

State-of-the-art Environmental Modeling for Surface- Subsurface Systems



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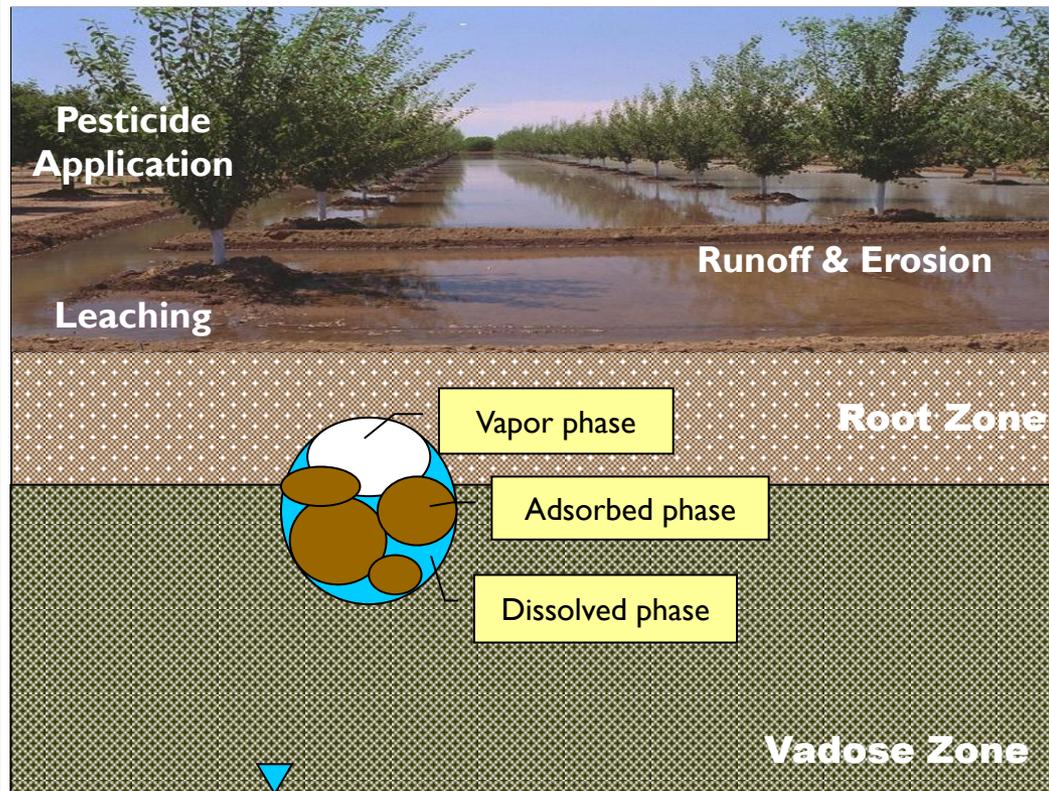


Part I

Windows-Based Integrated Pesticide Transport Model (IPTM)

- **Theoretical Background**
- **Windows-based Software**

Pesticide Transport Modeling in the Canopy Zone, Surface Runoff and the Unsaturated Zone



Major processes in Canopy Zone: degradation, volatilization, and washoff

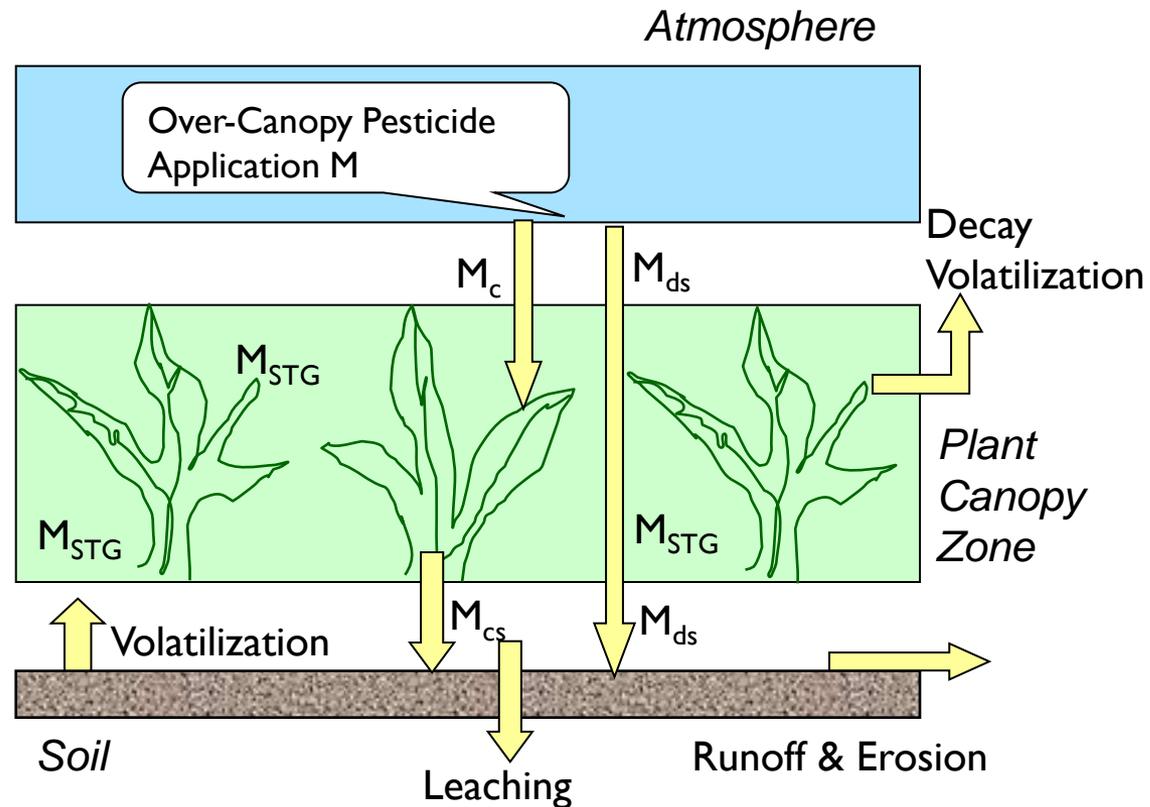
Major processes in Surface Zone: advection, dispersion, sorption, liquid-vapor partitioning, degradation, volatilization, runoff, and erosion.

Major processes in Root Zone: advection, dispersion, sorption, liquid-vapor partitioning, degradation, and root uptake.

Major processes in Vadose Zone: advection, dispersion, sorption, liquid-vapor partitioning, and degradation.

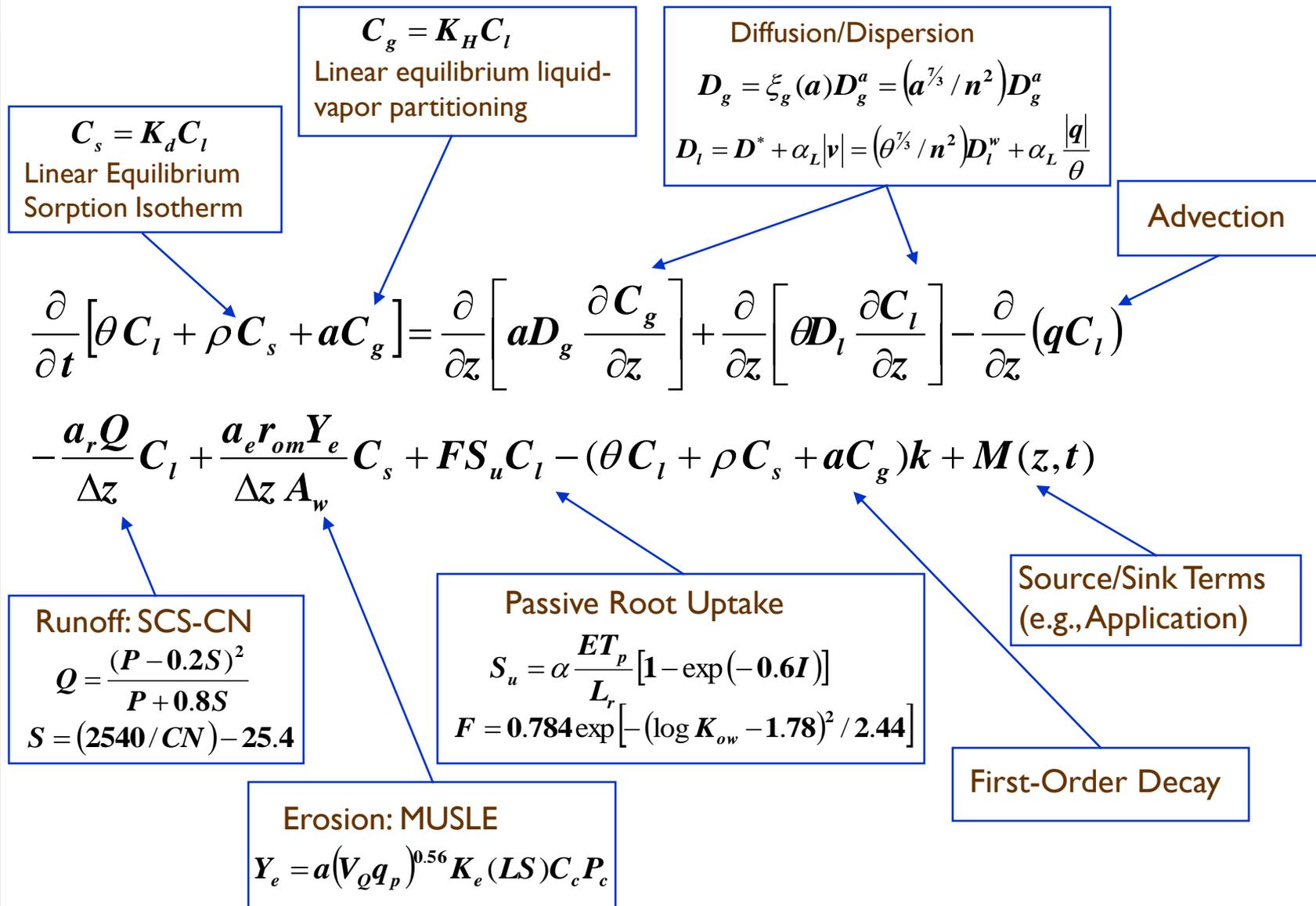
4-Zone System: Canopy Zone, Surface Zone, Crop Root Zone, and Deep Vadose Zone

Pesticide Processes and Modeling in the Canopy Zone



$$\frac{dM_{STG}(t)}{dt} = m_c(t) - m_{cs}(t) - k_c(t)M_{STG}(t)$$

Mathematical Expressions for Simulating I-D Three-Phase Pesticide Transport in the Unsaturated Zone



TC-SD Semidiscrete Method (Time Continuous & Space Discrete)

Second-Order PDE

$$\frac{\partial}{\partial t} [(\theta + \rho K_d + a K_H) C] = \frac{\partial}{\partial z} \left[a D_g \frac{\partial}{\partial z} (K_H C) \right] + \frac{\partial}{\partial z} \left[\theta D_l \frac{\partial C}{\partial z} \right] - \frac{\partial}{\partial z} (qC) - r_0 C - (\theta + \rho K_d + a K_H) k C + M(z, t)$$

$$C(z, t_0) = C_0(z)$$

$$-E^g \frac{\partial C_g}{\partial z} - E^l \frac{\partial C_l}{\partial z} + qC_l = qC_l^{in} - \frac{D_a}{d} (C_g - C_g^a) \quad \text{For } t > 0 \text{ and } z = 0$$

$$-E^g \frac{\partial C_g}{\partial z} - E^l \frac{\partial C_l}{\partial z} + qC_l = qC_l^{out} \quad \text{For } t > 0 \text{ and } z = L$$

TC-SD Semidiscrete Method



First-Order ODE System

$$\dot{\mathbf{C}}(t) = \mathbf{A}(t)\mathbf{C}(t) + \mathbf{M}(t)$$

Closed-Form Solution

$$\mathbf{C}(t) = \Phi(t, t_0)\mathbf{C}(t_0) + \int_{t_0}^t \Phi(t, \tau)\mathbf{M}(\tau)d\tau$$

State Transition Matrix Φ

$$\begin{aligned}\Phi(t, t_0) &= \lim_{j \rightarrow \infty} \left\{ \mathbf{I} + \sum_{k=0}^{j-1} \int_{t_0}^t \mathbf{A}(\tau_1) \int_{t_0}^{\tau_1} \mathbf{A}(\tau_2) \cdots \int_{t_0}^{\tau_k} \mathbf{A}(\tau_{k+1}) d\tau_{k+1} \cdots d\tau_1 \right\} \\ &= \mathbf{I} + \int_{t_0}^t \mathbf{A}(\tau_1) d\tau_1 + \int_{t_0}^t \mathbf{A}(\tau_1) \left[\int_{t_0}^{\tau_1} \mathbf{A}(\tau_2) d\tau_2 \right] d\tau_1 + \cdots\end{aligned}$$


$$\mathbf{C}(t) = \mathbf{e}^{\mathbf{A}(t-t_{0,i})} \mathbf{C}(t_{0,i}) + \int_{t_{0,i}}^t \mathbf{e}^{\mathbf{A}(t-\tau)} \mathbf{M}(\tau) d\tau$$

For instantaneous application

$$\mathbf{C}(t) = \mathbf{e}^{\mathbf{A}(t-t_{0,i})} [\mathbf{C}(t_{0,i}) + \mathbf{m}]$$

For continuous application

$$\mathbf{C}(t) = \mathbf{e}^{\mathbf{A}(t-t_{0,i})} \mathbf{C}(t_{0,i}) + \mathbf{A}^{-1} [\mathbf{e}^{\mathbf{A}(t-t_{0,i})} - \mathbf{I}] \mathbf{m}$$

Solution Methods in IPTM

Two-point first-order upwind scheme

Second-order central differencing

Multi-point high-order linear upwind-biased schemes

Nonlinear van Leer flux limiter



Pesticide Application Methods in IPTM

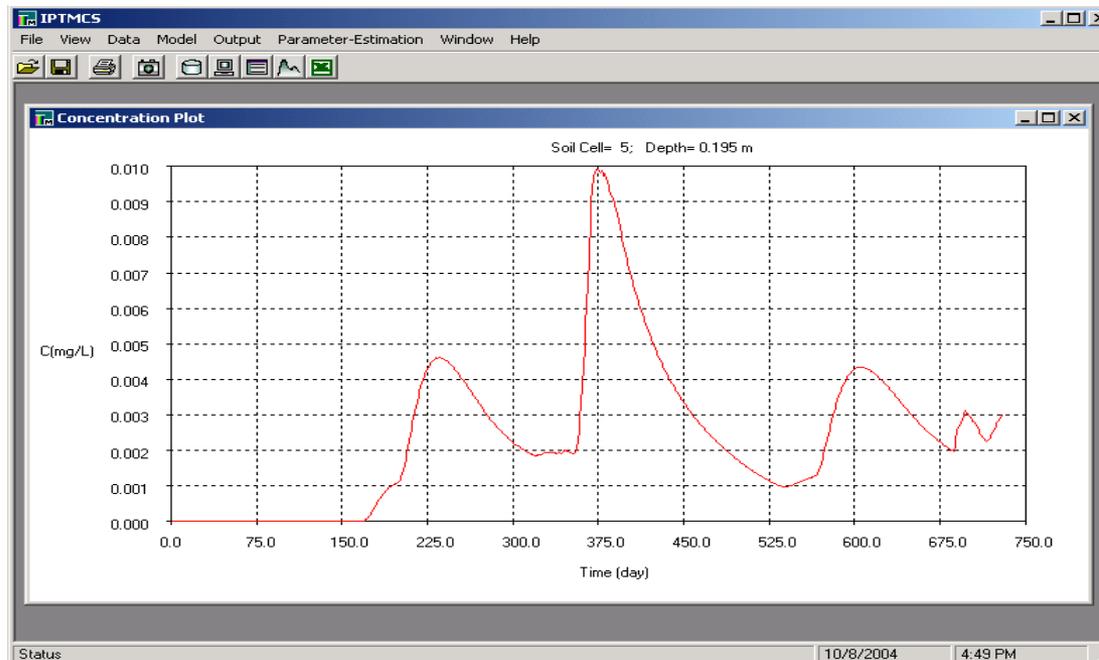
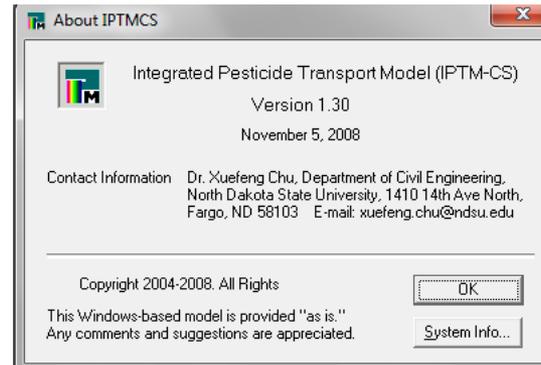
Over-canopy

Under-canopy

Combined foliar and soil surface spray

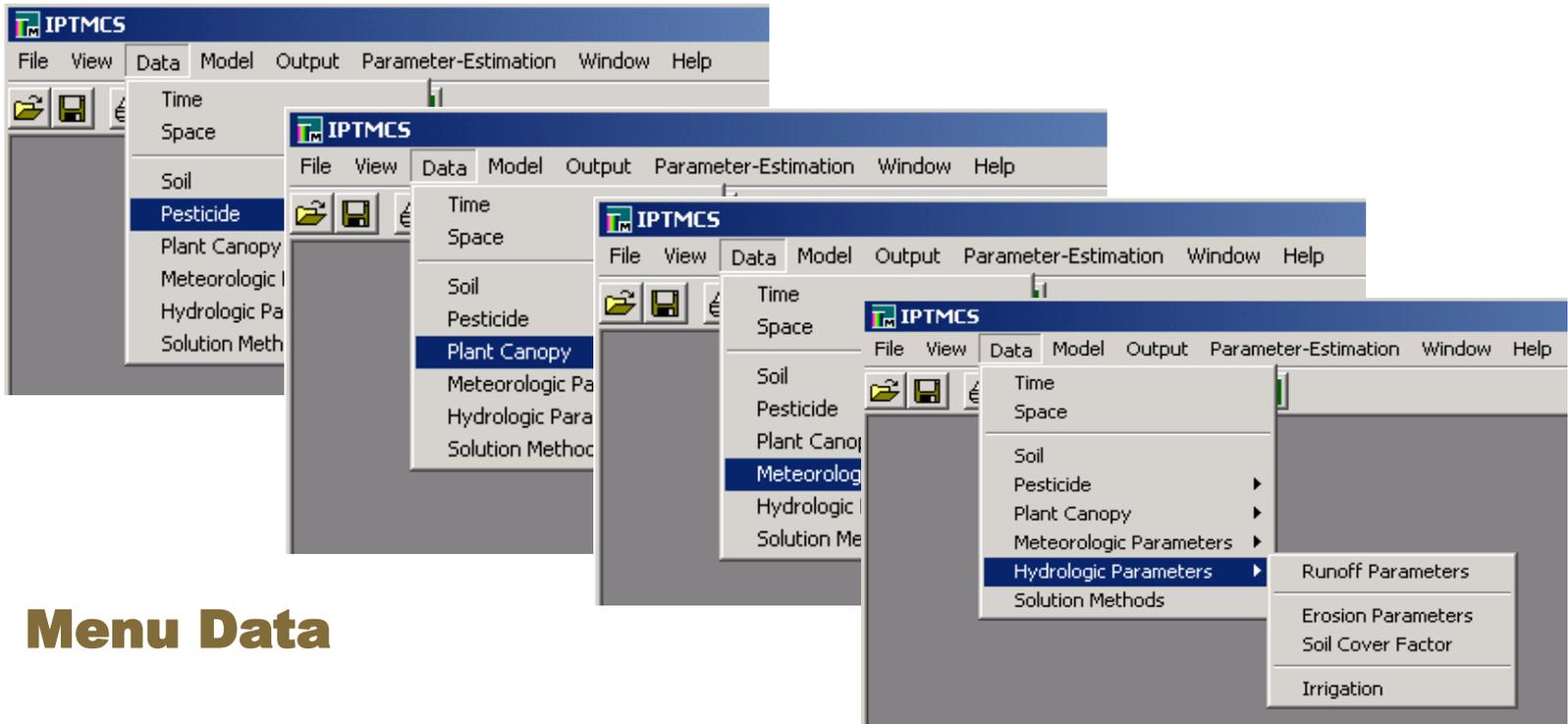
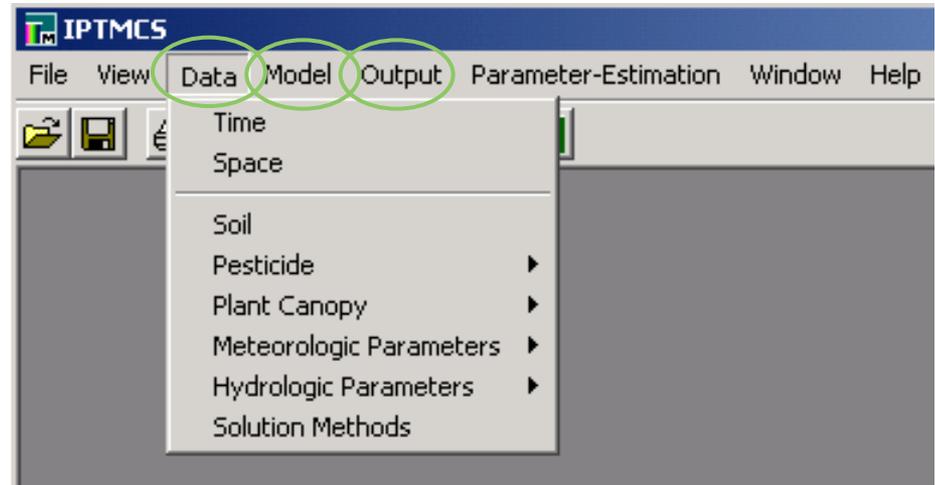
Soil-incorporated applications.

Windows-Based IPTM: Integrated Pesticide Transport Modeling System



IPTM-CS:

Three modeling steps –
Three major menus (Data,
Model, Output)



Menu Data

Menu Output (post-processing)

IPTMCS
File View Data Model Output Parameter-Estimation Window Help

Concentration Table
Concentration Graph
Concentration Excel

Water Table for Canopy
Water Table for Soil Surface
Soil Water Content

Pesticide Table for Canopy
Pesticide Table for Soil Surface

Pesticide Runoff
Pesticide Erosion

Pesticide Concentrations
Pesticide Concentration Table (mg/L)

No.	Depth (m)		
1	0.010	0.00000000	0.0000
2	0.045	0.00000000	0.0000
3	0.095	0.00000000	0.0000
4	0.145	0.00000000	0.0000
5	0.195	0.00000000	0.0000
6	0.245	0.00000000	0.0000
7	0.295	0.00000000	0.0000
8	0.345	0.00000000	0.0000
9	0.395	0.00000000	0.0000
10	0.445	0.00000000	0.0000
11	0.495	0.00000000	0.0000
12	0.545	0.00000000	0.0000
13	0.595	0.00000000	0.0000
14	0.645	0.00000000	0.0000
15	0.695	0.00000000	0.0000
16	0.745	0.00000000	0.0000
17	0.795	0.00000000	0.0000
18	0.845	0.00000000	0.0000
19	0.895	0.00000000	0.0000
20	0.945	0.00000000	0.0000
21	0.995	0.00000000	0.0000
22	1.045	0.00000000	0.0000
23	1.095	0.00000000	0.0000
24	1.145	0.00000000	0.0000

Water-Canopy.txt
Water Table for the Plant Canopy Zone (unit: cm)

No.	Date	Rain	RainC	RainS0	RainS1	RainS	Irri	IrriC
1	1/ 1/1996	.000000	.0					
2	1/ 2/1996	.000000	.0					
3	1/ 3/1996	.000000	.0					
4	1/ 4/1996	.000000	.0					
5	1/ 5/1996	.000000	.0					
6	1/ 6/1996	.000000	.0					
7	1/ 7/1996	.000000	.0					
8	1/ 8/1996	.000000	.0					
9	1/ 9/1996	.000000	.0					
10	1/10/1996	.000000	.0					
11	1/11/1996	.000000	.0					
12	1/12/1996	.000000	.0					
13	1/13/1996	.000000	.0					
14	1/14/1996	.000000	.0					
15	1/15/1996	.228400	.1					
16	1/16/1996	1.548000	.9					
17	1/17/1996	.050800	.0					
18	1/18/1996	.228400	.1					
19	1/19/1996	.2	.0					
20	1/20/1996	.0	.0					

Transfer Data to Excel

The concentration data are transferred to Excel..
It may take a minute depending on the numbers of the discretized cells and simulation time steps.

Please wait!!

Graphs

Time-Conc Graph
Depth-Conc Graph

Select a soil cell number

OK

Concentration Plot
Soil Cell= 3; Depth= 0.095 m

Plot Parameters

Plot Parameters

Xmin: 0 Xmax: 731
Ymin: 0 Ymax: 0.02396

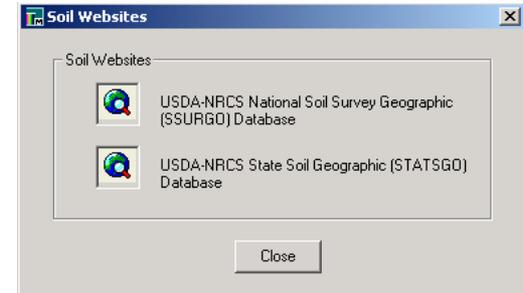
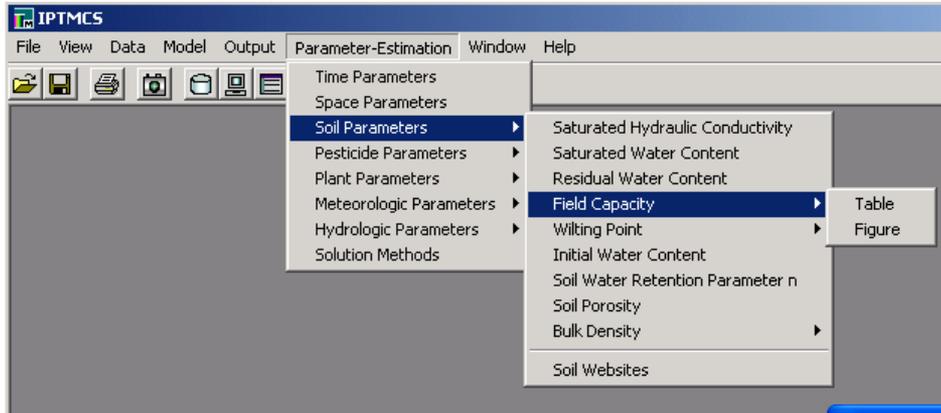
Number of X ticks: 10
Number of Y ticks: 10

Decimal digit of marked X values: ###0.0 (e.g., ###0.0, ### 0.000)
Decimal digit of marked Y values: ###0.000

Index of gridlines: 2
0 solid; 1 dash; 2 dot; 3 dash+dot; 4 dash+2dots; 5 no gridline

OK

Menu Parameter-Estimation

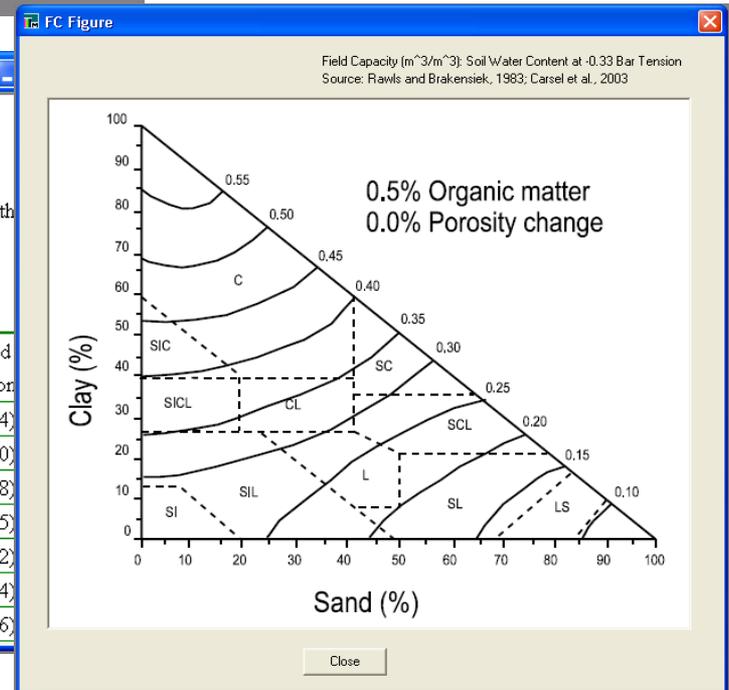


Field Capacity

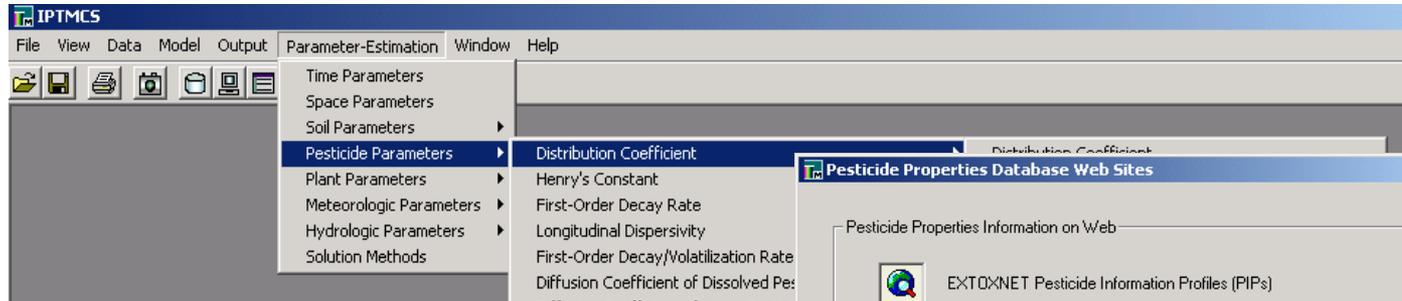
Field Capacity (m^3/m^3): FC
 Input FC values for both surface/root zone and deep vadose zone. FC can be estimated using the following table.

Field Capacity FC^a (m^3/m^3)

Soil Texture Class	Textural Properties (%)			FC (Water Retained at -0.33 Bar Tension)
	Sand	Silt	Clay	
Sand	85-100	0-15	0-10	0.091 (0.018-0.164)
Loamy Sand	70-90	0-30	0-15	0.125 (0.060-0.190)
Sandy Loam	45-85	0-50	0-20	0.207 (0.126-0.288)
Loam	25-50	28-50	8-28	0.270 (0.195-0.345)
Silt Loam	0-50	50-100	8-28	0.330 (0.258-0.402)
Sandy Clay Loam	45-80	0-28	20-35	0.257 (0.186-0.324)
Clay Loam	20-45	15-55	28-50	0.318 (0.250-0.386)



Menu Parameter-Estimation



Sw

Water Solubility S_w (20°C)

Chemical Name
1,2-Dichloropropane
1,3-Dichloropropene
1-Naphthaleneacetamide
2,4,5-T Amine Salts
2,4,5-T Esters
2,4-D Acid
2,4-D Esters or Oil-Soluble Salts
2,4-D Dimethylamine Salts
2,4-DB Acid
2,4-DB Butoxyethyl Esters
2,4-DB Dimethylamine Salts
2,4,5-T Acid
3-CPA Sodium Salt
Abamectin (Avermectin B1a)
Acephate

KH Calculator

KH Calculator

Vapor pressure (mmHg)

Solubility (mg/L)

Molecular weight (g/mol)

Temperature (Celsius)

Henry's Constant

Pesticide Properties Database Web Sites

Pesticide Properties Information on Web

- [EXTOXNET Pesticide Information Profiles \(PIPs\)](#)
- [USDA ARS Pesticide Properties Database](#)
- [Pesticide Properties Database - Oregon State University Extension](#)
- [USDA-ARS, GLEAMS](#)
- [ChemFinder Database and Internet Searching](#)
- [Jinno Laboratory Pesticide Database](#)

<http://extoxnet.orst.edu/pips/diazinon.htm>

Address: <http://extoxnet.orst.edu/pips/diazinon.htm>

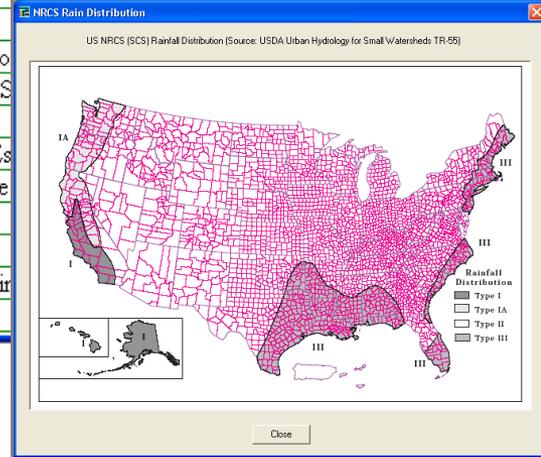
Diazinon

Trade and Other Names: Trade names of this product include Basudin, Dazal, Gardentox, Kayazol, Knox-Out, Nucidol, and Spectracide. Diazinon may be found in formulations with a variety of other pesticides such as pyrethrins, lindane, and disulfoton.

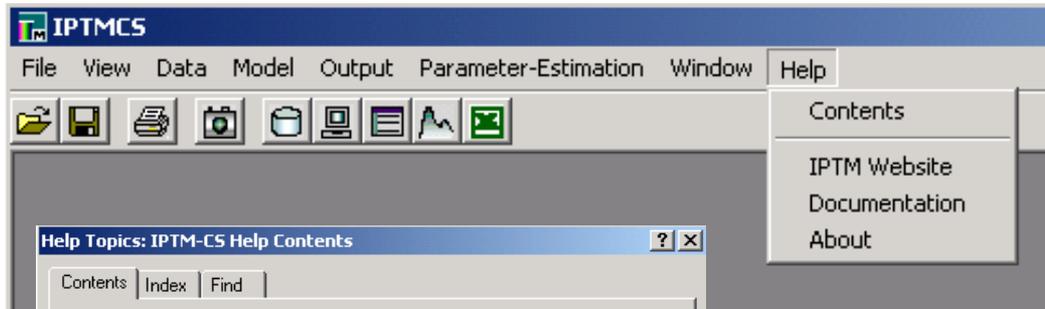
Regulatory Status: Diazinon is classified as a Restricted Use Pesticide (RUP) and is for professional pest control operator use only. In 1988, EPA canceled registration of diazinon for use on golf courses and sod farms because of die offs of birds that often congregated in these areas. It is classified toxicity class II - moderately toxic, or toxicity class III - slightly toxic, depending on the formulation. Products containing diazinon bear the Signal Word WARNING or CAUTION.

Chemical Class: organophosphate

Introduction: Diazinon is a nonsystemic organophosphate insecticide used to control cockroaches, silverfish, ants, and fleas in residential non-food buildings. Bait is used to control scavenger yellow



Menu Help



Help Topics: IPTM-CS Help Contents

Contents Index Find

Click a book, and then click Open. Or click another tab, such as Index.

- Introduction
- Getting Started
- File
- Data
- Model
- Output
- Parameter Estimation
- Documentation and Support

Open

Help Topics: IPTM-CS Help Contents

Contents Index Find

- 1 Type the first few letters of the word you're
 - 2 Click the index entry you want, and then clic
- 2-Year, 24-Hour Rainfall
 - AC
 - Air Boundary Layer Thickness
 - AMC
 - AP
 - Application Date
 - Application Depth
 - Application Times
 - AW
 - BAS
 - BD
 - Bulk Density
 - Canopy Decay Rate
 - Canopy-Soil Application Partition Factor
 - CC
 - Central Differencing
 - Check

Display

Documentation

Documentation



Introduction



User's Manual



Reference Paper 1: Chu, Xuefeng and M. A. Marino. 2004. J. Hydrol. 285:19-40.



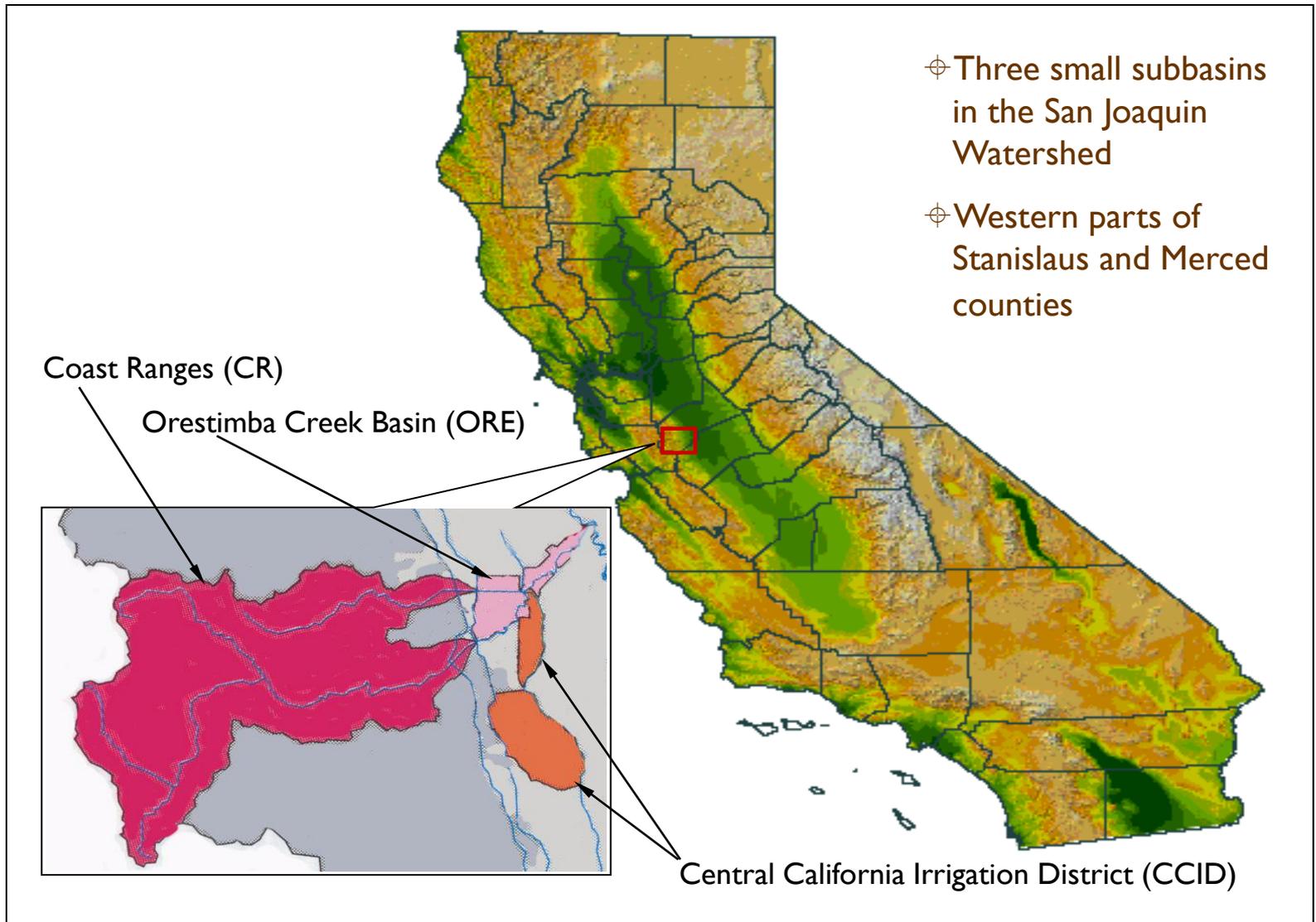
Reference Paper 2: Chu, Xuefeng and M.A. Marino. 2006. J. Environ Engng. ASCE. 132(2):211-219.



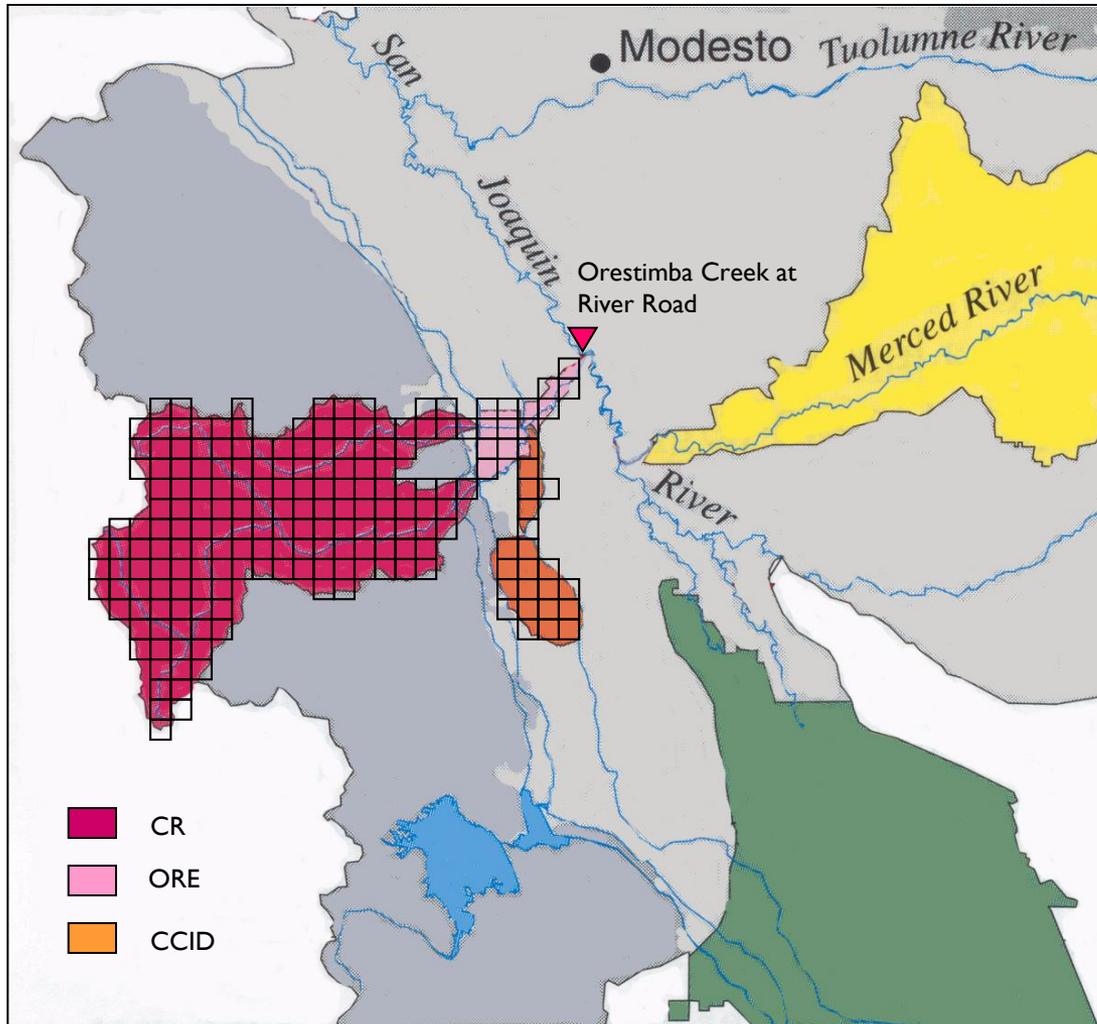
Reference Paper 3: Chu, Xuefeng and M.A. Marino. 2007. Environ. Model. Softw. 22(9):1316-1327.

Close

Application - Study Area and Location



Section Map and Areas



- Orestimba Creek Basin (ORE): 13 sections, 33,670,000 m²
- Central California Irrigation District (CCID): 22 sections, 56,980,000 m²
- Coast Ranges (CR): 164 sections, 424,760,000 m²
- Total 199 sections

Simulation Period

1/1/1996 - 12/31/1997
(731 days)

Pesticide Applications

Pesticide: diazinon

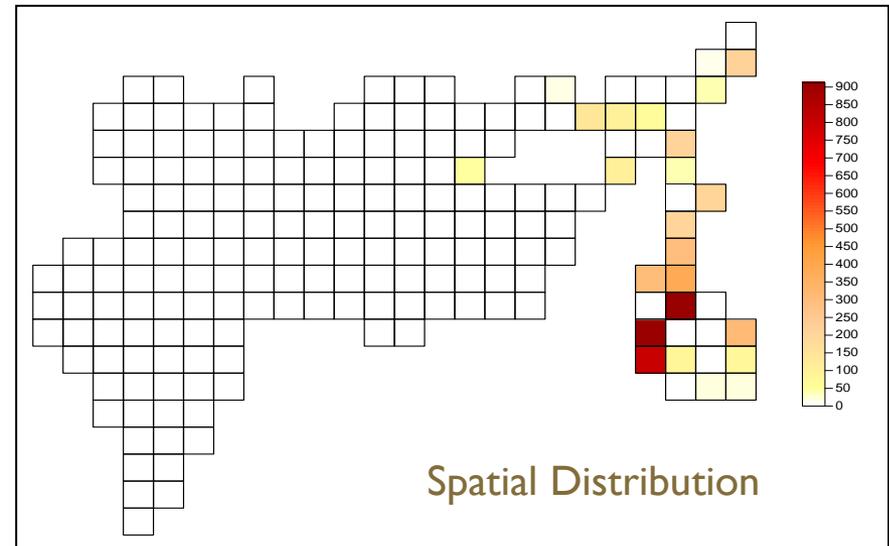
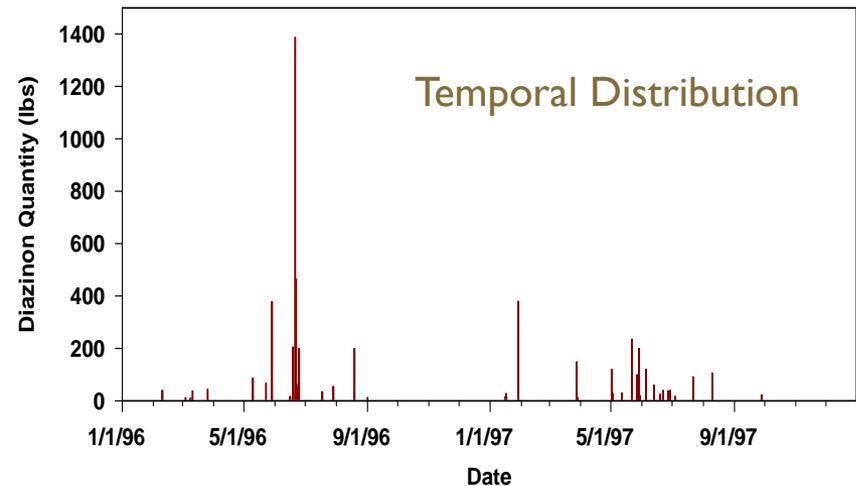
24 diazinon-applied sections

Crops

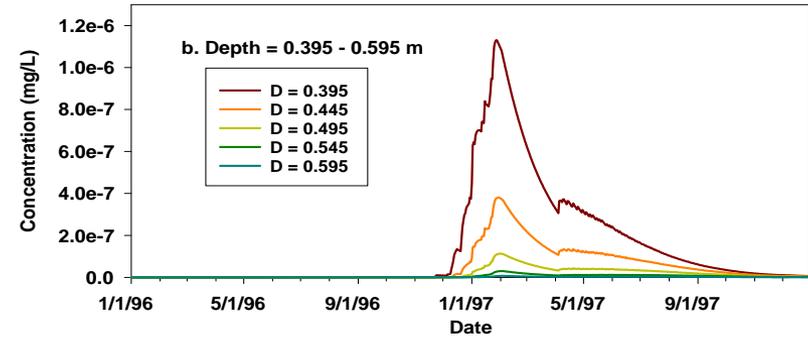
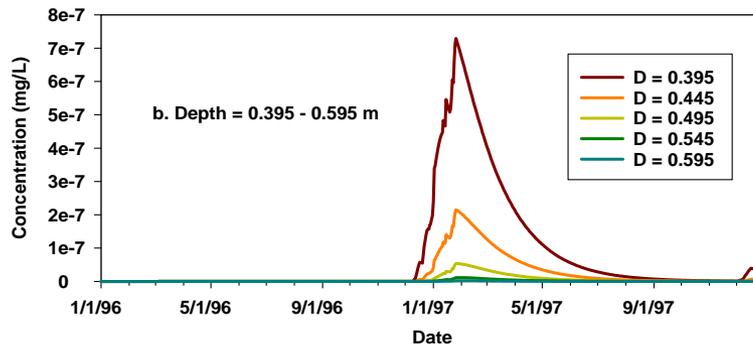
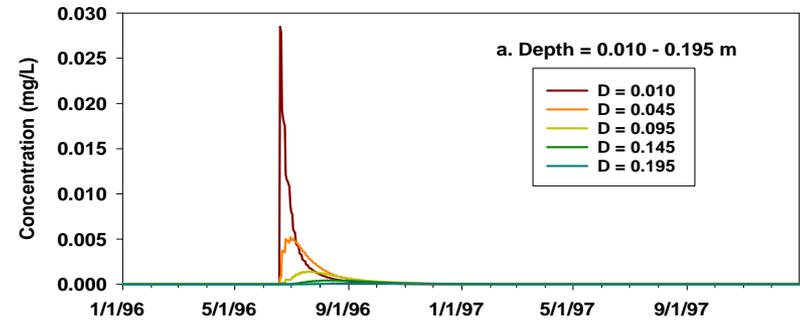
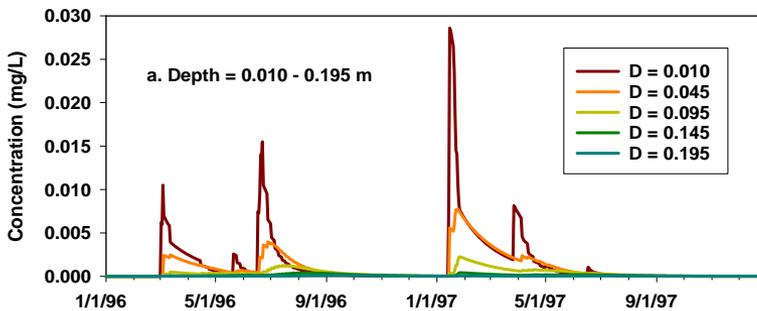
Almond and walnut (orchard crops), and tomatoes, beans, and alfalfa (vegetable, field, or pasture crops).

Soils

Clay loam, loam, and sandy loam are three major soil types

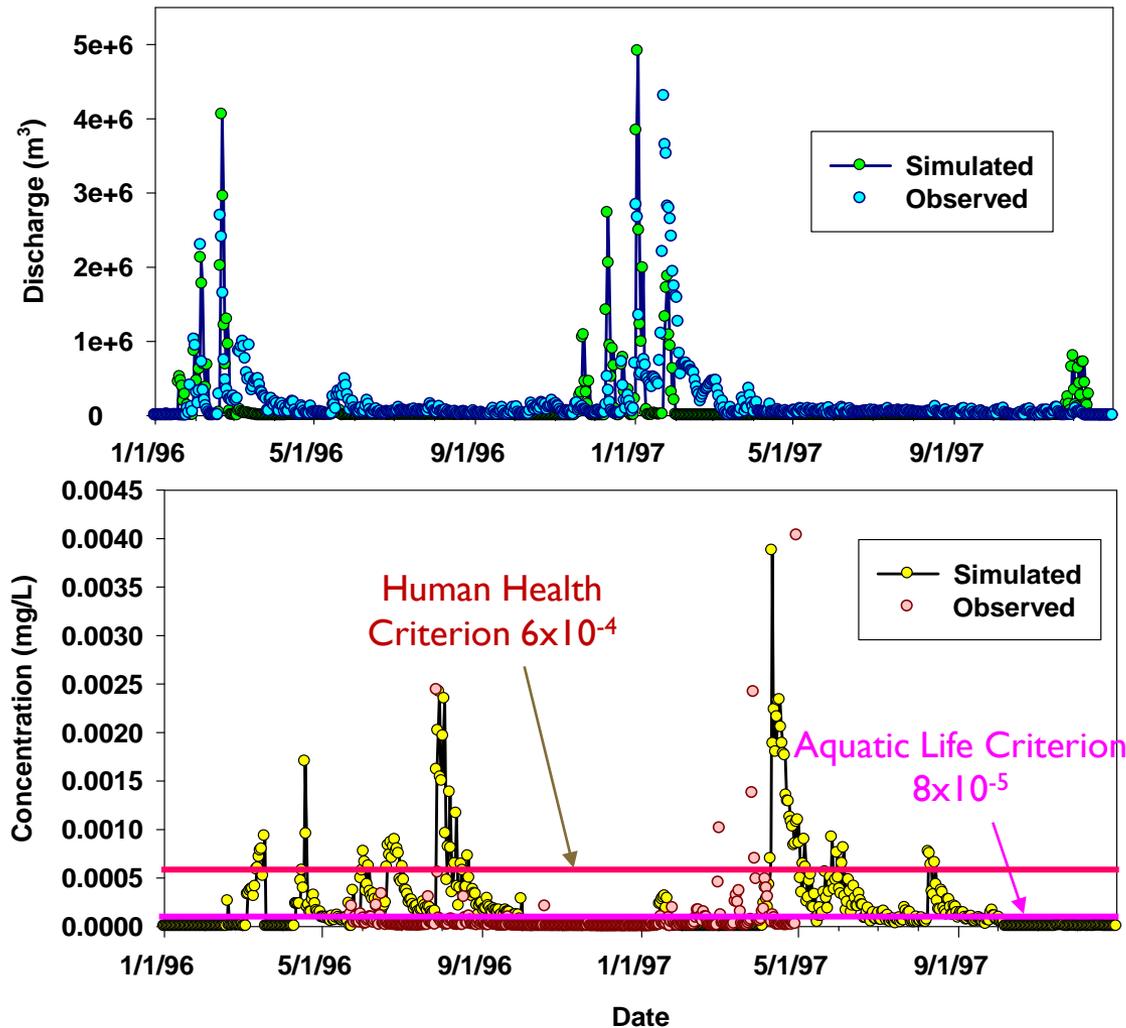


Diazinon in the Subsurface Environment



- ✦ The combined timing of pesticide application and rainfall/irrigation dominates the exposure levels of diazinon in the subsurface environment
- ✦ In the deeper soil, diazinon peaks generally follow the heavy rainfall season (end of January or early February).
- ✦ Diazinon concentrations decrease rapidly along the soil profile and contamination is limited within the soil less than 1 m.

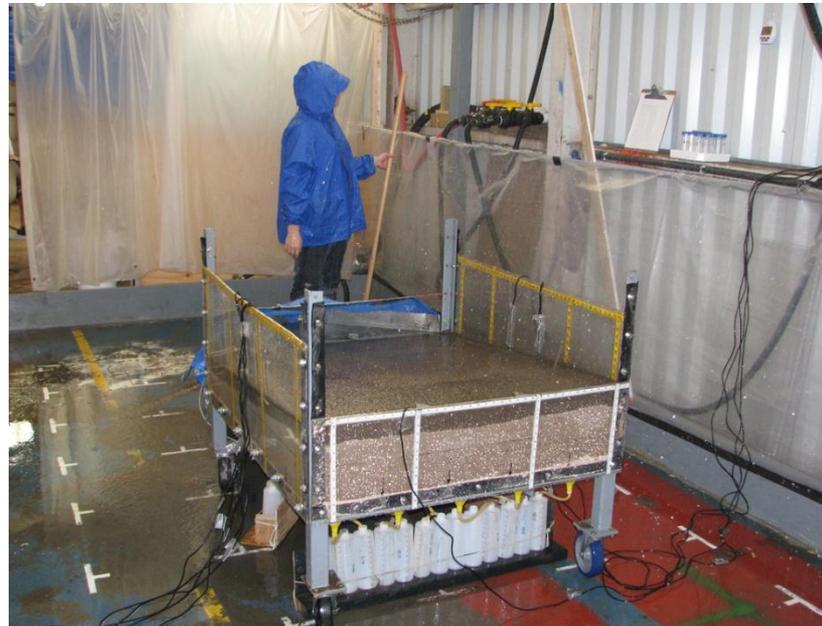
Diazinon in the Creek (at the Outlet)



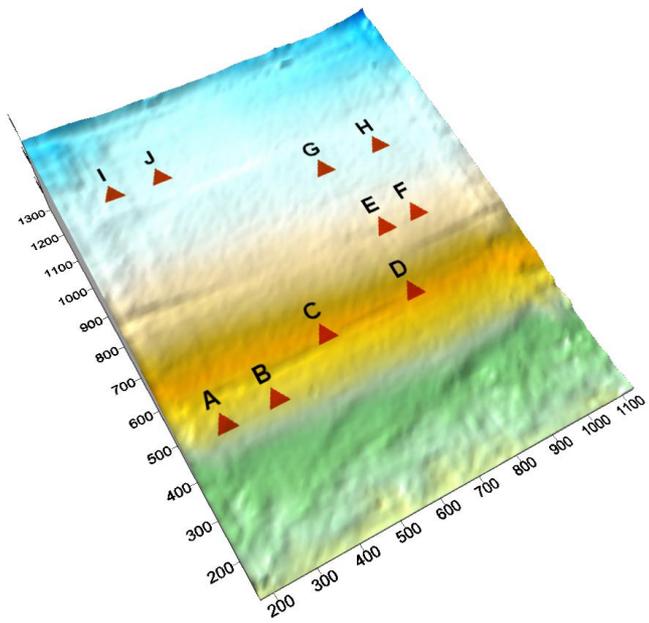
Diazinon in the Orestimba Creek Basin frequently exceeds criteria for aquatic life ($0.08 \mu\text{g/L}$). Worse of all, diazinon concentrations even exceed the human-health criterion ($0.6 \mu\text{g/L}$). Such high peak pulses may last up to a half month..

Part II

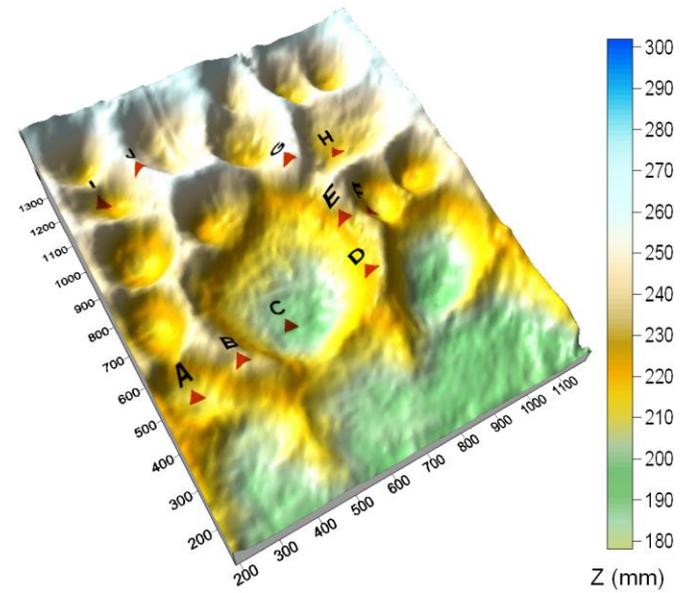
Tracer (Br) Transport under the Influence of Surface Microtopography



Smooth vs. Rough Soil Surfaces Tracer Sampling Locations

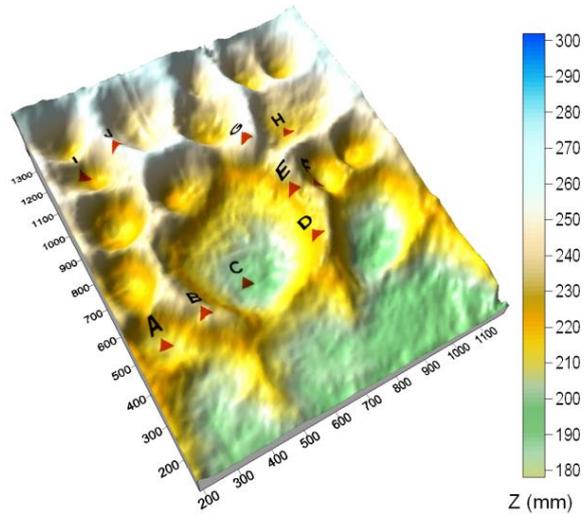


Z (mm)

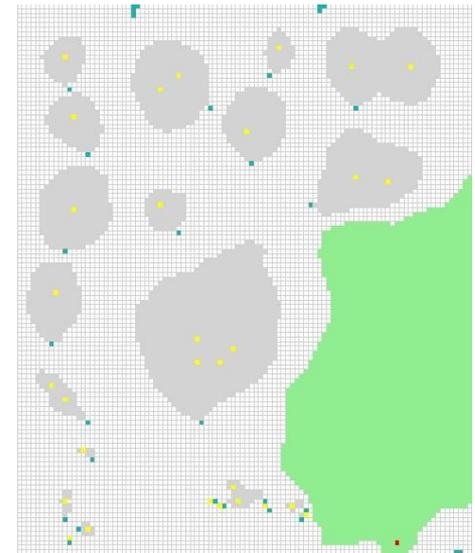
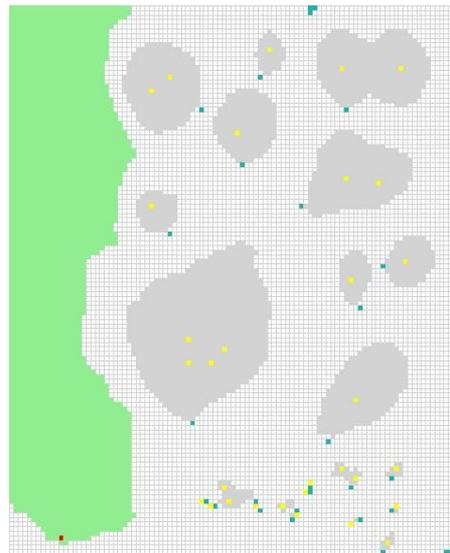
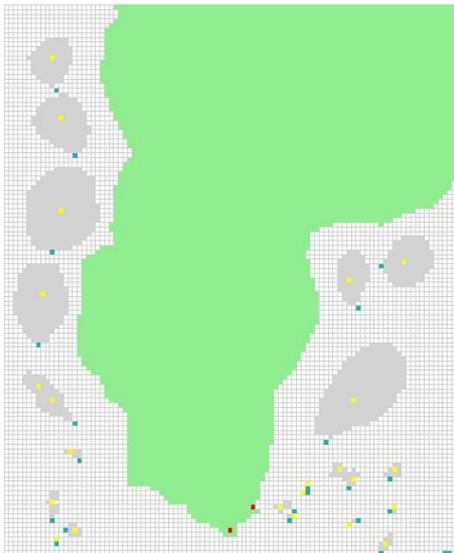


Z (mm)

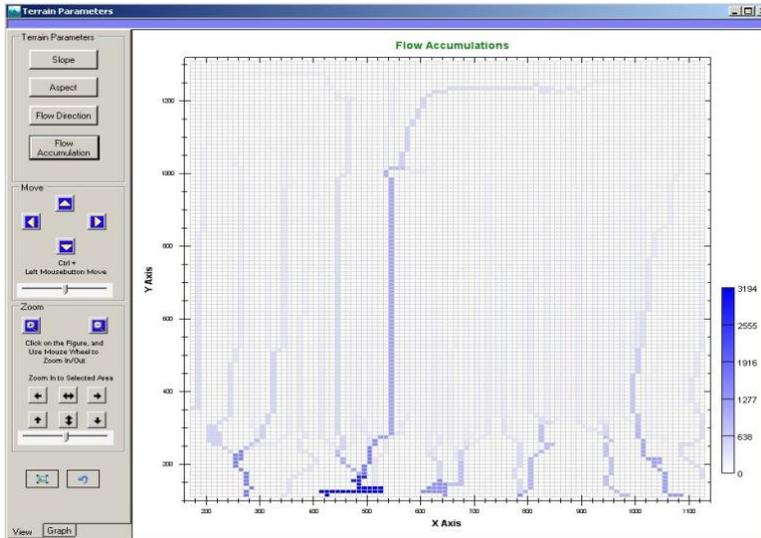
Puddle Delineation



Three mini-basins delineated for the rough soil surface

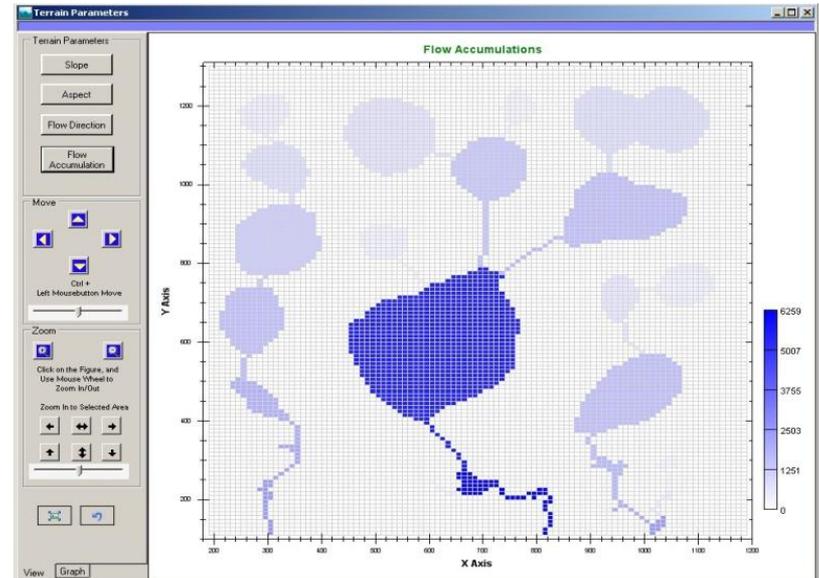


Puddle Delineation – Flow Accumulations

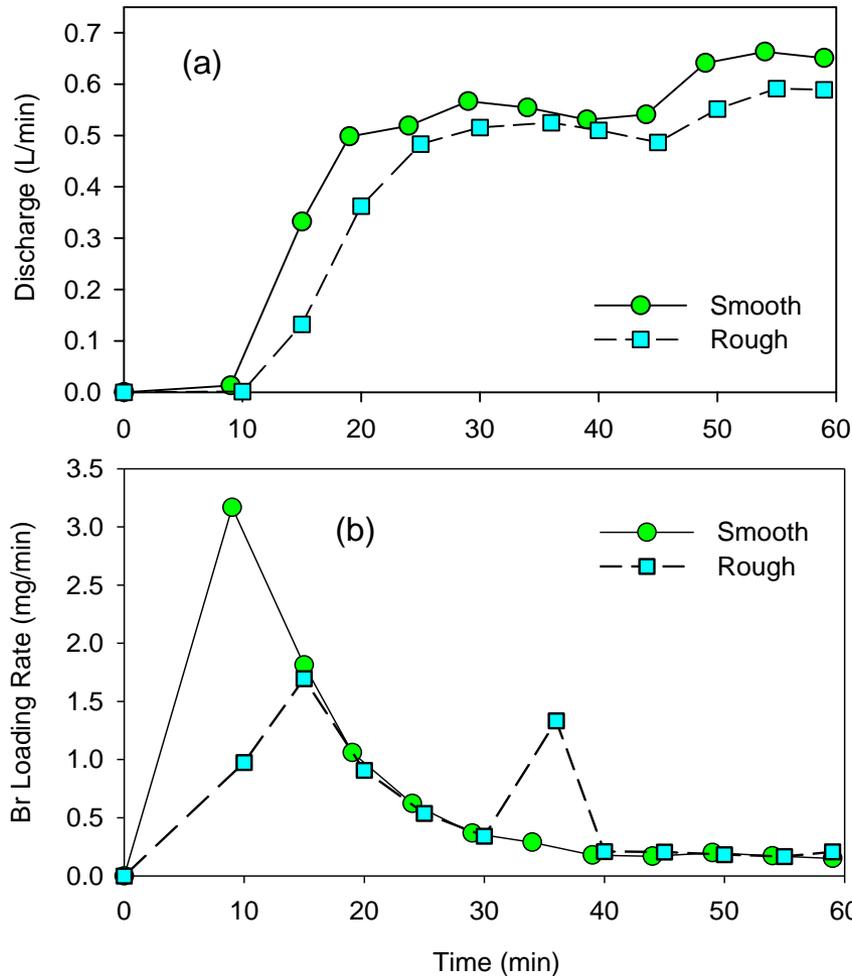


Smooth Surface

Rough Surface



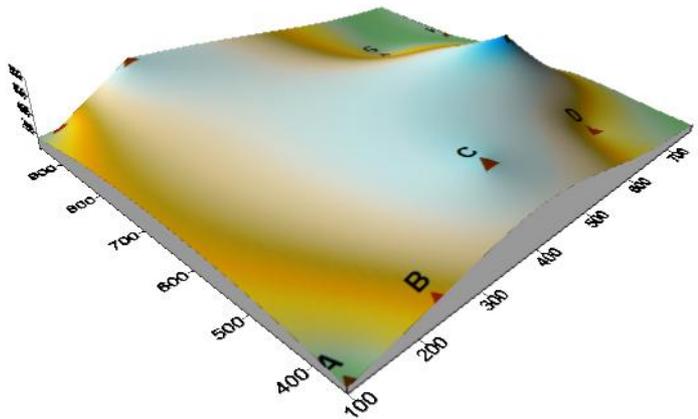
Hydrograph and Chemograph



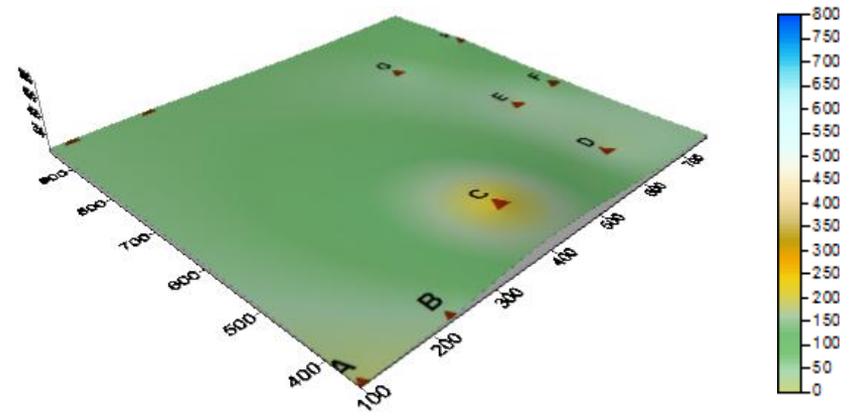
The smooth surface had earlier and greater contributions of both runoff water and tracer than the rough surface. An increase in surface roughness (microtopography) significantly reduced the tracer loading at the outlet and delayed the occurrence of tracer concentration peaks.

Overland flow and tracer transport on the rough soil surface featuring a variety of depressions exhibited a threshold behavior affected by surface microtopography.

Smooth Soil Surface: Spatial Distributions of Br Concentrations in soil



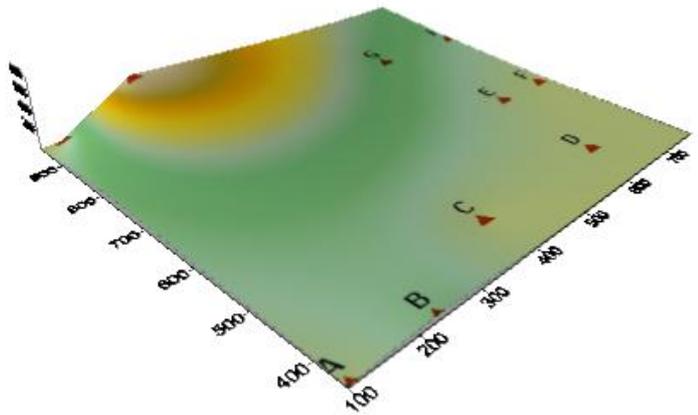
D=4 cm



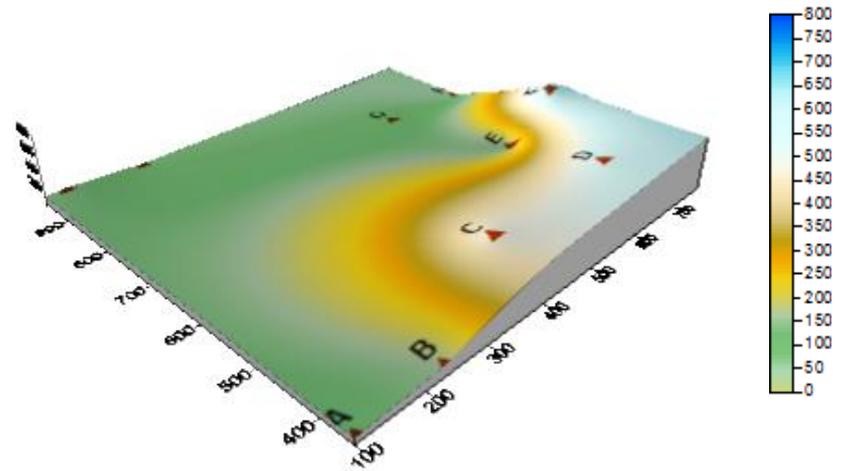
D=8 cm

Close correlations between the tracer spatial distribution in soil and surface microtopography were identified. The discrepancy in tracer levels and distributions in the subsurface system can be attributed primarily to the effect of surface microtopography on the infiltration and tracer leaching processes.

Rough Soil Surface: Spatial Distributions of Br Concentrations in soil



$D=4$ cm



$D=8$ cm

Microtopography-controlled preferential flow under the centers of surface depressions transported more solute into deep soil, which led to higher concentrations in deep soil under the depressions

Acknowledgements



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Thank You!

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February 29, 2012**