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

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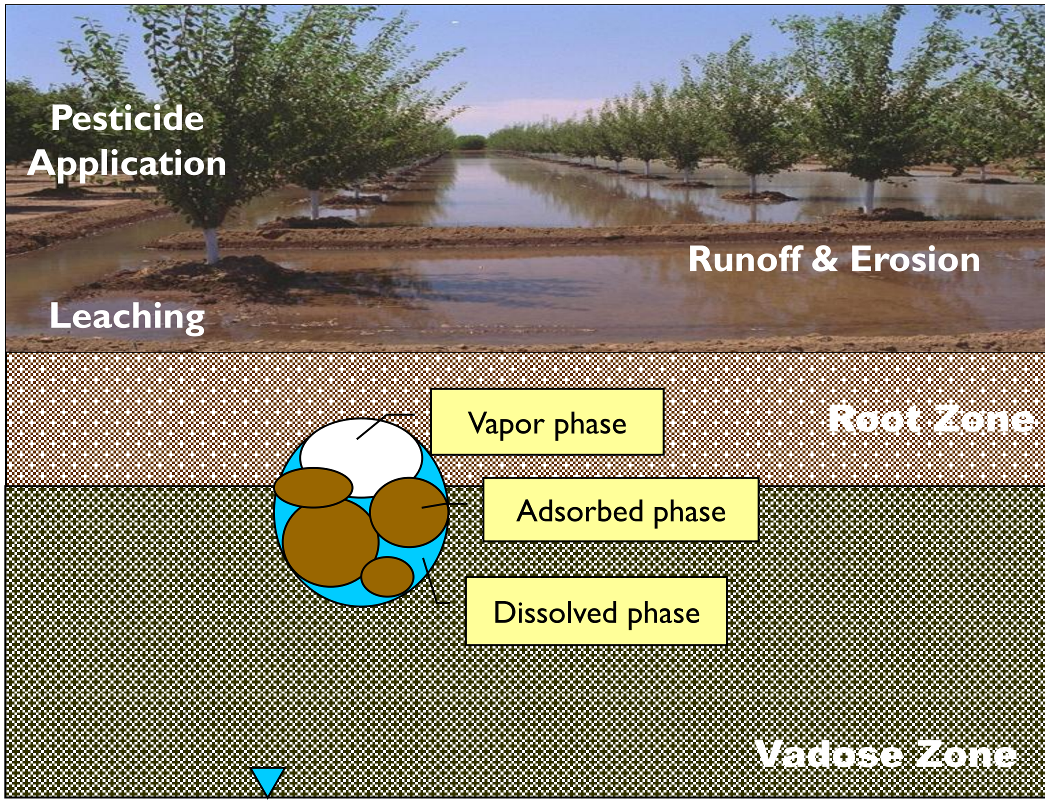
Part I
Windows-Based Integrated Pesticide Transport Model (IPTM)

- 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

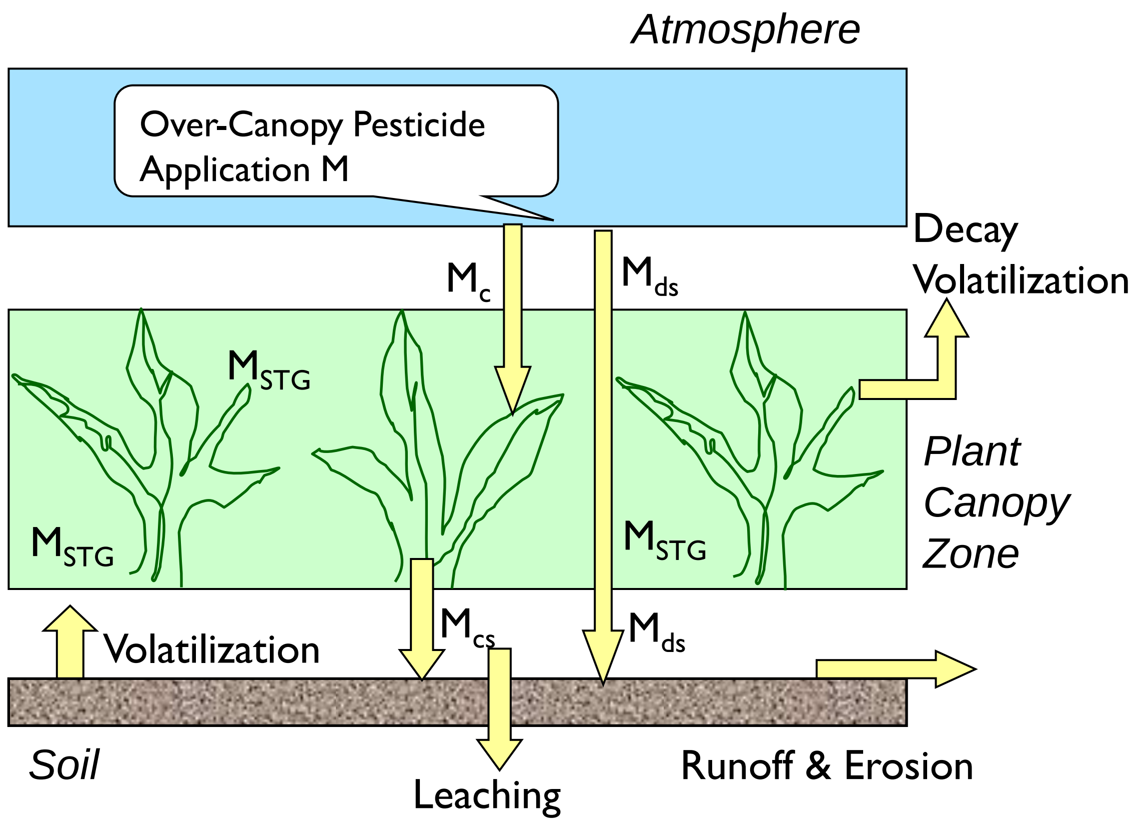
Major processes in Surface Zone: advection, dispersion, sorption, liquid-vapor partitioning, degradation, volatilization, runoff, and erosion.

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 1-D Three-Phase Pesticide Transport in the Unsaturated Zone

$$C_g = K_H C_l$$

Linear equilibrium liquid-vapor partitioning

Diffusion/Dispersion

$$D_g = \xi_g(a) D_g^a = \left(a^{7/3} / n^2\right) D_g^a$$

$$D_l = D^* + \alpha_L |v| = \left(\theta^{7/3} / n^2\right) D_l^w + \alpha_L \frac{|q|}{\theta}$$

$$C_s = K_d C_l$$

Linear Equilibrium Sorption Isotherm

Advection

$$\frac{\partial}{\partial t}\left[\theta C_l + \rho C_s + aC_g\right] = \frac{\partial}{\partial z}\left[aD_g \frac{\partial C_g}{\partial z}\right] + \frac{\partial}{\partial z}\left[\theta D_l \frac{\partial C_l}{\partial z}\right] - \frac{\partial}{\partial z}\left(qC_l\right)$$

$$-\frac{a_r Q}{\Delta z} C_l + \frac{a_e r_{om} Y_e}{\Delta z\, A_w} C_s + F S_u C_l - \left(\theta C_l + \rho C_s + aC_g\right)k + M(z,t)$$

Source/Sink Terms (e.g., Application)

Runoff: SCS-CN

$$Q = \frac{(P - 0.2S)^2}{P + 0.8S}$$

$$S = \left(2540 / CN\right) - 25.4$$

Passive Root Uptake

$$S_u = \alpha \frac{ET_p}{L_r}\left[1 - \exp\left(-0.6I\right)\right]$$

$$F = 0.784 \exp\left[-\left(\log K_{ow} - 1.78\right)^2 / 2.44\right]$$

First-Order Decay

Erosion: MUSLE

$$Y_e = a\left(V_Q q_p\right)^{0.56} K_e (LS) C_c P_c$$

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

Second-Order PDE

$$\frac{\partial}{\partial t}[(\theta+\rho K_d+aK_H)C]=\frac{\partial}{\partial z}\left[aD_g\frac{\partial}{\partial z}(K_H C)\right]+\frac{\partial}{\partial z}\left[\theta D_l\frac{\partial C}{\partial z}\right]$$

$$-\frac{\partial}{\partial z}(qC)-r_0 C-(\theta+\rho K_d+aK_H)kC+M(z,t)$$

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

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

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

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

State Transition Matrix Φ

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

$$= \mathbf{I} + \int_{t_0}^{t}\mathbf{A}(\tau_1)d\tau_1 + \int_{t_0}^{t}\mathbf{A}(\tau_1)\left[\int_{t_0}^{\tau_1}\mathbf{A}(\tau_2)d\tau_2\right]d\tau_1 + \cdots$$

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

For instantaneous application

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

For continuous application

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

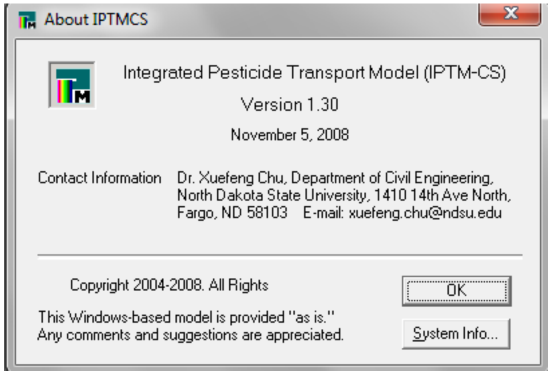
Solution Methods in IPTM

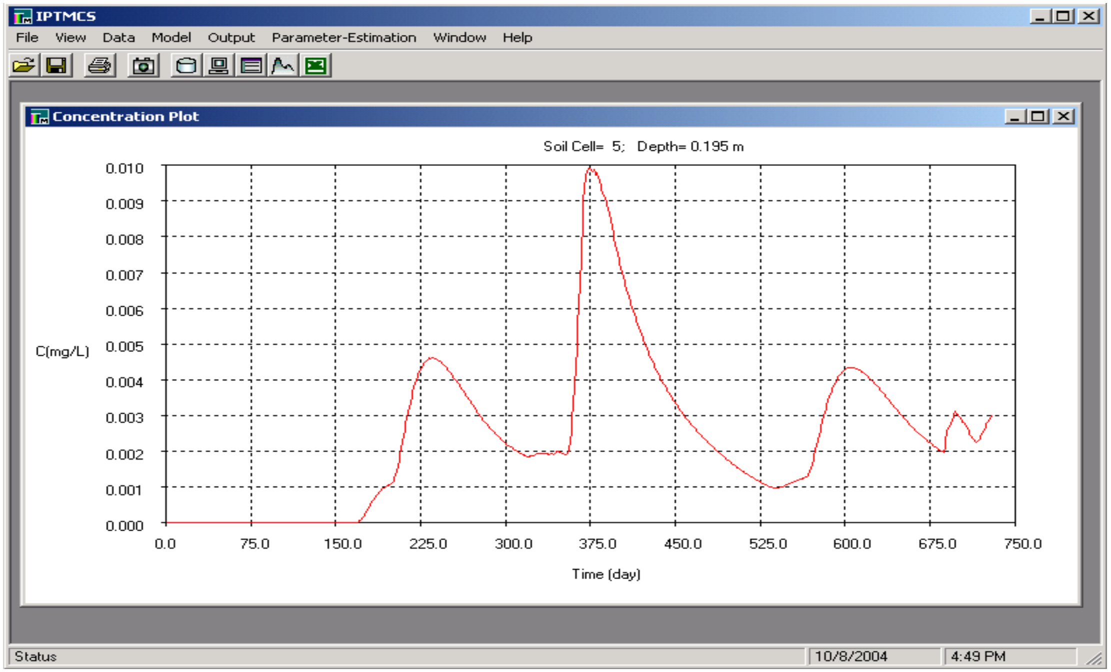
- Two-point first-order upwind scheme
- Second-order central differencing
- Multi-point high-order linear upwind-biased schemes
- Nonlinear van Leer flux limiter

Pesticide Application Methods in IPTM

- Over-canopy
- Under-canopy
- Combined foliar and soil surface spray
- Soil-incorporated applications.

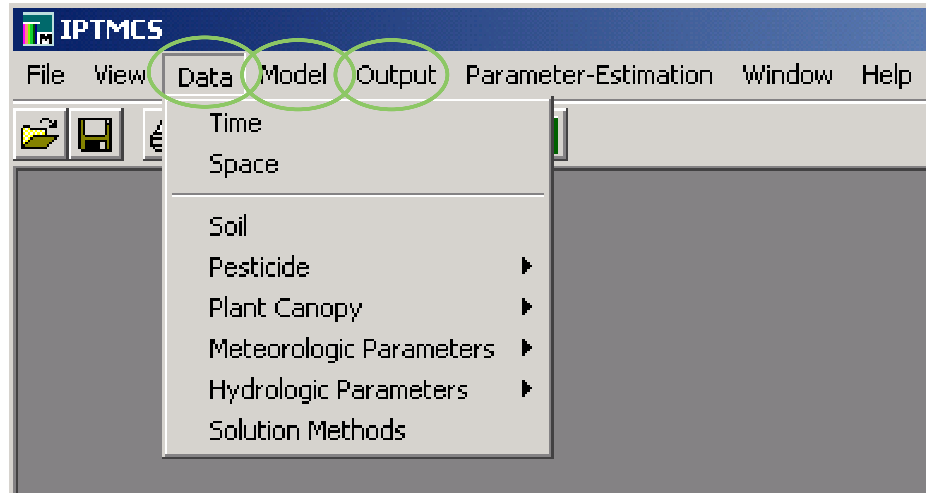
Windows-Based IPTM: Integrated Pesticide Transport Modeling System

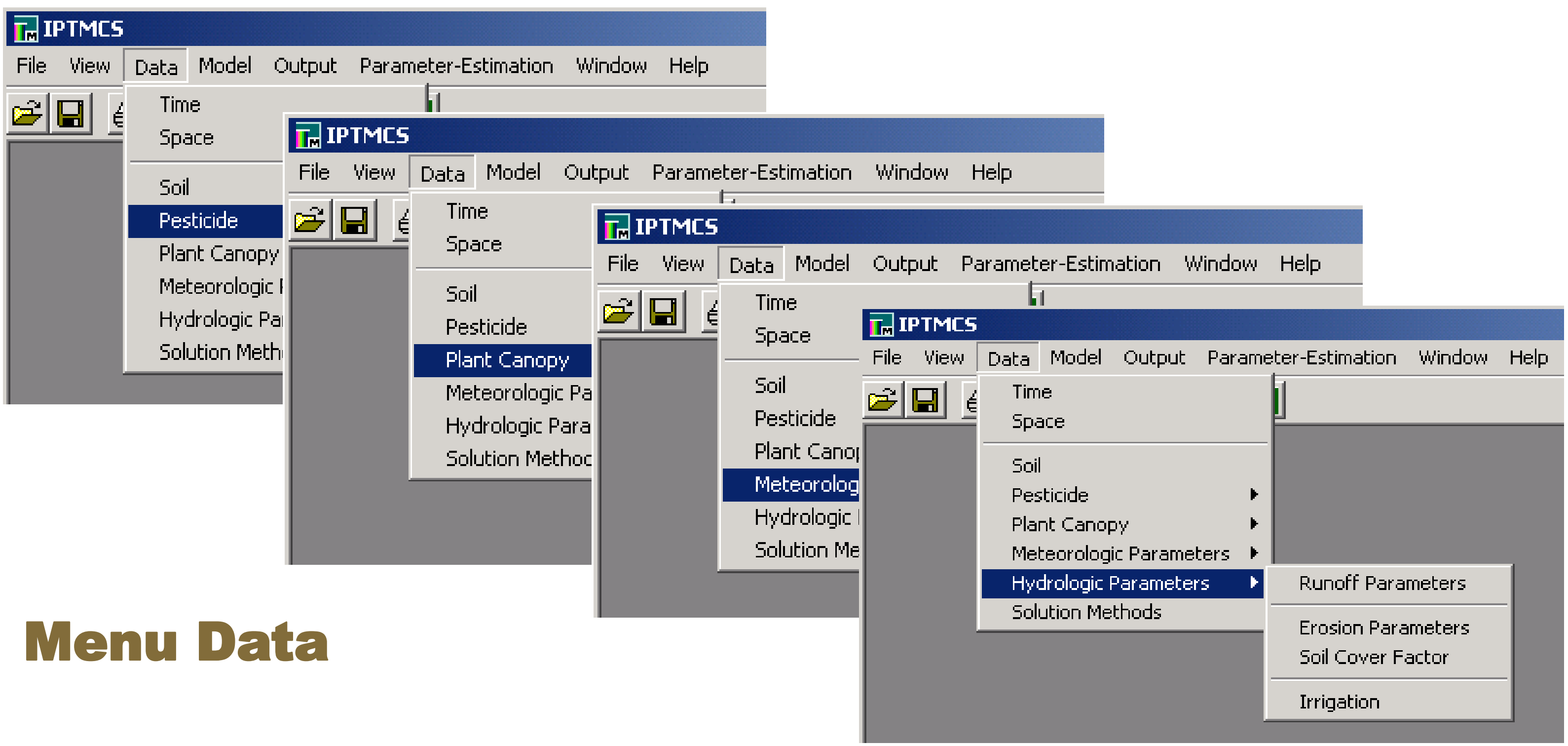




IPTM-CS:

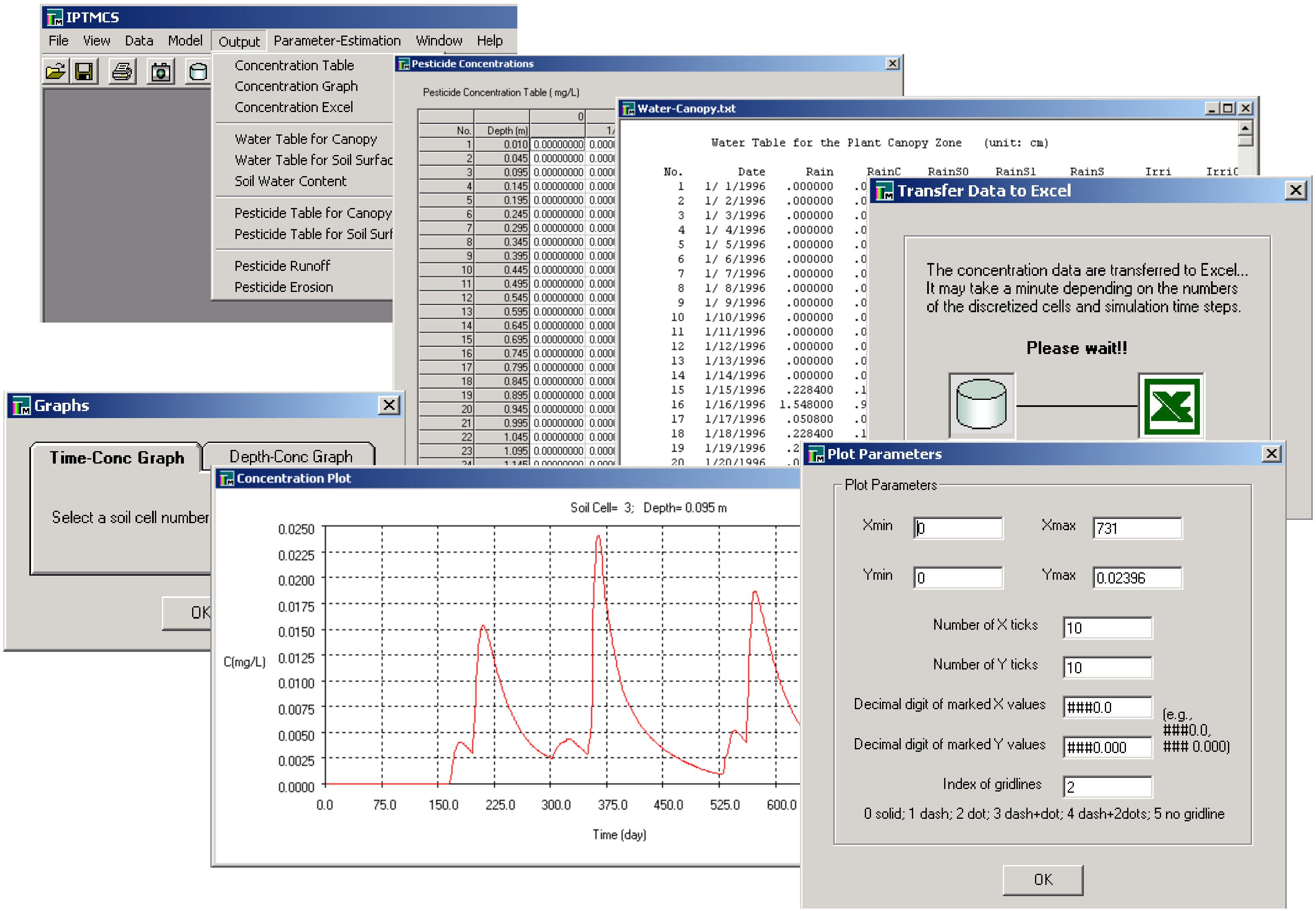
Three modeling steps – Three major menus (Data, Model, Output)



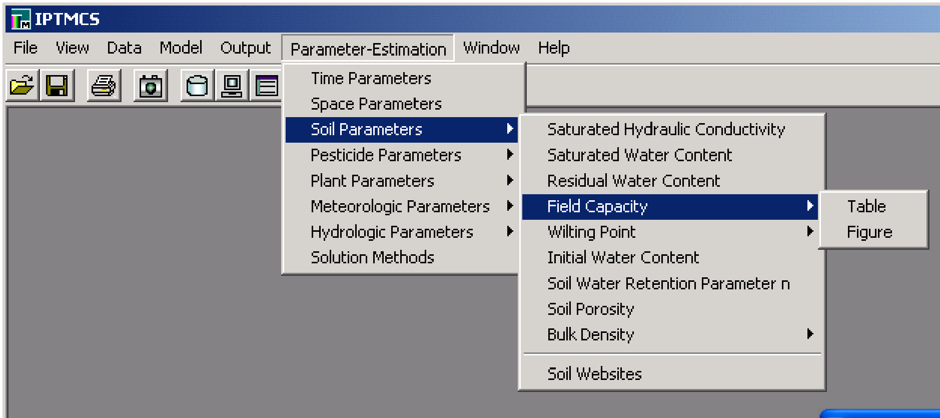


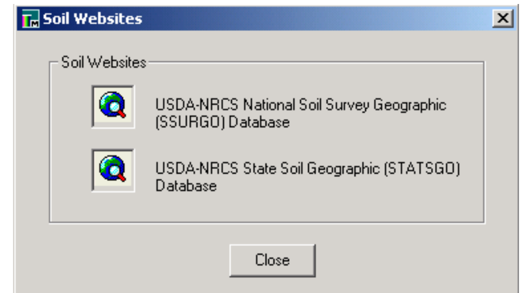
Menu Data

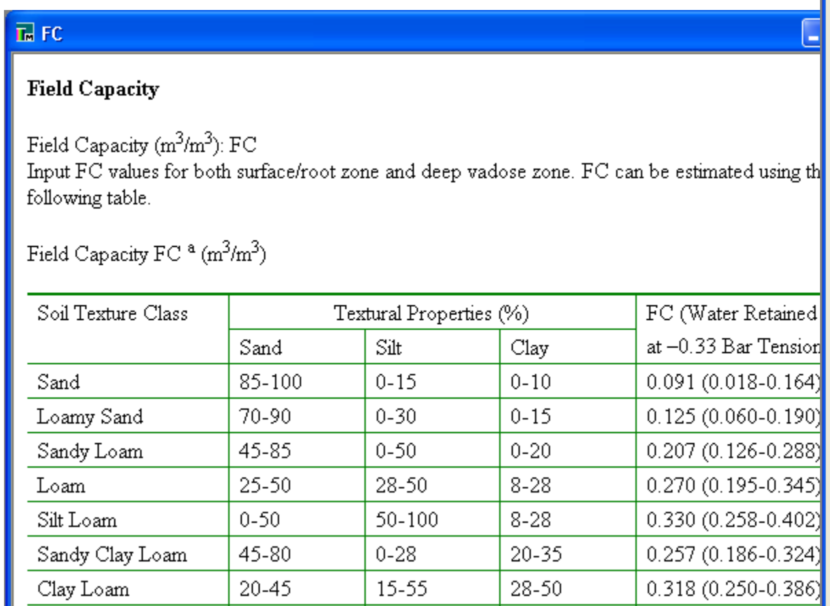
Menu Output (post-processing)



Menu Parameter-Estimation





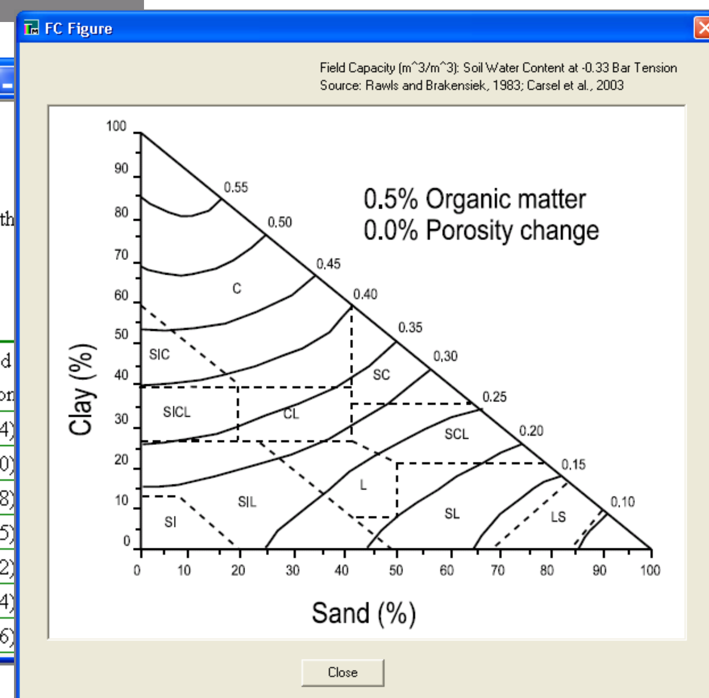

FC

Field Capacity

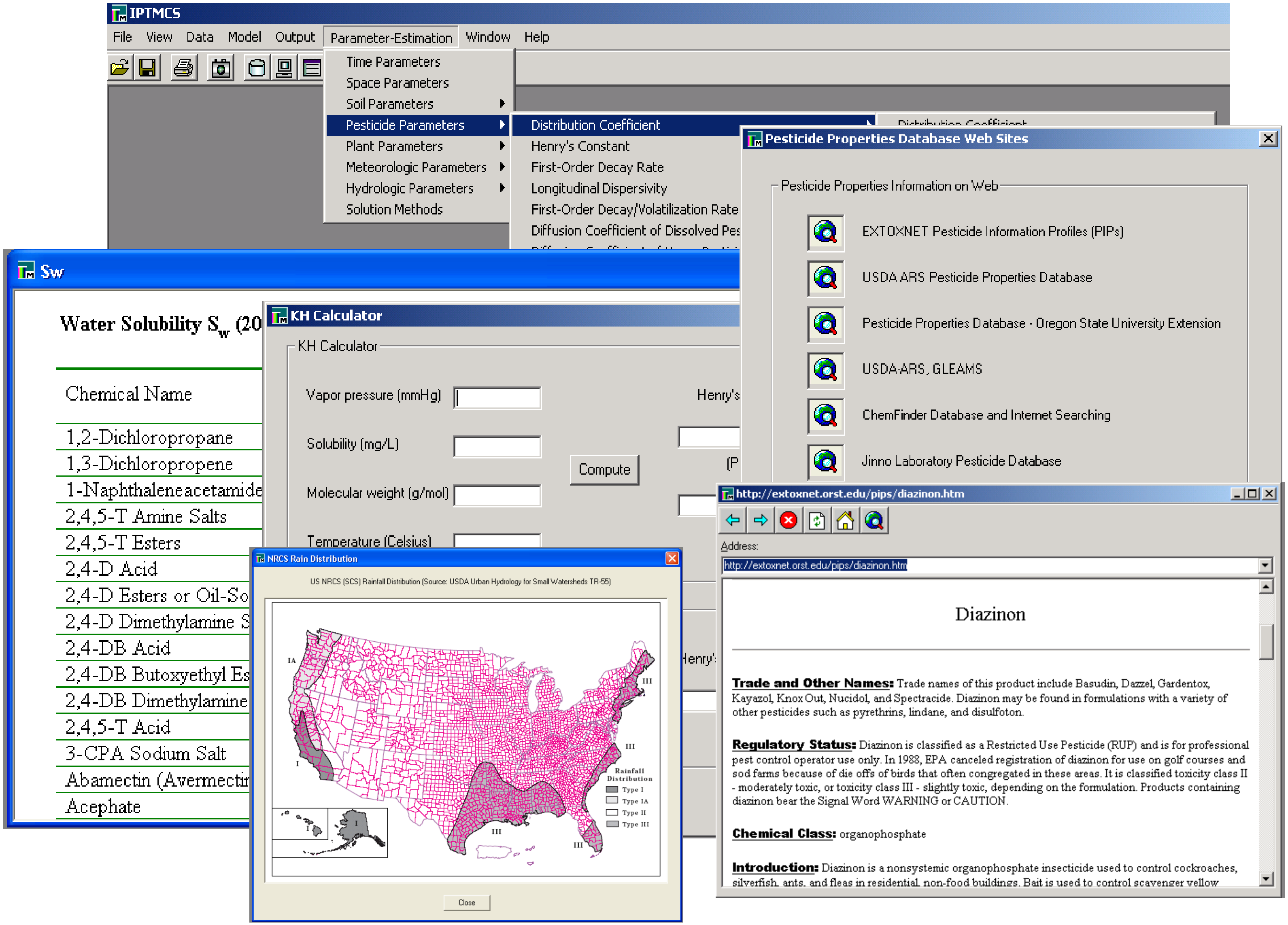
Field Capacity (m^3/m^3): FC
Input FC values for both surface/root zone and deep vadose zone. FC can be estimated using th
following table.

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

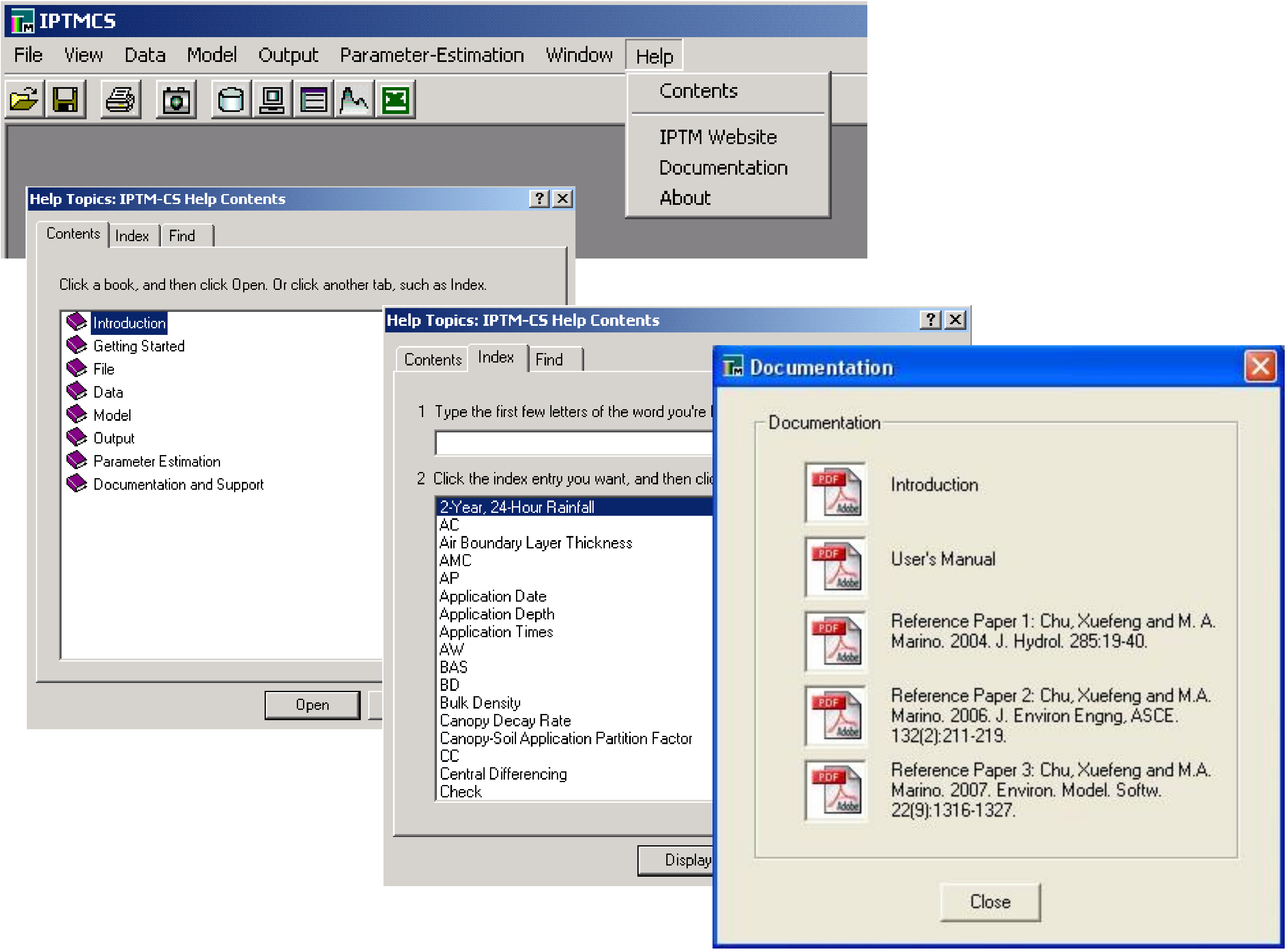
Soil Texture Class	Textural Properties (%)			FC (Water Retained at –0.33 Bar Tension
	Sand	Silt	Clay	
Sand	85-100	0-15	0-10	0.091 (0.018-0.164)
Loamy Sand	70-90	0-30	0-15	0.125 (0.060-0.190)
Sandy Loam	45-85	0-50	0-20	0.207 (0.126-0.288)
Loam	25-50	28-50	8-28	0.270 (0.195-0.345)
Silt Loam	0-50	50-100	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



Menu Help


IPTMCS
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Canopy-Soil Application Partition Factor
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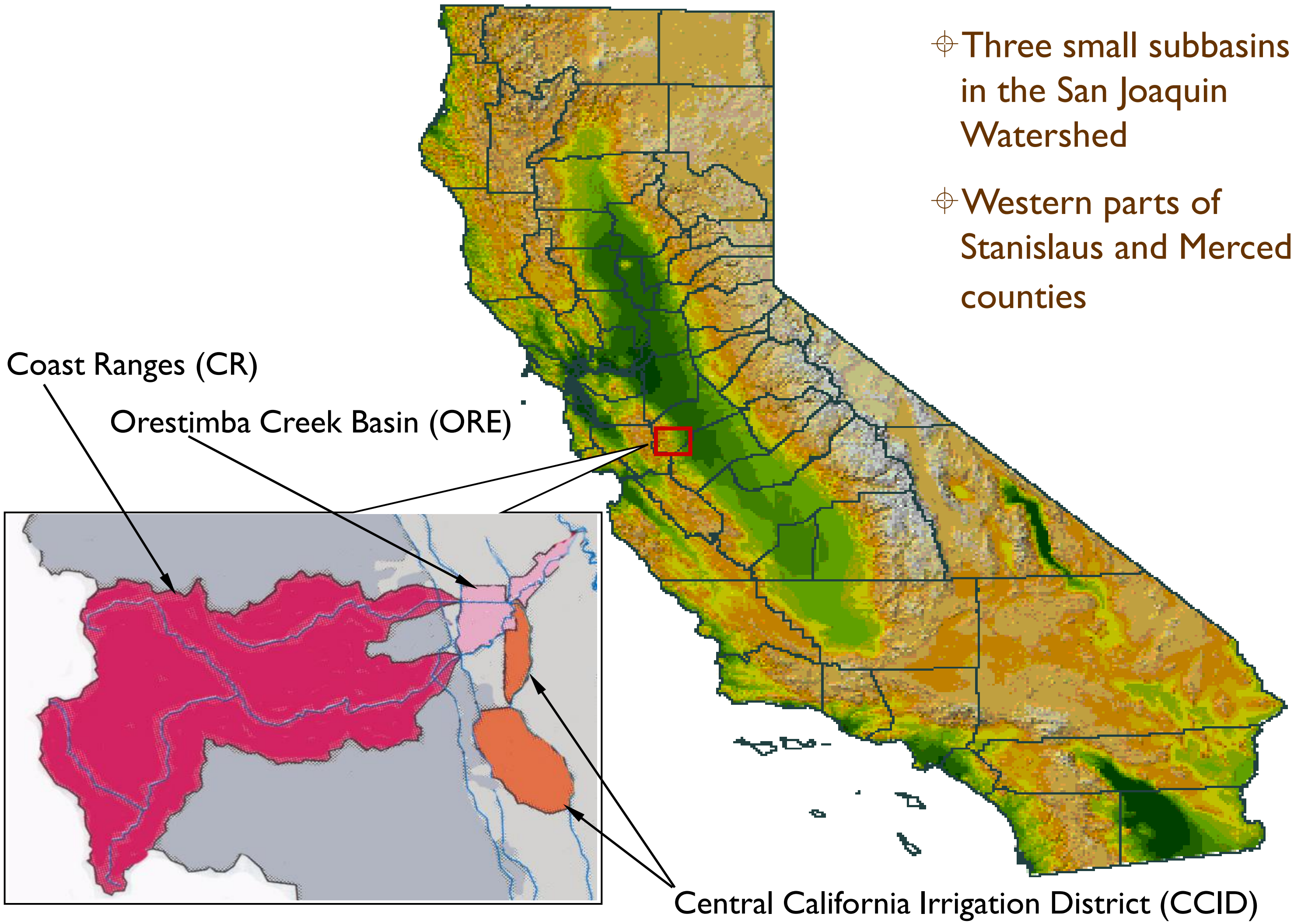
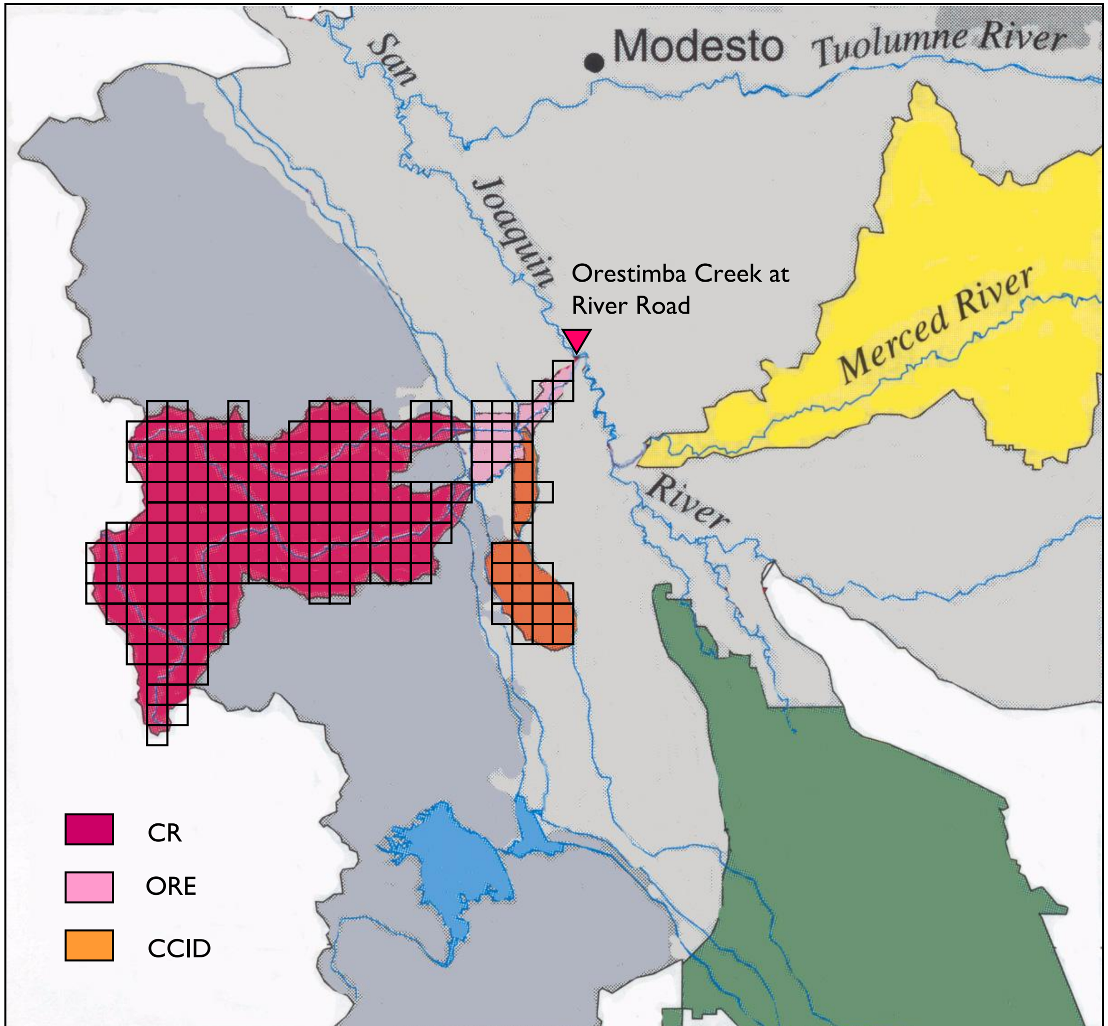
Reference Paper 1: Chu, Xuefeng and M. A. Marino. 2004. J. Hydrol. 285:19-40.
Reference Paper 2: Chu, Xuefeng and M.A. Marino. 2006. J. Environ Engng, ASCE. 132(2):211-219.
Reference Paper 3: Chu, Xuefeng and M.A. Marino. 2007. Environ. Model. Softw. 22(9):1316-1327.
Close

Application - Study Area and Location



- Three small subbasins in the San Joaquin Watershed
- Western parts of Stanislaus and Merced counties

Section Map and Areas



- Orestimba Creek Basin (ORE): 13 sections, 33,670,000 m^2
- Central California Irrigation District (CCID): 22 sections, 56,980,000 m^2
- Coast Ranges (CR): 164 sections, 424,760,000 m^2
- Total 199 sections

Simulation Period

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

Pesticide Applications

Pesticide: diazinon

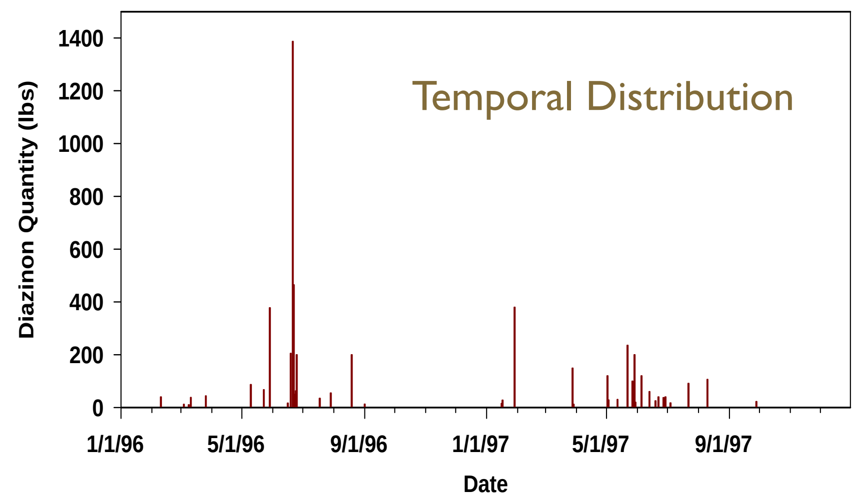
24 diazinon-applied sections

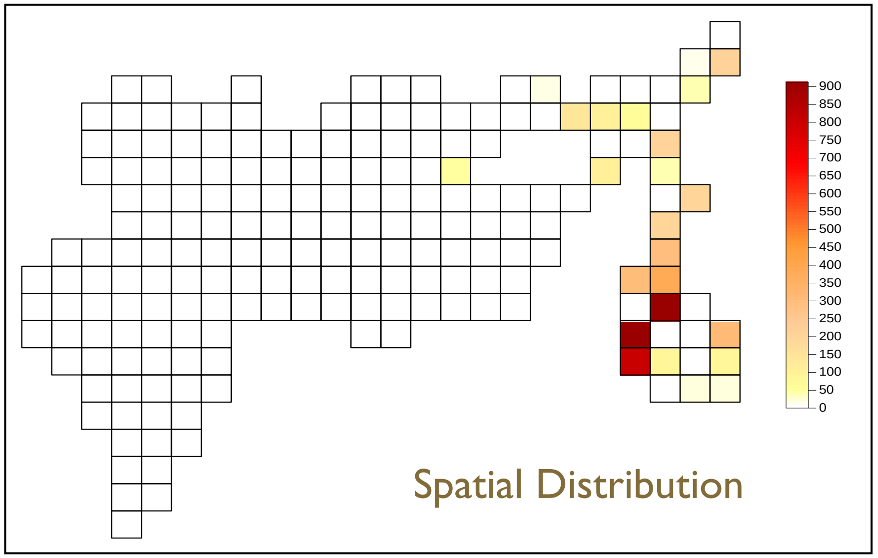
Crops

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

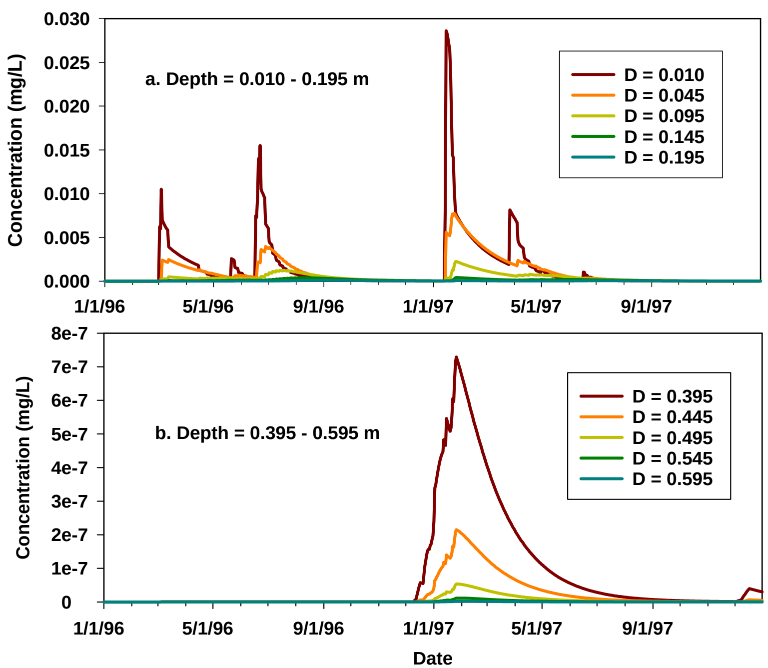
Soils

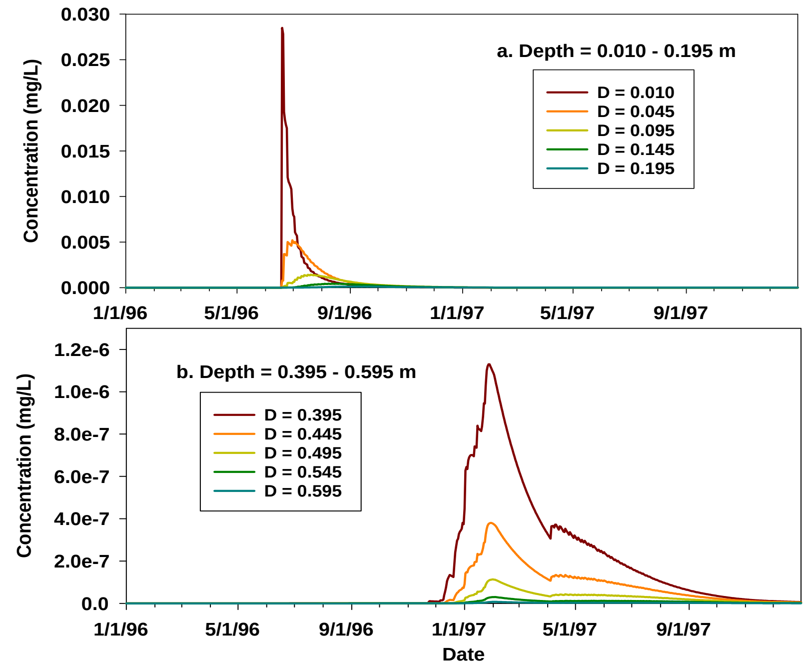
Clay loam, loam, and sandy loam are three major soil types





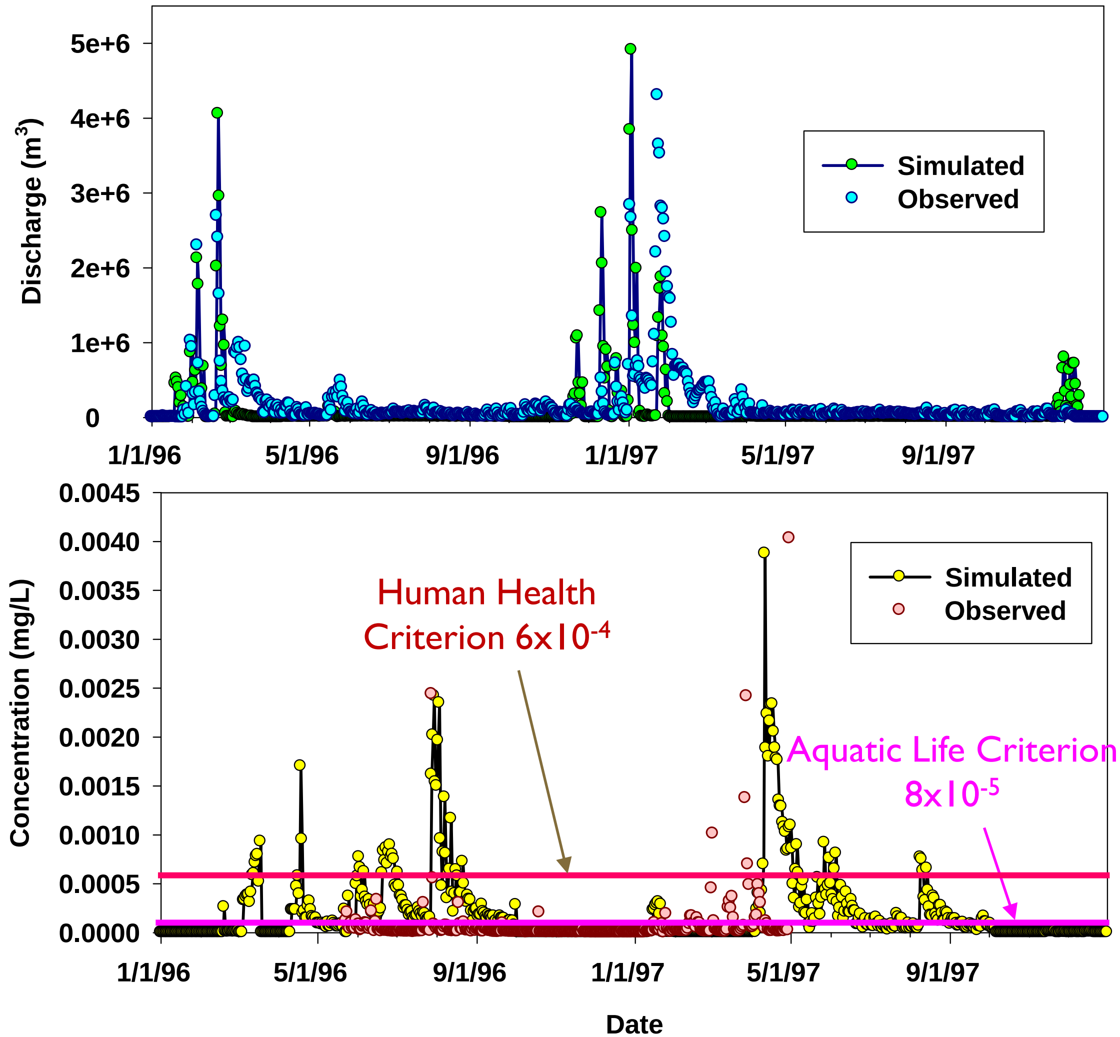
Diazinon in the Subsurface Environment





- 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)

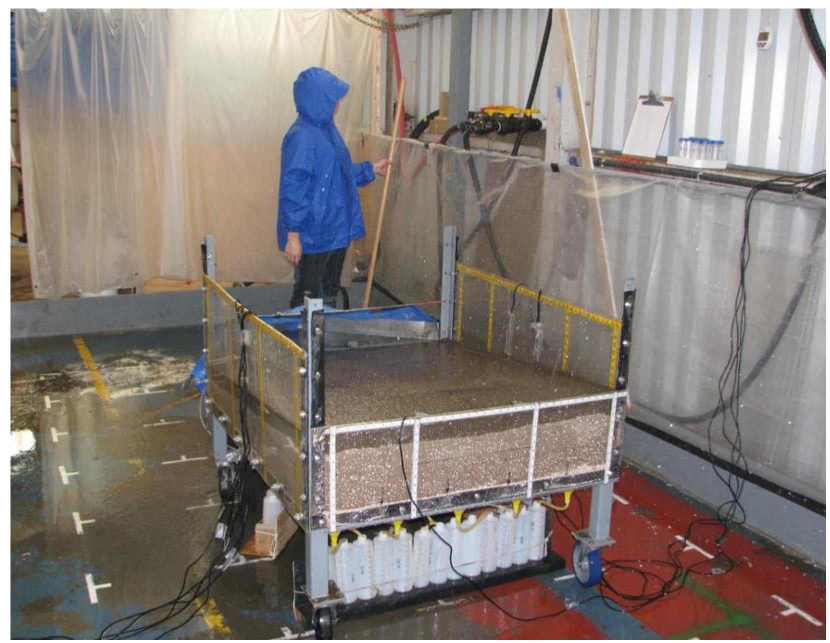


Diazinon in the Orestimba Creek Basin frequently exceeds criteria for aquatic life (0.08 μg/L). Worse of all, diazinon concentrations even exceed the human-health criterion (0.6 μg/L). Such high peak pulses may last up to a half month..

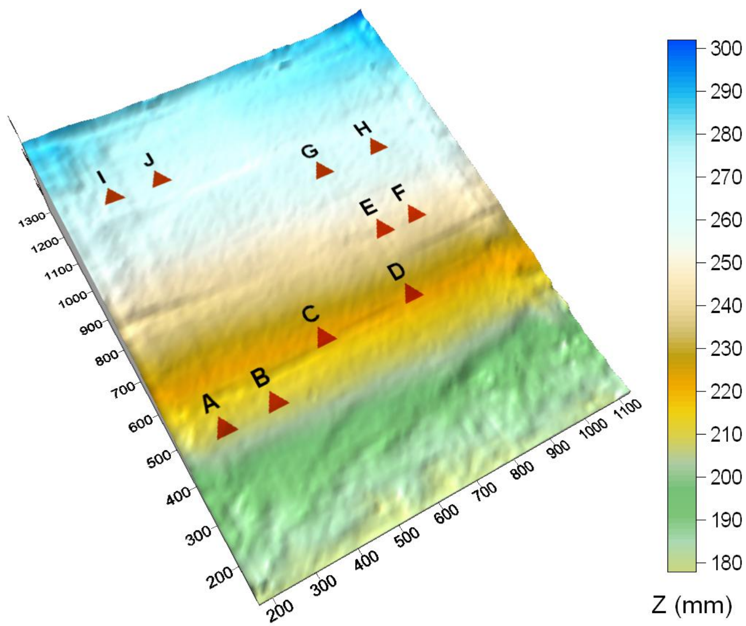
Part II
Tracer (Br) Transport under the Influence of Surface Microtopography

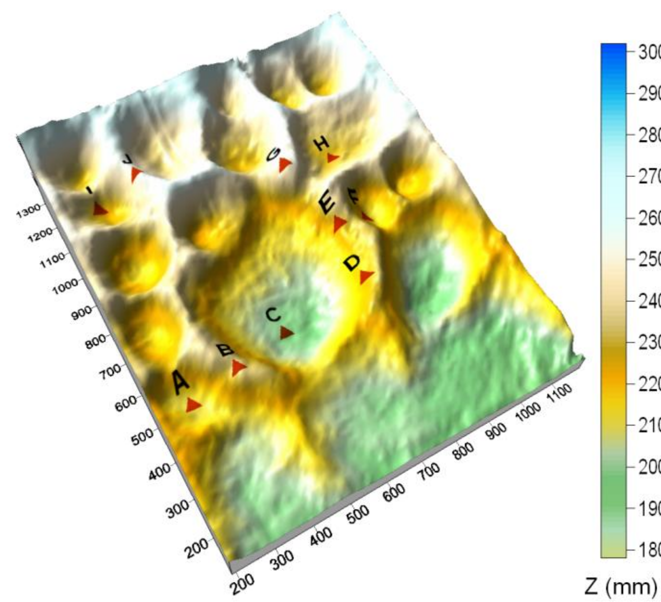




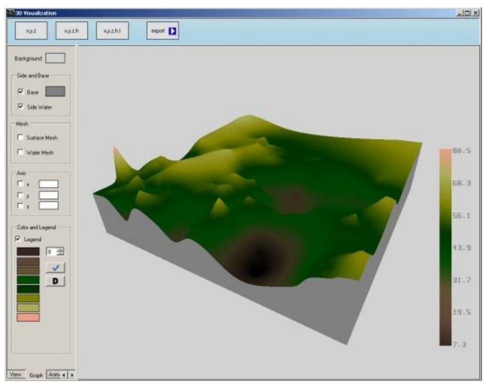


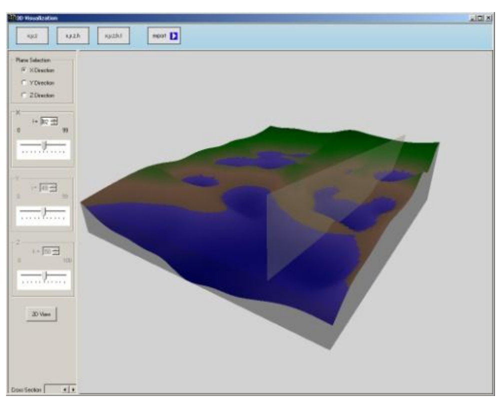
Smooth vs. Rough Soil Surfaces
Tracer Sampling Locations

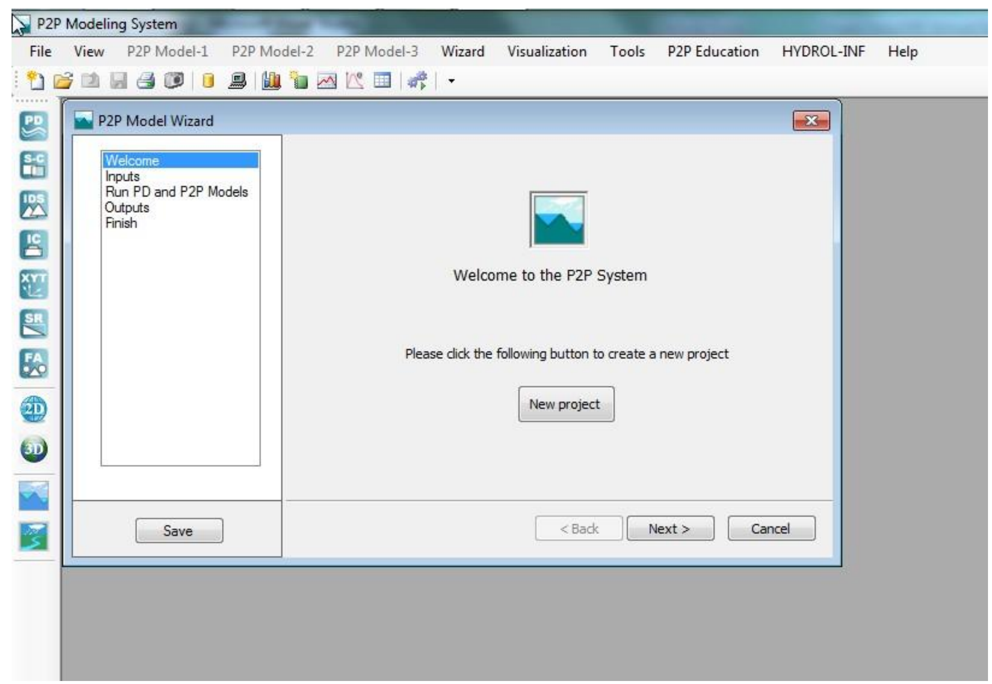




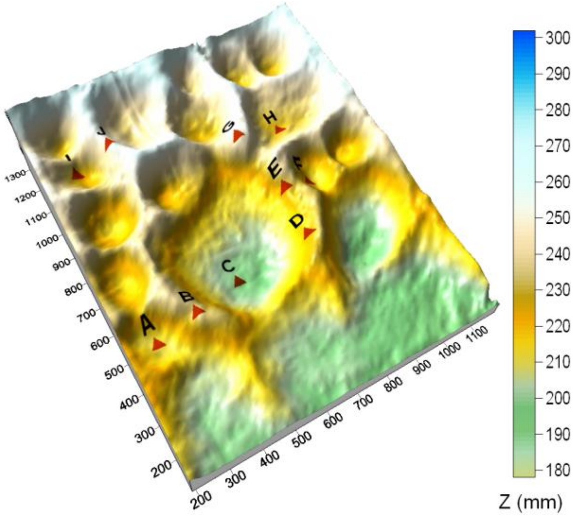
Windows-based P2P Modeling System
Puddle Delineation Tool



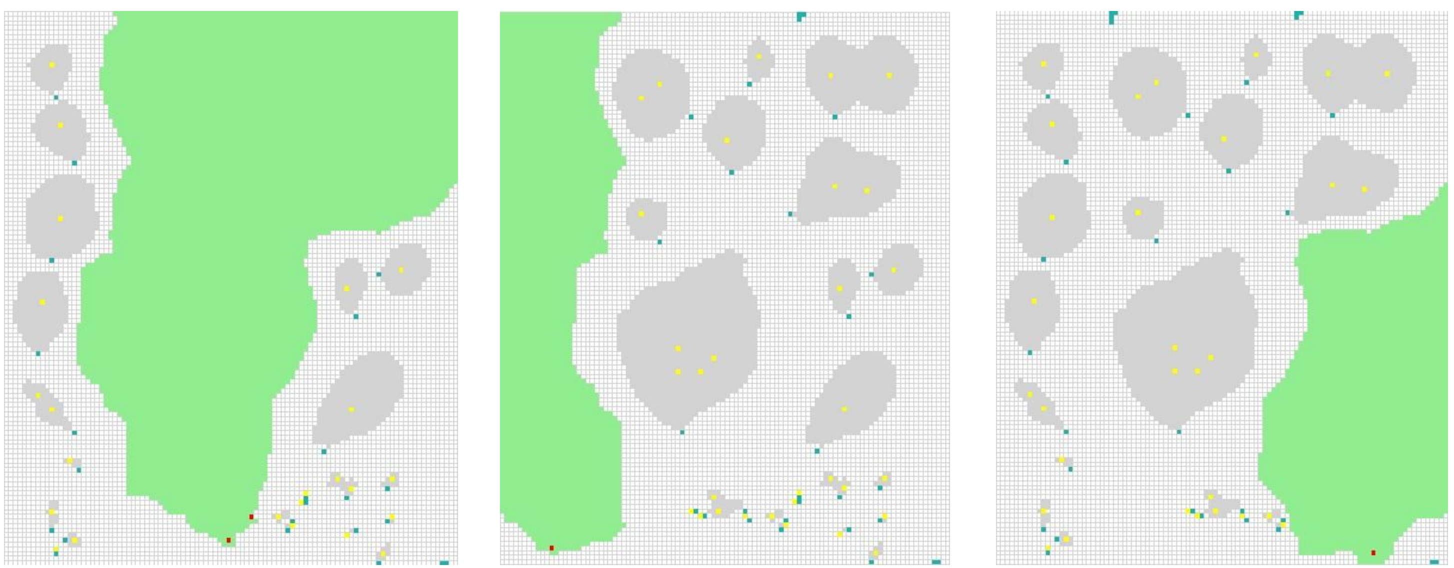




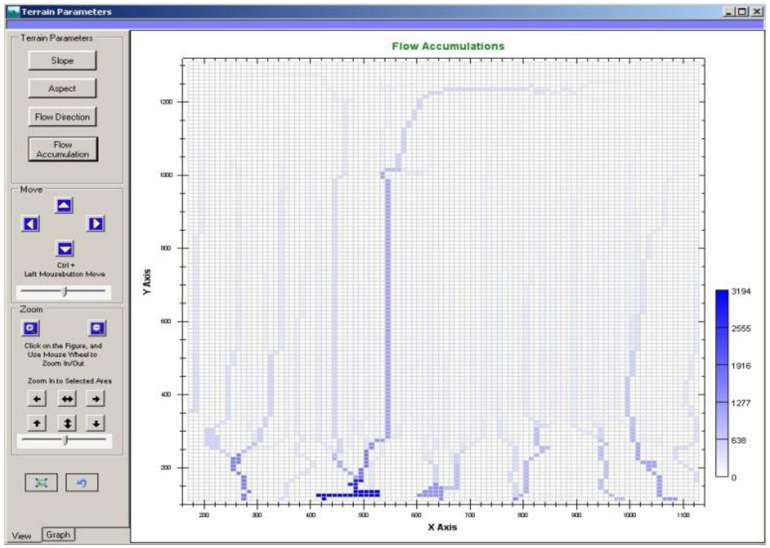
Puddle Delineation



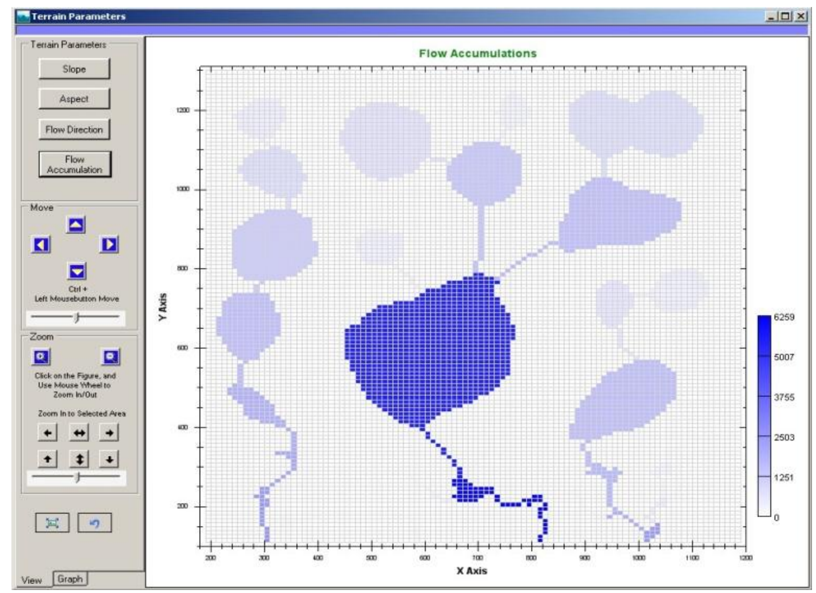
Three mini-basins delineated for the rough soil surface



Puddle Delineation – Flow Accumulations

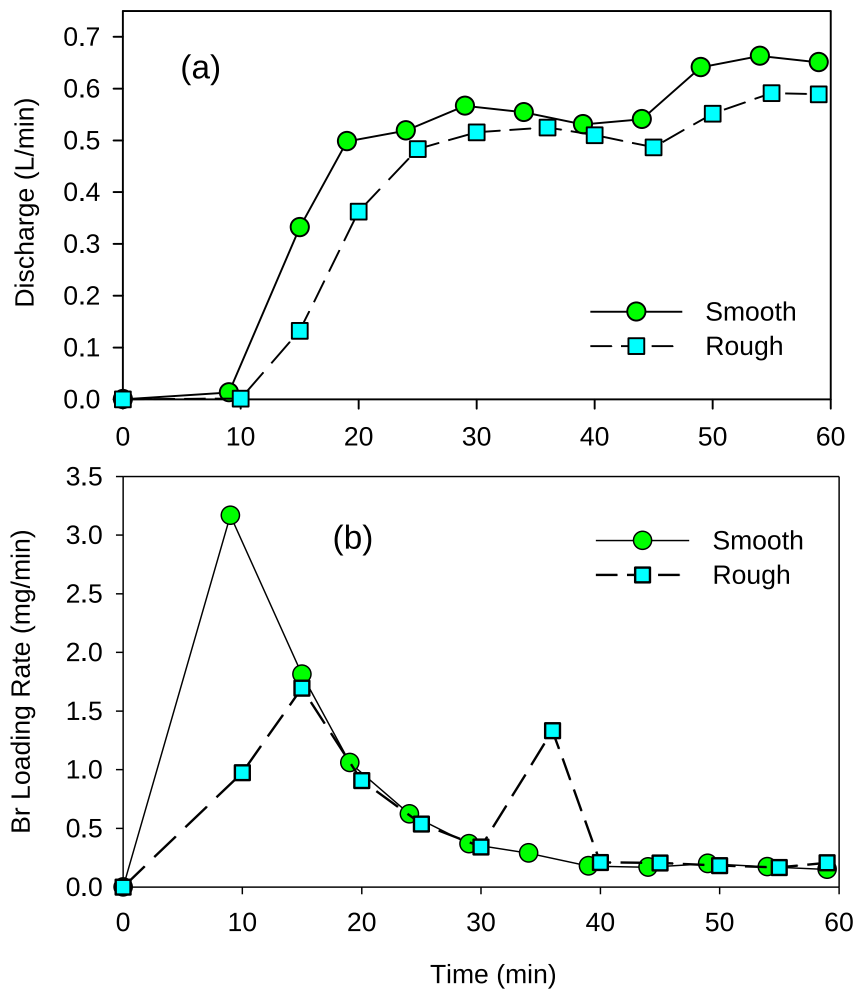


Smooth Surface



Rough Surface

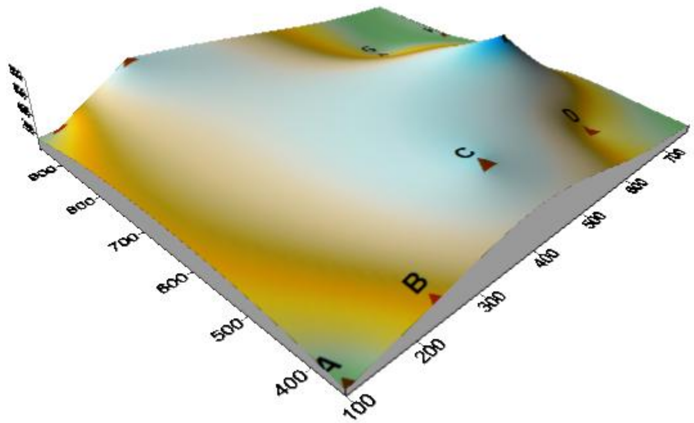
Hydrograph and Chemograph



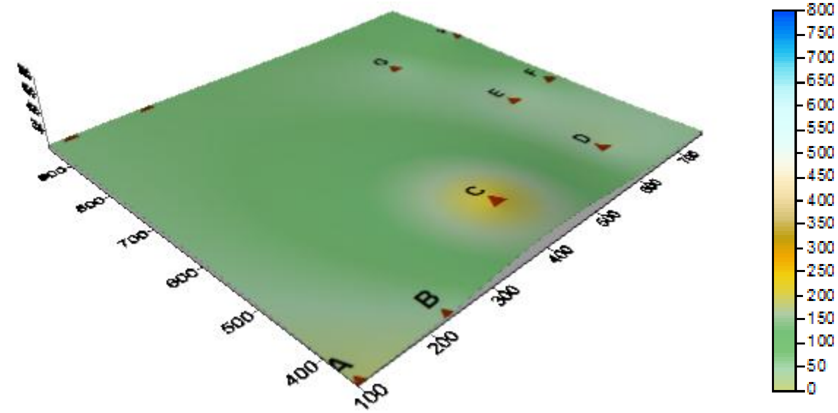
The smooth surface had earlier and greater contributions of both runoff water and tracer than the rough surface. An increase in surface roughness (microtopography) significantly reduced the tracer loading at the outlet and delayed the occurrence of tracer concentration peaks.

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



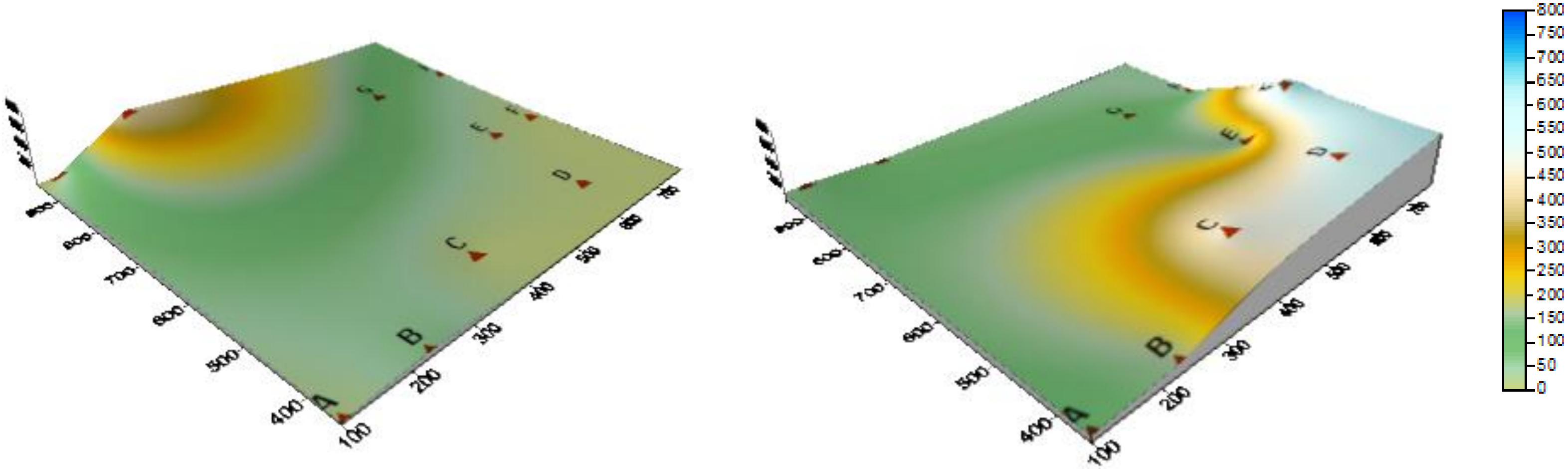
D=4 cm



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

This material is based upon work supported by the National Science Foundation under Grant No. EAR-0907588 and USEPA Center for Ecological Health Research (CEHR)

- Dr. Miguel Marino, Distinguished Professor, UC Davis
- Ms. Jessica Higgins, Grand Valley State University
- Dr. Richard Rediske, Grand Valley State University
- Dr. Jianli Zhang (postdoc) and all graduate students in my research group.

Thank You!

2012 North Dakota Water Quality Monitoring Conference
February 29, 2012