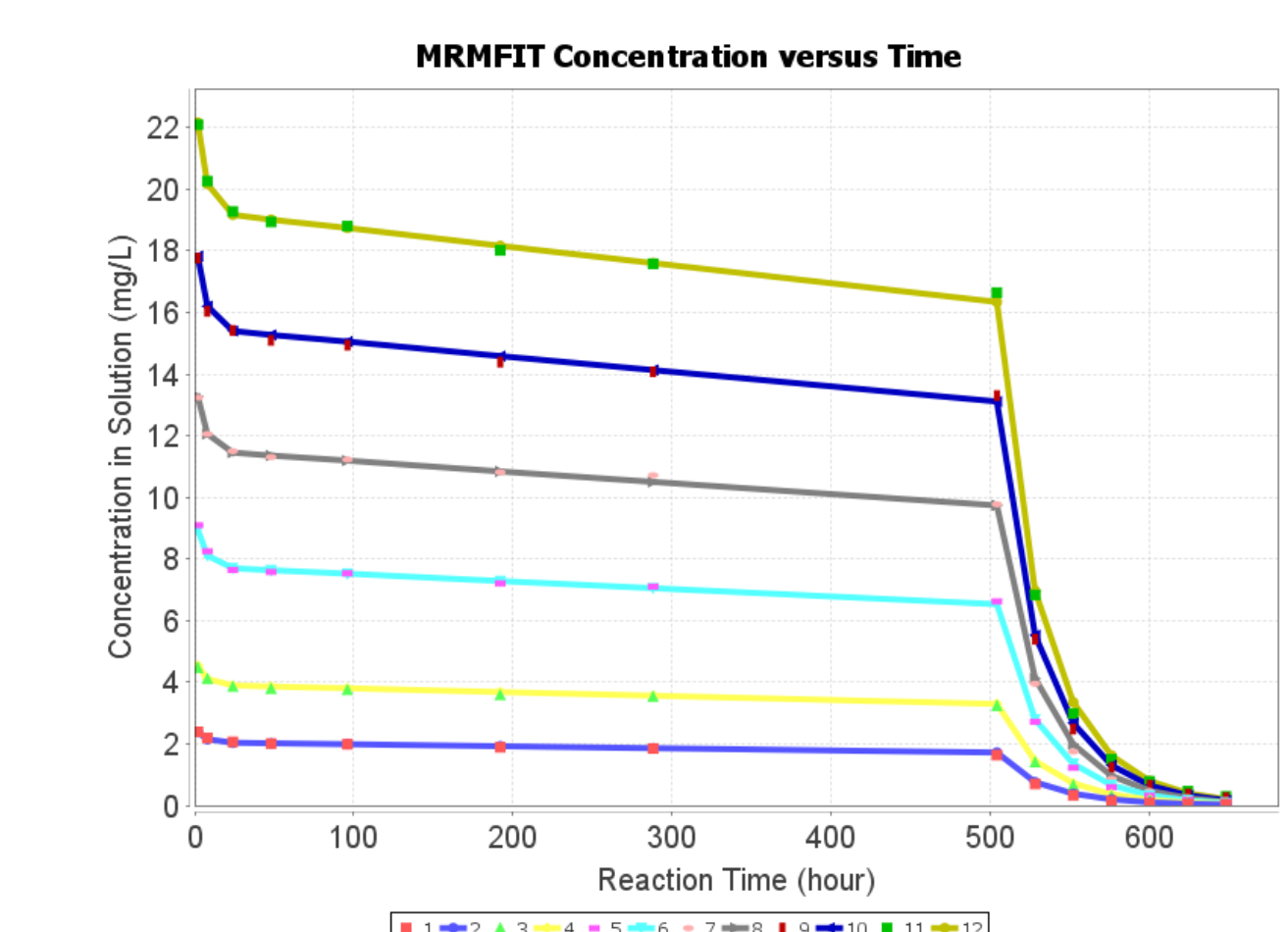
Input parameters	Case 1	Case 2	Case 3
Water Flux, CM/DAY (WFLX)	1.0000	1.0000	1.0000
Initial Concentration, MG/ML (CI)	0.0	0.0	0.0
Solute Conc. in Input Pulse, MG/ML (CS)	10.0	10.0	10.0
Duration of Input Pulse, DAYS (TPULSE)	12.0000	12.0000	12.0000
Total Simulation Time, DAYS (TOTAL)	40.0000	40.0000	40.0000
Printout Time Desired, DAYS (TPRINT)	0.5000	0.5000	1.0000
Initial Time Step, DT, DAYS (DT)	0.2000	0.2000	0.2000
Initial Increm. Distance, DX, CM (DX)	1.0000	1.0000	1.0000
Number of Soil Layer in Profile (NS)	001	001	001
Number of Iterations Desired (IT)	1	1	1
Thickness (CM) of Layer 1, (COL)	10	10	10
Soil Moisture Content of Layer 1, (TH)	0.4000	0.4000	0.4000
Soil Bulk Density of Layer 1, (ROU)	1.2500	1.2500	1.2500
Dispersion Coeff. of Layer 1, CM2/DAY (D)	1.000	1.000	1.000
Distribution Coeff. for Eq. CM3/G (KD)	1.00	1.00	1.00
Nonlinear Eq. Param. N, Layer 1 (NEQ)	0.5000	0.75000	1.0000
Forward Reaction Rate, K1, DAY-1, L-1 (K1)	0.0000	0.0000	0.0000
Backward Reaction Rate, K2, DAY-1, L-1 (K2)	0.000	0.000	0.000
Nonlinear Kinetic Para. W, Layer 1 (W)	0.000	0.000	0.000
Forward Reaction Rate, K3, DAY-1, L-1 (K3)	0.000	0.000	0.000
Backward Reaction Rate, K4, DAY-1, L-1 (K4)	0.0000	0.0000	0.0000
Nonlinear Kinetic Para. U, Layer 1 (U)	0.000	0.000	0.000
Irreversible Rate Coefficient, DAY-1 (KS)	0.000	0.000	0.000
Forward Reaction Rate, K5, DAY-1, L-1 (K5)	0.0000	0.0000	0.0000
Backward Reaction Rate, K6, DAY-1, L-1 (K6)	0.000	0.000	0.000



Template for the MRM-FIT model

Model selected is MRM-FIT
Title: DATA FROM ATRAZINE-SUGARCANE RESIDUE-ADSOR. DESOR. REQ (2005) 34:325-335, Pgs. 5&6:1

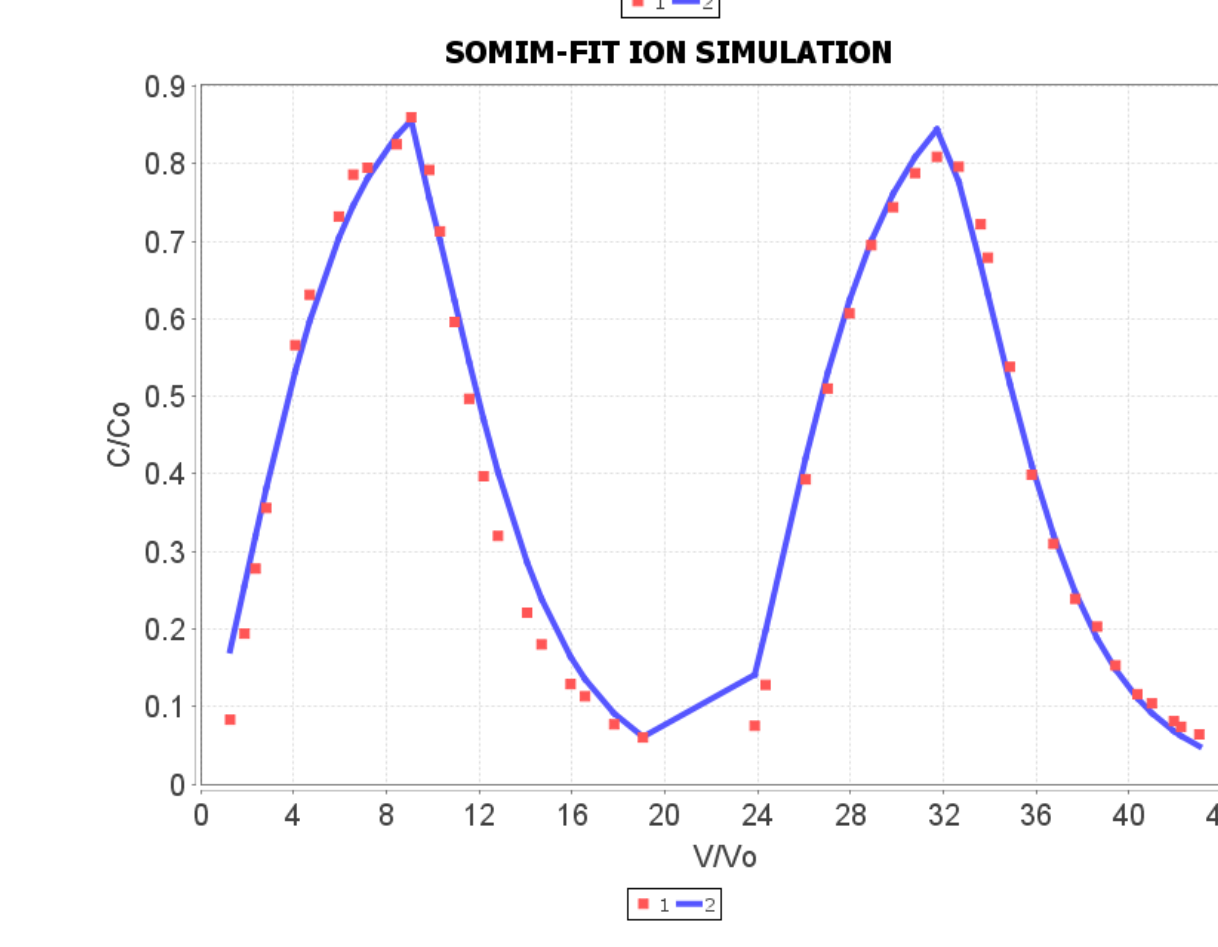
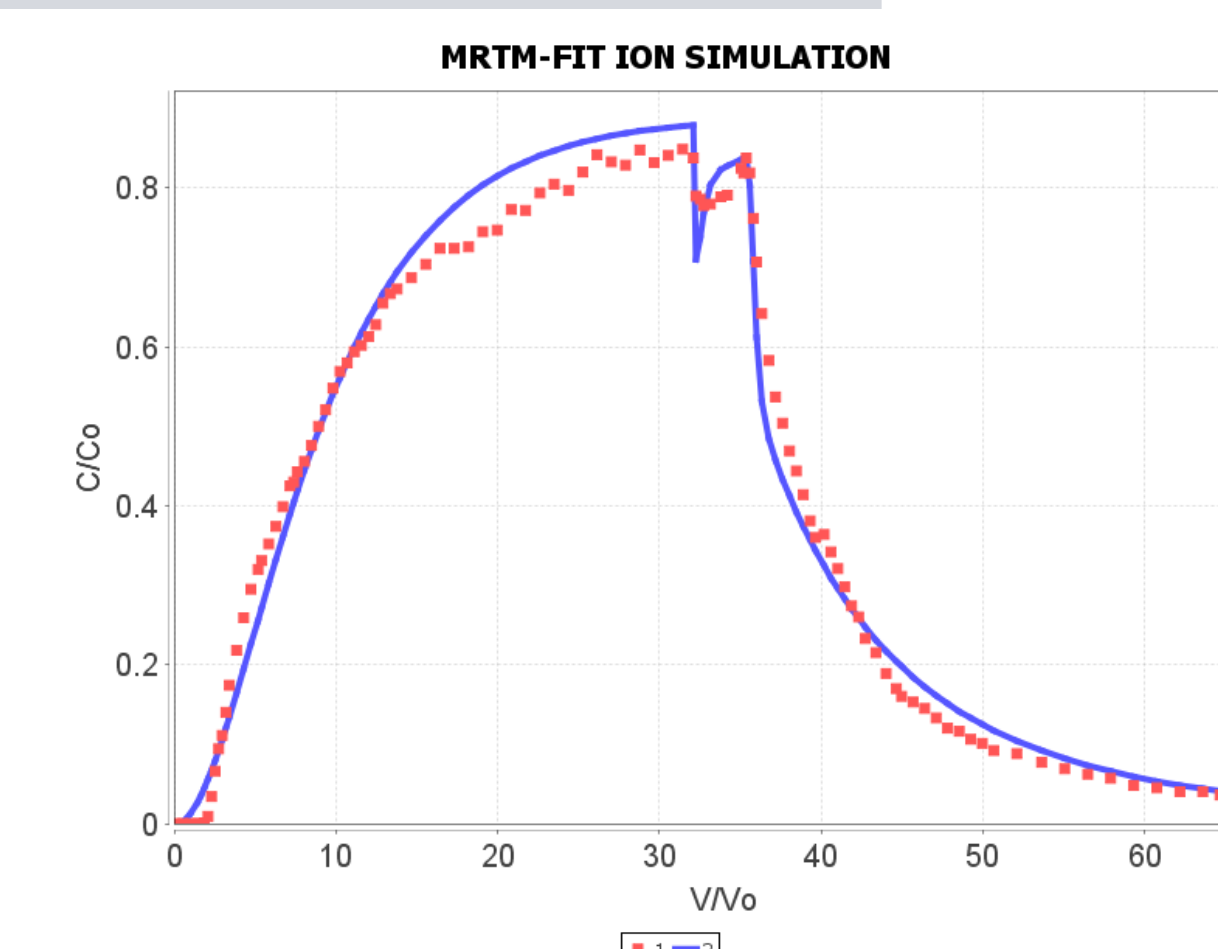
Input parameters	Value
Initial Concentration, MG/L (CI)	0.0000E00
Incremental Time Step, HOUR (DT)	0.1000E00
Printout Time Interval, (PRQOUT)	2.0000E00
Maximum Number of Iterations (MIT)	40
Distrib. Coeff. for Eq. SORP, CM3/G (KF)	0.8000E00
Nonlinear Param. for Eq. MECH. (NF)	0.9477E00
Irreversible Reaction Rate, KS, HR-1 (KIRR)	0.0000E00
Forward Rate Reaction, K1, HR-1 (K1)	0.0000E00
Backward Rate Reaction, K2, HR-1 (K2)	0.0000E00
Nonlinear Kinetic Parameter, W, (NS1)	0.0000E00
Forward Rate Reaction, K3, HR-1 (K3)	0.3500E00
Backward Rate Reaction, K4, HR-1 (K4)	0.1100E00
Nonlinear Kinetic Parameter, U, (NS2)	0.9477E00
Forward Rate Reaction, K5, HR-1 (K5)	0.0002E00
Backward Rate Reaction, K6, HR-1 (K6)	0.0000E00
Number of Fitted Parameters (NP)	4



Template for the MRTM-FIT model

Model selected is MRTM-FIT
Title: SILVER TRANSPORT CASE FOR LOW WATER AND SOIL K1 (4:2)

Input parameters	Value
Moisture Content (CM3/CM3) (THETA)	0.559
Bulk Density (G/CM3) (ROU)	1.156
Column Length (CM) (LENGTH)	5.0
Initial Solute Concentration (UG/ML) (C0)	0.000
Diffusion Coeff. in Water (CM2/HR) (DIPWATER)	0.000472
Interaction Step in Time (HR) (DT)	0.5
Interaction Step in Length (CM) (DX)	0.4
Output Frequency (HOURS) (FREQU)	10
Maximum Iteration Number (MIT)	35
Dispersion Coefficient (D)	0.754
Equilibrium Coefficient (KE)	0.0
Nonlinear Equilibrium Parameter (NE)	0.426
Irreversible Coeff. KIRR (C--SRR)	0.000
Rate Coefficient K1 (C--S1)	0.000
Nonlinear Kinetic Parameter (U)	0.426
Rate Coefficient K2 (S1--C)	0.0
Rate Coefficient K3 (C--S2)	0.08
Rate Coefficient K4 (S2--C)	0.08
Nonlinear Kinetic Parameter (W)	0.426
Rate Coefficient K5 (S2--S3)	0.005
Rate Coefficient K6 (S3--S2)	0.000
Number of Fitted Parameters (NP)	3
Number of Applied Pulses (DSET)	1
Input Concentr. (UG/ML)	207.9000
Darcy Flux (CM/HR)	0.310000
Pulse Start P.V. (P.V.)	0.000000
Pulse Stop P.V. (P.V.)	35.310000
Flow Interruption Starts At (P.V.)	32.200000
Duration of Flow Interruption (HOURS)	48.000000



Template for the SOMIM-FIT model

Model selected is SOMIM-FIT
Title: DATA FROM ATRAZINE-SUGARCANE RESIDUE-ADSOR. DESOR. REQ (2005) 34:325-335, Pgs. 5&6:1

Input parameters	Value
Moisture Content (CM3/CM3) (THETA)	0.4000
Soil Water Fraction (FM)	0.318
Soil Aggregate Size (CM) (RADIUS)	0.007
Soil Bulk Density (G/CM3) (ROU)	1.000
Column Length (CM) (LENGTH)	10.0
Initial Solute Concentration (UG/ML) (C0)	0.000
Water Diffusion Coefficient (CM2/HR) (DIPWATER)	0.000472
Interaction Step in Time (HR) (DT)	0.5
Interaction Step in Length (CM) (DX)	0.2
Output Frequency (HOURS) (FREQU)	10
Maximum Iteration Number (MIT)	10
NP	1.00000
NS1	184.62
NS2	0.00040
NS3	0.000
NS4	0.000
NS5	0.000
NS6	0.000
NS7	0.000
NS8	0.000
NS9	0.000
NS10	0.000
NS11	0.000
NS12	0.000
NS13	0.000
NS14	0.000
NS15	0.000
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NS85	0.000
NS86	0.000
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NS89	0.000
NS90	0.000
NS91	0.000
NS92	0.000
NS93	0.000
NS94	0.000
NS95	0.000
NS96	0.000
NS97	0.000
NS98	0.000
NS99	0.000
NS100	0.000

MEASURED DATA
NUMBER OF OBSERVATION DATA POINTS: 49

V/V0	C/C0
1.274	0.083
1.898	0.194
2.366	0.278
2.834	0.356
4.082	0.566
4.706	0.631
5.955	0.732
6.579	0.788
7.203	0.795
8.451	0.825
9.075	0.860
9.855	0.792
10.323	0.713
10.947	0.596
11.571	0.497
12.195	0.397
12.819	0.320
14.067	0.221
14.691	0.180
15.939	0.129
16.563	0.113
17.812	0.077
19.060	0.060
23.871	0.075
24.242	0.158