Modeling of Water Flow and Solute Transport in the Vadose Zone

Introduction to Hydrus Models

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1

Program Developers – Jirka Šimůnek

A Professor of Hydrology with the Department of Environmental Sciences of the University of California, Riverside. Received an M.S. in Civil Engineering from the Czech Technical University, Prague, Czech Republic, and a Ph.D. in Water Management from the Czech Academy of Sciences, Prague.

Expertise in numerical modeling of subsurface water flow and solute transport processes, equilibrium and nonequilibrium chemical transport, multicomponent major ion chemistry, field-scale spatial variability, and inverse procedures for estimating soil hydraulic and solute transport parameters.

He has authored and coauthored over 190 peer-reviewed journal publications, over 20 book chapters, and 2 books. His numerical HYDRUS models are used by virtually all scientists, students, and practitioners modeling water flow, chemical movement, and heat transport through variably saturated soils. Dr. Simunek is a recipient of the Soil Science Society of America's Don and Betty Kirkham Soil Physics Award, Fellow and the past chair of the Soil Physics (S1) of Soil Sciences Society of America. He is an associate editor of Vadose Zone Journal, Journal of Hydrological Sciences, Journal of Hydrology and Hydromechanics, and a past AE of Water Resources Research.

2

Program Developers – Rien van Genuchten

A soil physicist originally with the George E. Brown, Jr. Salinity Laboratory, USDA, ARS, Riverside, CA. Received a B.S. and M.S. in irrigation and drainage from Wageningen University in The Netherlands, and a Ph.D. in soil physics from New Mexico State University.

Dr. van Genuchten is a recipient of the Soil Science Society of America's Don and Betty Kirkham Soil Physics Award, of the EGU Dalton Medal, and fellow of the Soil Science Society of America, American Society of Agronomy, American Geophysical Union and American Association for the Advancement of Sciences. Founding Editor of the Vadose Zone Journal. Currently with the University of Rio de Janeiro, Brazil.

Research on variably-saturated water flow and contaminant transport, analytical and numerical modeling, nonequilibrium transport, preferential flow, characterization and measurement of the unsaturated soil hydraulic functions, salinity management, and root-water uptake. Most often referenced researcher in the field of Soil Physics. Dr. van Genuchten is probably best known for the theoretical equations he developed for the nonlinear constitutive relationships between capillary pressure, water content and the hydraulic conductivity of unsaturated media.

3

Program Developers – Miroslav Šejna

A Director and Development Lead of PC-Progress, a Software company located in Prague, Czech Republic. Received B.S. and M.S. from the Charles University of Prague, Faculty of Mathematics and Physics, Prague, Czechoslovakia, and a PhD. from the Czech Academy of Sciences, Prague, Czech Republic.

Expertise in numerical modeling of Transonic Flow with homogeneous and heterogeneous condensation and chemicals in steam through Turbine Cascade (Euler and Navier-Stokes equations).

Recently specializes in the development of GUI (Graphical User Interfaces) for FEM/CFD software packages for Windows. He has more than twenty years of experience in developing programs for numerical modeling in Fluid Mechanics and Structural Engineering. His software helps thousands of scientists and engineers from around the world.

Selected Software Projects:

- RFEM, RSTAB - Structural Engineering Software packages, 1995-2009, Ing.-Software Dlubal, GmbH, Germany
- HYDRUS 2D/3D - Software package for simulating water, heat, and solute transport in variably saturated porous media.
- MESHGEN Plus - FE-mesh generator and open modeling environment for Finite-Element and Finite-Volume applications.
- COCHEM Flow - Software package simulating 2D water steam flow with homogeneous and heterogeneous Condensation.

4

HP1 Model Developer - Diederik Jacques

Diederik Jacques is a researcher at the Section Radiological impact and performance assessment studies, Institute of Environment, Health and Safety of the Belgian Nuclear Research Centre (SCK•CEN) in Mol, Belgium.

He received a B.S. and M.S. in Bio-engineering land and forest management at the Catholique University of Leuven, Belgium, a Master of Statistic at the Catholique University of Leuven, and a Ph.D. in soil physics at the Catholique University of Leuven.

His expertise is in modeling water flow and solute transport in unsaturated porous media including characterizing spatial variability and estimating parameters. He has some experience with experiments at the field scale. He is working on different aspects of coupling unsaturated water flow, solute transport and geochemical reaction including the development and testing of the coupled code HP1, application to (long-term) solute transport in soils and interaction between different systems (clay – concrete, or soil – concrete).

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Czech Republic (Czechoslovakia)

Known for:
1. Beer (Pilsner Urquel)
2. Ice Hockey (Jágr, Hašek)
3. Vaclav Havel (former president)
4. Beauty of its capital (Prague)
5. HYDRUS

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Holland (Netherlands) + Belgium

Known for:
1. Beer (Grolsch, Heineken)
2. Soccer (Robben, Sneijder)
3. Beatrix (Queen)
4. Beauty of its towns (A'dam, Utrecht)
5. Herrings and Cheese
6. HYDRUS

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Subsurface Flow and Transport

Hydrus-1D and Hydrus (2D/3D)

- numerical models that simulate

a) Water flow:

b) Solute Transport

c) Heat Transport

in unsaturated, partially saturated, or fully saturated one-, two-, or three-dimensional porous media, i.e., in nonuniform soils

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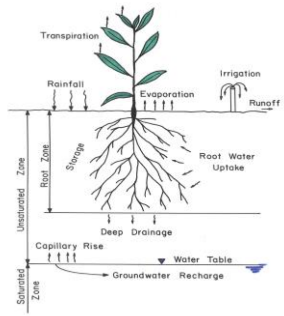
Agricultural Applications

- Precipitation
- Irrigation
- Runoff
- Evaporation
- Transpiration
- Root Water Uptake
- Capillary Rise
- Deep Drainage
- Fertigation
- Pesticides
- Fumigants
- Colloids
- Pathogens



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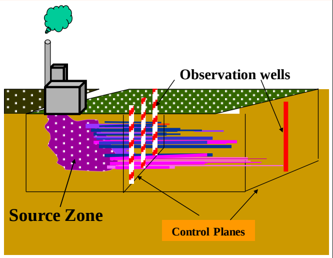
Industrial Applications

- Industrial Pollution
- Municipal Pollution
- Landfill Covers
- Waste Repositories
- Radioactive Waste Disposal Sites
- Remediation
- Brine Releases
- Contaminant Plumes
- Seepage of Wastewater from Land Treatment Systems



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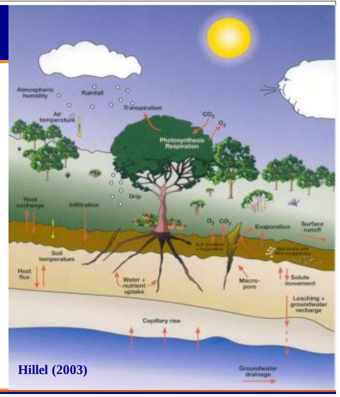
Environmental Applications

- Ecological Apps
- Carbon Storage and Fluxes
- Heat Exchange and Fluxes
- Nutrient Transport
- Soil Respiration
- Microbiological Processes
- Effects of Climate Change
- Riparian Systems
- Stream-Aquifer Interactions



Hillel (2003)

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Governing Equations

Variably-Saturated Water Flow (Richards Equation)

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z}\left[K(h)\frac{\partial h}{\partial z} - K(h)\right] - S$$

Heat Movement

$$\frac{\partial C_p(\theta)T}{\partial t} = \frac{\partial}{\partial z}\left[\lambda(\theta)\frac{\partial T}{\partial z}\right] - C_w\frac{\partial qT}{\partial z} - C_w ST$$

Solute Transport (Convection-Dispersion Equation)

$$\frac{\partial(\rho s)}{\partial t} + \frac{\partial(\theta c)}{\partial t} = \frac{\partial}{\partial z}\left(\theta D\frac{\partial c}{\partial z} - qc\right) - \phi$$

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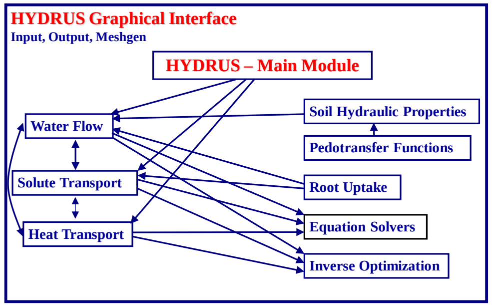
HYDRUS –Modular Structure



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HYDRUS Software Packages

Water Flow:
- Richards equation for variably-saturated water flow
- Various models of soil hydraulic properties
- Hysteresis
- Sink term to account for water uptake by plant roots

Heat Transport:
- Conduction and convection with flowing water

Solute Transport:
- Convective-dispersive transport in the liquid phase, diffusion in the gaseous phase
- Nonlinear nonequilibrium reactions between the solid and liquid phases
- Linear equilibrium reactions between the liquid and gaseous phases
- Zero-order production
- First-order degradation reactions
- Physical nonequilibrium solute transport

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The HYDRUS Software Packages

- **Variably-Saturated Flow (Richards Eq.)**
- Root Water Uptake (water and salinity stress)
- Solutes Transport (decay chains, ADE)
  - Sorption (linear and nonlinear)
  - Chemical Nonequilibrium
  - Physical Nonequilibrium
- Heat Transport
- Parameter Estimation
- Interactive Graphics-Based Interface
- Additional Modules

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Water Flow in Soils

- **Groundwater flow** (Darcy's Law)

$$q = K_s \frac{\Delta(P+z)}{\Delta L} = -K_s \frac{dH}{dz}$$

- **Unsaturated water flow** (Darcy-Buckingham Law)

$$q = K(h) \frac{\Delta(h+z)}{\Delta L} = -K(h) \frac{dH}{dz}$$

H - sum of the matric (h) and gravitational (z) head ($H=h+z$)

Water Flow - Richards Equation

The governing flow equation for one-dimensional isothermal Darcian flow in a variably-saturated isotropic rigid porous medium:

$$\frac{\partial \theta(h)}{\partial t} = -\frac{\partial q}{\partial z} - S(h)$$

$$\frac{\partial \theta(h)}{\partial t} = \frac{\partial}{\partial z}\left[K(h)\frac{\partial h}{\partial z} + K(h) \right] - S(h)$$

θ - volumetric water content [L^3L^{-3}]
h - pressure head [L]
K - unsaturated hydraulic conductivity [LT^{-1}]
z - vertical coordinate positive upward [L]
t - time [T]
S - root water uptake [T^{-1}]

Water Flow - Richards Equation

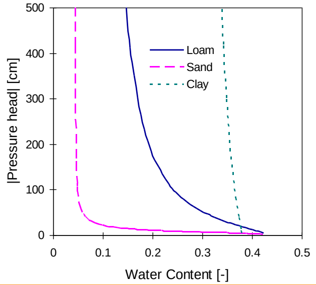
The governing flow equation for two-dimensional isothermal Darcian flow in a variably-saturated isotropic rigid porous medium:

$$\frac{\partial \theta(h)}{\partial t} = \frac{\partial}{\partial x_i}\left[K(h)\left(K_{ij}^A \frac{\partial h}{\partial x_j} + K_{iz}^A \right) \right] - S(h)$$

θ - volumetric water content [L^3L^{-3}]
h - pressure head [L]
K - unsaturated hydraulic conductivity [LT^{-1}]
K_{ij}^A - components of a anisotropy tensor [-]
x_i - spatial coordinates [L]
z - vertical coordinate positive upward [L]
t - time [T]
S - root water uptake [T^{-1}]

Retention Curve, $\theta(h)$

Soil-water characteristic curve
Characterizes the energy status of the soil water



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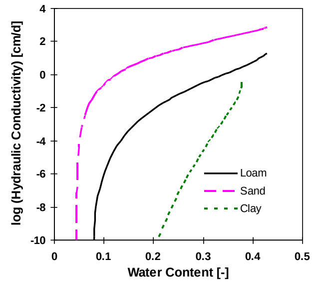
Hydraulic Conductivity, $K(\theta)$

- characterizes resistance of porous media to water flow



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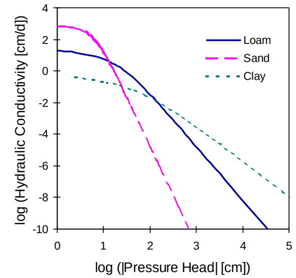
Hydraulic Conductivity, $K(h)$

- characterizes resistance of porous media to water flow



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Retention Curve Models

- **Brooks and Corey [1964]:** $S_e = \begin{cases} |\alpha h|^{-n} & h < -1/\alpha \\ 1 & h \geq -1/\alpha \end{cases}$
- **van Genuchten [1980]:** $S_e = \dfrac{1}{(1+|\alpha h|^n)^{1-1/n}}$
- **Kosugi [1996]:** $S_e = \dfrac{1}{2} erfc\left\{\dfrac{\ln(h/h_0)}{\sqrt{2}\sigma}\right\}$

θ_s - saturated water content [-]
θ_r - residual water content [-]
α, n, h_0, σ - empirical parameters [L^{-1}], [-], [L], [-]
S_e - effective water content [-]

$$S_e = \frac{\theta - \theta_r}{\theta_s - \theta_r}$$

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Hydraulic Conductivity Functions

- **Brooks and Corey [1964]:** $K(h) = K_s S_e^{2/n+l+2}$
- **van Genuchten [1980]: (Mualem [1976])** $K(h) = K_s S_e^l \left[1 - \left(1 - S_e^{1/m}\right)^m\right]^2$
- **Kosugi [1996]: (Mualem [1976])** $K(h) = K_s S_e^l \left\{\dfrac{1}{2} erfc\left[\dfrac{\ln(h/h_0)}{\sqrt{2}\sigma} + \dfrac{\sigma}{\sqrt{2}}\right]\right\}^2$

θ_s - saturated water content [-]
θ_r - residual water content [-]
α, n, h_0, σ, l - empirical parameters [L^{-1}], [-], [L], [-], [-]
S_e - effective water content [-]
K_S - saturated hydraulic conductivity [LT^{-1}]

$$S_e = \frac{\theta - \theta_r}{\theta_s - \theta_r}$$

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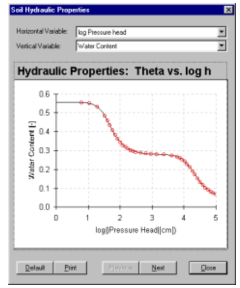
RETC, version 6.0

The RETC program for quantifying the hydraulic functions of unsaturated soils

Old functions:
- **van Genuchten (1980)**
- **Brooks and Corey (1964)**

New functions:
- **Lognormal distribution model (Kosugi, 1996)**
- **Dual-porosity model (Durner, 1994)**



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Richards Equation - Assumptions

- Effect of air phase is neglected
- Darcy's equation is valid at very low and very high velocities
- Osmotic gradients in the soil water potential are negligible
- Fluid density is independent of solute concentration
- Matrix and fluid compressibilities are relatively small

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Richards Equation - Complications

- Hysteresis in the soil water retention function
- Extreme nonlinearity of the hydraulic functions
- Lack of accurate and cheap methods for measuring the hydraulic properties
- Extreme heterogeneity of the subsurface
- Inconsistencies between scale at which the hydraulic and solute transport parameters are measured, and the scale at which the models are being applied

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Boundary Conditions (System-Independent)

- Pressure head (Dirichlet type) boundary conditions:

$$h(z,t) = h_0(z,t) \quad \text{for} \quad z=0 \quad \text{or} \quad z=L$$

- Flux (Neumann type) boundary conditions:

$$-K\left(\frac{\partial h}{\partial z}+1\right) = q_0(z,t) \quad \text{for} \quad z=0 \quad \text{or} \quad z=L$$

- Gradient boundary conditions:

$$\frac{\partial h}{\partial z}=1 \quad \text{for} \quad z=L$$

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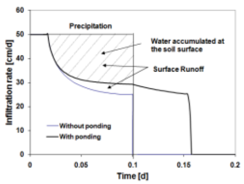
Boundary Conditions (System-Dependent)

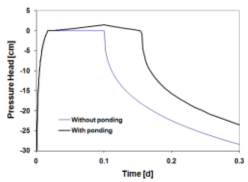
Atmospheric boundary condition:

$$\left| -K\frac{\partial h}{\partial x} - K \right| \le P \qquad h_A \le h \le h_S$$

Precipitation and Infiltration Fluxes



Pressure Heads (Stage I and II)



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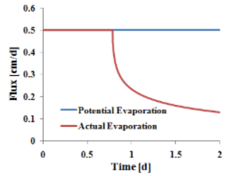
Boundary Conditions (System-Dependent)

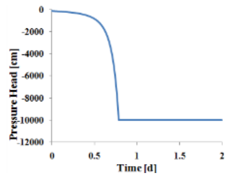
Atmospheric boundary condition:

$$\left| K(h)\left(\frac{\partial h}{\partial x} + 1\right) \right| \le E \qquad h_A \le h \le h_S$$

Actual and Potential Evaporation



Pressure Heads (Stage I and II)



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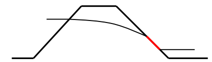
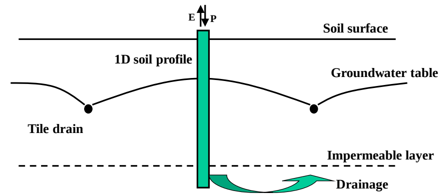
Boundary Conditions (System-Dependent)

- **Seepage face** (free draining lysimeter, dike)
  if(h<0) => q=0
  if(h=0) => q=?



- **Tile drains**



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The HYDRUS Software Packages

- Variably-Saturated Flow (Richards Eq.)
- **Root Water Uptake (water and salinity stress)**
- Solutes Transport (decay chains, ADE)
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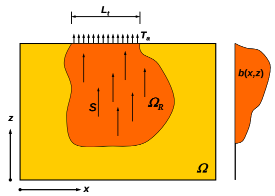
Root Water Uptake

Feddes et al. [1978]

$$S_p(z,t) = b(z)T_p$$



b	normalized water uptake distribution [L^{-1}]
S_p	potential root water uptake [T^{-1}]
T_p	potential transpiration [LT^{-1}]

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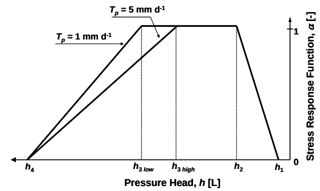
Root Water Uptake

Feddes et al. [1978] $S(z,t) = \alpha(h)S_p(z,t) = \alpha(h)b(z)T_p$



b	normalized water uptake distribution [L^{-1}]
S_p	potential root water uptake [T^{-1}]
S	actual root water uptake [T^{-1}]
T_p	potential transpiration [LT^{-1}]
α	stress response function [-]

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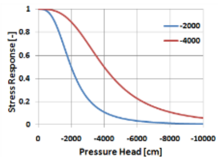
Stress Response Functions

Water and solute stress:

$$\alpha(h,h_\phi)=\frac{1}{1+\left(\frac{h+h_\phi}{h_{50}}\right)^p}$$

$$\alpha(h,h_\phi)=\frac{1}{1+\left(\frac{h}{h_{50}}\right)^{p_1}}*\frac{1}{1+\left(\frac{h_\phi}{h_{\phi 50}}\right)^{p_2}}$$



α	stress response function [-]
h	pressure head [L]
h_f	osmotic head [L]
h_{50}	pressure head at which water extraction rate is reduced by 50% [L]
$h_{\phi 50}$	ditto for osmotic head [L]
p_1, p_2	experimental constants [-] (=3)

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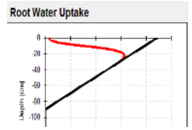
Transpiration Rates

$$T_p=\int_{L_R} S_p(h,z)\,dz$$

$$T_a=\int_{L_R} S(h,z)\,dz=T_p\int_{L_R} a(h,z)\,b(z)\,dz$$



b	normalized water uptake distribution [L^{-1}]
α	stress response function [-]
S_p	potential root water uptake [T^{-1}]
S	actual root water uptake [T^{-1}]
T_p	potential transpiration [LT^{-1}]
T_a	actual transpiration [LT^{-1}]

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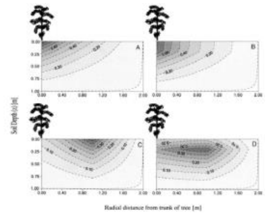
Spatial Root Distribution Function

$$b(x,y,z)=\left(1-\frac{x}{X_m}\right)\left(1-\frac{y}{Y_m}\right)\left(1-\frac{z}{Z_m}\right)e^{-\left(\frac{p_x}{X_m}|x^*-x|+\frac{p_y}{Y_m}|y^*-y|+\frac{p_z}{Z_m}|z^*-z|\right)}$$

$$b(x,z)=\left(1-\frac{z}{Z_m}\right)\left(1-\frac{x}{X_m}\right)e^{-\left(\frac{p_z}{Z_m}|z^*-z|+\frac{p_r}{X_m}|x^*-x|\right)}$$



(Vrugt et al., 2001)

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Root Growth

$$L_R(t) = L_m f(t)$$

$$f(t) = \frac{L_0}{L_0 + (L_m - L_0)e^{-rt}}$$

L_R rooting depth [L]
L_0 initial rooting depth [L]
L_m maximum rooting depth [L]
f root growth coefficient (Verhulst-Pearl logistic function)
r growth rate [T^{-1}]

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- **Solutes Transport (decay chains, ADE)**
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Solute Transport - Convection-Dispersion Equation

One-dimensional chemical transport during transient water flow in a variably saturated rigid porous medium

$$\frac{\partial(\theta c)}{\partial t} + \frac{\partial(\rho s)}{\partial t} = \frac{\partial}{\partial z}\left(\theta D \frac{\partial c}{\partial z} - qc\right) - \phi$$

c - solution concentration [ML^{-3}]
s - adsorbed concentration [MM^{-1}]
θ - water content [L^3L^{-3}]
ρ - soil bulk density [ML^{-3}]
D - dispersion coefficient [L^2T^{-1}]
q - volumetric flux [LT^{-1}]
ϕ - rate constant representing reactions [$ML^{-3}T^{-1}$]

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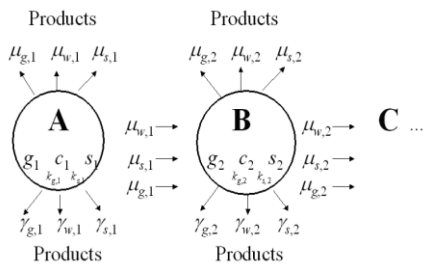
General Structure of the System of Solutes



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HYDRUS – Solute Transport

- **Transport of single ions**
- **Transport of multiple ions (sequential first-order decay)**
  - **Radionuclides:** ^{238}Pu -> ^{234}U -> ^{230}Th -> ^{226}Ra
  - **Nitrogen:** $(NH_2)_2CO$ -> NH_4^+ -> NO_2^- -> NO_3^-
  - **Pesticides:** aldicarb (oxime) -> sulfone (sulfone oxime) -> sulfoxide (sulfoxide oxime)
  - **Chlorinated Hydrocarbons:** PCE -> TCE -> c-DCE -> VC -> ethylene
  - **Pharmaceuticals, hormones:** Estrogen (17bEstradiol -> Estrone -> Estriol), Testosterone
  - **Explosives:** TNT (-> 4HADNT -> 4ADNT -> TAT), RDX HMX

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Governing Solute Transport Equations

$$\frac{\partial(\theta c)}{\partial t} + \frac{\partial(\rho s)}{\partial t} = \frac{\partial}{\partial z}\left(\theta D \frac{\partial c}{\partial z} - qc\right) - \phi$$

$$\frac{\partial \theta c_k}{\partial t} + \frac{\partial \rho s_k}{\partial t} + \frac{\partial a g_k}{\partial t} = \frac{\partial}{\partial z}\left(\theta D_k^w \frac{\partial c_k}{\partial z}\right) + \frac{\partial}{\partial z}\left(a D_k^g \frac{\partial g_k}{\partial z}\right) - \frac{\partial q c_k}{\partial z} -$$
$$-(\mu_{w,k} + \mu'_{w,k})\theta c_k - (\mu_{s,k} + \mu'_{s,k})\rho s_k - (\mu_{g,k} + \mu'_{g,k}) a g_k + \mu'_{w,k-1}\theta c_{k-1} +$$
$$-\mu'_{s,k-1}\rho s_{k-1} - \mu'_{g,k-1} a g_{k-1} + \gamma_{w,k}\theta + \gamma_{s,k}\rho + \gamma_{g,k} a - Sc_{r,k} \qquad k \varepsilon (2, n_s)$$

w, s, g **subscripts corresponding with the liquid, solid and gaseous phases, respectively**

c, s, g **concentration in liquid, solid, and gaseous phase, respectively**

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Solute Transport - Boundary Conditions

- **First-type (or Dirichlet type) boundary conditions**

$$c(x,z,t) = c_0(x,z,t) \qquad \text{for } (x,z)\ \varepsilon\ \Gamma_D$$

- **Third-type (Cauchy type) boundary conditions**

$$-\theta D_{ij}\frac{\partial c}{\partial x_j} n_i + q_i n_i c = q_i n_i c_0 \qquad \text{for } (x,z)\ \varepsilon\ \Gamma_C$$

- **Second-type (Neumann type) boundary conditions**

$$\theta D_{ij}\frac{\partial c}{\partial x_j} n_i = 0 \qquad \text{for } (x,z)\ \varepsilon\ \Gamma_N$$

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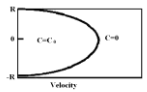
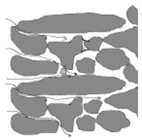
Solute Transport – Dispersion Coefficient





***Bear* [1972]:**

$$\theta D = \lambda |q| + \theta D_d \tau$$

- D_d - ionic or molecular diffusion coefficient in free water [L^2T^{-1}]
- τ - tortuosity factor [-]
- λ - longitudinal dispersivity [L]
- θ - water content [L^3L^{-3}]
- q - Darcy's flux [LT^{-1}]

***Millington and Quirk* [1961]:**

$$\tau = \frac{\theta^{7/3}}{\theta_s^2}$$

- θ_s - saturated water content [-]

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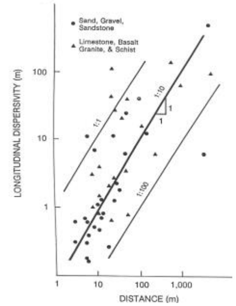
Dispersivity as a Function of Scale



Gelhar et al. (1985)

50

The HYDRUS Software Packages

- Variably-Saturated Flow (Richards Eq.)
- Root Water Uptake (water and salinity stress)
- **Solutes Transport (decay chains, ADE)**
  - **Sorption (linear and nonlinear)**
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  - Physical Nonequilibrium
- Heat Transport
- Parameter Estimation
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- Additional Modules

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Convection-Dispersion Equation

Linear Adsorption

$$s = K_d c \qquad R = 1 + \frac{\rho K_d}{\theta}$$

$$\frac{\partial R\theta c}{\partial t} = \frac{\partial}{\partial x_i}\left(\theta D_{ij}\frac{\partial c}{\partial x_j} - q_i c\right) + \phi$$

K_d - distribution coefficient [L^3M^{-1}]
R - retardation factor [-]
s - solid phase concentration [MM^{-1}]
c - liquid phase concentration [ML^{-3}]

52

Nonlinear Equilibrium Adsorption

- HYDRUS assumes nonequilibrium interactions between the solution (*c*) and adsorbed (*s*) concentrations, and equilibrium interaction between the solution (*c*) and gaseous (*g*) concentrations of the solute in the soil system.
- Liquid - Solid: a generalized nonlinear (Freundlich-Langmuir) empirical equation

$$s = \frac{k_s c^\beta}{1 + \eta c^\beta}$$

- k_s, η, β empirical constants

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- Additional Modules

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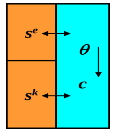
Nonequilibrium Two-Site Adsorption Model

$$s = s^e + s^k$$



s^e Type-1 sites with instantaneous sorption

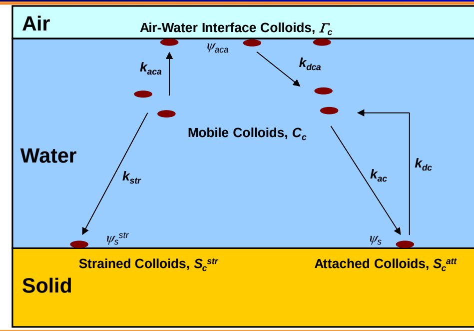
s^k Type-2 sites with kinetic sorption

$$\frac{\partial s^k}{\partial t} = \alpha[(1-f)K_d c - s^k]$$

f fraction of exchange sites assumed to be at equilibrium

55

Colloid, Virus, and Bacteria Transport



56

Colloid, Virus, and Bacteria Transport

$$\theta\frac{\partial c}{\partial t}+\rho\frac{\partial s_1}{\partial t}+\rho\frac{\partial s_2}{\partial t}=\theta D\frac{\partial^2 c}{\partial x^2}-\theta v\frac{\partial c}{\partial x}$$

Attachment/Detachment

$$\rho\frac{\partial s_1}{\partial t}=\theta k_a\psi_t c-k_d\rho s_1$$

$$\psi_t=\frac{s_{\max}-s}{s_{\max}}=1-\frac{s}{s_{\max}}$$

Straining

$$\rho\frac{\partial s_2}{\partial t}=\theta k_{str}\psi_{str}c$$

$$\psi_{str}=\left(\frac{d_c+x-x_0}{d_c}\right)^{\beta}$$

k_{str} - straining [T^{-1}]
k_a - deposition (attachment) coefficient [T^{-1}]
k_d - entrainment (detachment) coefficient [T^{-1}]
ψ - reduction of attachment coefficient due to blockage of sorption sites

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The HYDRUS Software Packages

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  - **Chemical Nonequilibrium**
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- Additional Modules

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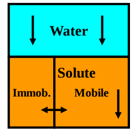
Two-Region Physical Nonequilibrium Transport



$$\theta=\theta_{im}+\theta_{mo}$$

$$\frac{\partial}{\partial t}(\theta_m+f\rho k_d)c_m=\frac{\partial}{\partial z}\left(\theta_m D_m\frac{\partial c_m}{\partial z}-qc_m\right)-\alpha(c_m-c_{im})$$

$$[\theta_{im}+(1-f)\rho k_d]\frac{\partial c_{im}}{\partial t}=\alpha(c_m-c_{im})$$

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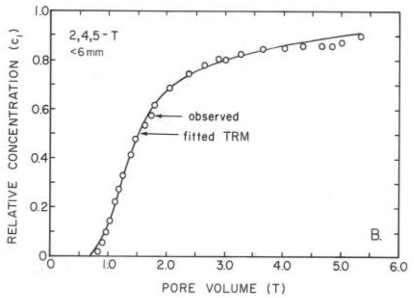
Two-Region Physical Nonequilibrium Transport



60

Interaction Among Phases

Liquid - Gas: a linear relation (Henry's Law)

$$g = k_g c$$

k_g	**empirical constant equal to $(K_H R T_A)^{-1}$**
K_H	**Henry's Law constant**
R	**universal gas constant**
T_A	**absolute temperature**

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Temperature Dependence of Transport and Reaction Coefficients

Most of the diffusion (D_w, D_g), distribution (k_s, k_g), and reaction rate (γ_w, γ_s, γ_g, μ_w', μ_s', μ_g', μ_w, μ_s, and μ_g) coefficients are strongly temperature dependent. HYDRUS assumes that this dependency can be expressed by an Arrhenius equation [Stumm and Morgan, 1981].

$$a_T = a_r \exp\left[\frac{E(T^A - T_r^A)}{RT^A T_r^A}\right]$$

a_r, a_T	**coefficient values at a reference absolute temperature, T_r^A, and absolute temperature, T^A, respectively**
E	**activation energy of the reaction or process**

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The HYDRUS Software Packages

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  - Physical Nonequilibrium
- Heat Transport
- **Parameter Estimation**
- Interactive Graphics-Based Interface
- Additional Modules

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Parameter Estimation with HYDRUS

Parameter Estimation:
- Soil hydraulic parameters
- Solute transport and reaction parameters
- Heat transport parameters

Sequence:
- Independently
- Simultaneously
- Sequentially

Method:
- Marquardt-Levenberg optimization

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Formulation of the Inverse Problem

The problem can be simplified into
the Weighted Least-Squares Problem

$$\Phi(\beta) = \sum_{i=1}^{n} w_i \left[q_i^* - q_i(\beta) \right]^2$$

w_i - weight of a particular measured point

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The HYDRUS Software Packages

- Variably-Saturated Flow (Richards Eq.)
- Root Water Uptake (water stress)
- Solutes Transport (decay chains, ADE)
  - Nonlinear Sorption
  - Chemical Nonequilibrium
  - Physical Nonequilibrium
- Heat Transport
- Pedotransfer Functions (hydraulic properties)
- Parameter Estimation
- <u>**Interactive Graphics-Based Interface**</u>
- HYDRUS (2D/3D) and Additional Modules

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The HYDRUS Software Packages

- Variably-Saturated Flow (Richards Eq.)
- Root Water Uptake (water stress)
- Solutes Transport (decay chains, ADE)
  - Sorption (linear and nonlinear)
  - Chemical Nonequilibrium
  - Physical Nonequilibrium
- Heat Transport
- Parameter Estimation
- <u>**Interactive Graphics-Based Interface**</u>
- Additional Modules

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Traditional Input to Hydrological Models

```
*** BLOCK A: BASIC INFORMATION ******************
Heading
'Example 4 - Infiltration Test '
LUnit  TUnit  MUnit  (indicated units are obligatory for all data)
'cm'   'min'  '-'
Kat (0:horizontal plane, 1:axisymmetric vertical flow, 2:vertical )
1
MaxIt   TolTh   TolH   (maximum number of iterations)
20   .0005   0.1
lWAt lChem     CheckF  ShortF  FluxF   AtmInF  SeepF  FreeD
t    t    f    f    t    f    f      f      f
*** BLOCK B: MATERIAL INFORMATION ***************
NMat    NLay    hTab1   hTabN   NPar
  2       2      .001    200.    9
thr     ths     tha     thm     Alfa    n       Ks      Kk      thk
.0001   .399    .0001   .399    .0174   1.3757  .0207   .0207   .399
.0001   .339    .0001   .339    .0139   1.6024  .0315   .0315   .339
*** BLOCK C: TIME INFORMATION *******************
dt      dtMin   dtMax   DMul    DMul2   MPL
.1      .001    100.    1.33    .33     10
TPrint(1),TPrint(2),...,TPrint(MPL)                (print-time array)
 60 180 360 720 1440 2160 2880 4320 5760 7200
*** BLOCK G: SOLUTE TRANSPORT INFORMATION *****
Epsi lUpW    lArtD   PeCr
0.5  t       f       0.
Bulk.d. Difus.   Disper.    Adsorp.   SinkL1  SinkS1   SinkL0
1.4  0.026     0.50  0.10   0.100   -3.472E-5 -6.9444E-6   0.     0.
1.4  0.026     0.50  0.10   0.100   -3.472E-5 -6.9444E-6   0.     0.
KodCB(1),KodCB(2),.....,KodCB(NumBP)
1    1    1    1    1
cTop   cBot
1.   0.   0.   0.   0.   0.
tPulse
7200
*** END OF INPUT FILE 'SELECTOR.IN' ****************
```

```
*** BLOCK H: NODAL INFORMATION **********************************
    NumNP     NumEl       IJ       NumBP    NObs
     380       342        19          5      0
  n  Code    x      z          h      Conc        Q       M   B
  1   1    0.00  230.00      0.00  0.00E+00  0.00E+00  1  0.00
  2   0    0.00  228.00   -145.50  0.00E+00  0.00E+00  1  0.00
  3   0    0.00  226.00   -143.40  0.00E+00  0.00E+00  1  0.00
  4   0    0.00  224.00   -141.00  0.00E+00  0.00E+00  1  0.00
  5   0    0.00  220.00   -135.60  0.00E+00  0.00E+00  1  0.00
  6   0    0.00  215.00   -127.70  0.00E+00  0.00E+00  1  0.00
  7   0    0.00  210.00   -119.00  0.00E+00  0.00E+00  1  0.00
  8   0    0.00  205.00   -109.90  0.00E+00  0.00E+00  1  0.00
  9   0    0.00  200.00   -100.50  0.00E+00  0.00E+00  1  0.00
 10   0    0.00  190.00    -82.80  0.00E+00  0.00E+00  1  0.00
 11   0    0.00  180.00    -71.00  0.00E+00  0.00E+00  2  0.00
 12   0    0.00  170.00    -60.30  0.00E+00  0.00E+00  2  0.00
 13   0    0.00  160.00    -49.80  0.00E+00  0.00E+00  2  0.00
 14   0    0.00  150.00    -39.60  0.00E+00  0.00E+00  2  0.00
 15   0    0.00  140.00    -29.50  0.00E+00  0.00E+00  2  0.00
 16   0    0.00  130.00    -19.40  0.00E+00  0.00E+00  2  0.00
 17   0    0.00  120.00     -9.40  0.00E+00  0.00E+00  2  0.00
 18   0    0.00  110.00      0.60  0.00E+00  0.00E+00  2  0.00
 19   0    0.00  100.00     10.20  0.00E+00  0.00E+00  2  0.00
 20   1    5.00  230.00      0.00  0.00E+00  0.00E+00  1  0.00
 21   0    5.00  228.00   -145.50  0.00E+00  0.00E+00  1  0.00
 22   0    5.00  226.00   -143.40  0.00E+00  0.00E+00  1  0.00
 23   0    5.00  224.00   -141.00  0.00E+00  0.00E+00  1  0.00
 24   0    5.00  220.00   -135.60  0.00E+00  0.00E+00  1  0.00
 25   0    5.00  215.00   -127.70  0.00E+00  0.00E+00  1  0.00
 26   0    5.00  210.00   -119.00  0.00E+00  0.00E+00  1  0.00
 27   0    5.00  205.00   -109.90  0.00E+00  0.00E+00  1  0.00
 28   0    5.00  200.00   -100.50  0.00E+00  0.00E+00  1  0.00
 29   0    5.00  190.00    -82.80  0.00E+00  0.00E+00  1  0.00
 30   0    5.00  180.00    -71.00  0.00E+00  0.00E+00  2  0.00
 31   0    5.00  170.00    -60.30  0.00E+00  0.00E+00  2  0.00
 32   0    5.00  160.00    -49.80  0.00E+00  0.00E+00  2  0.00
 33   0    5.00  150.00    -39.60  0.00E+00  0.00E+00  2  0.00
 34   0    5.00  140.00    -29.50  0.00E+00  0.00E+00  2  0.00
 35   0    5.00  130.00    -19.40  0.00E+00  0.00E+00  2  0.00
```

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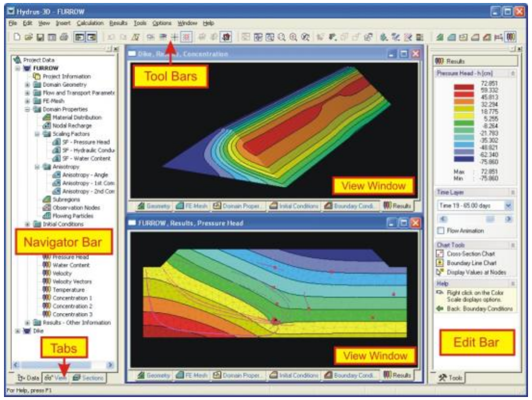
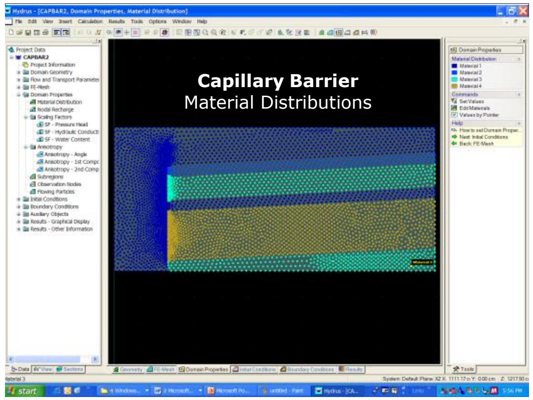
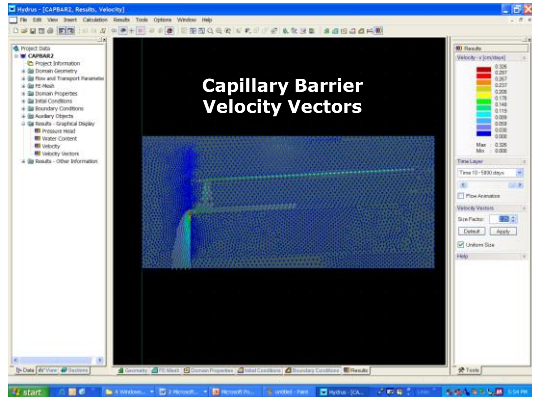

Tool Bars
View Window
Navigator Bar
View Window
Tabs
Edit Bar

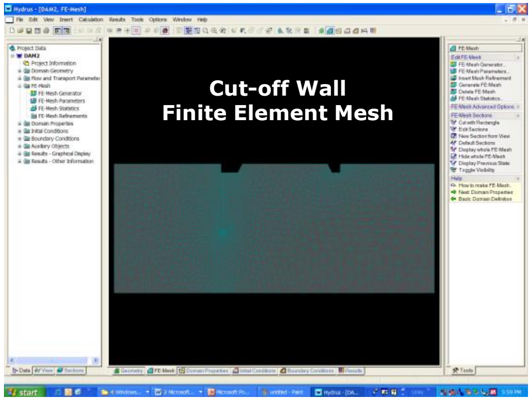
73


Capillary Barrier
Material Distributions

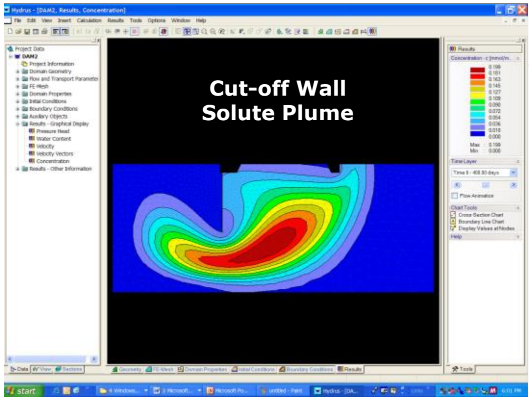
74


Capillary Barrier
Velocity Vectors

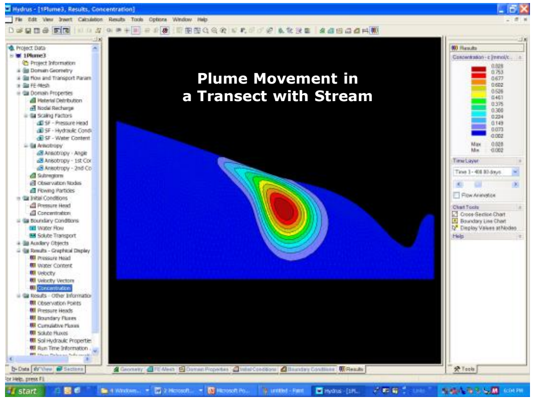
75


Cut-off Wall
Finite Element Mesh

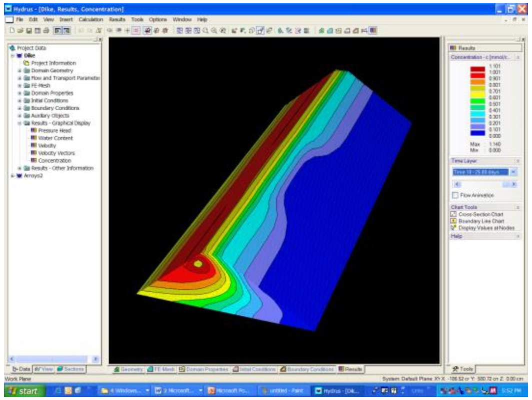
76


Cut-off Wall
Solute Plume

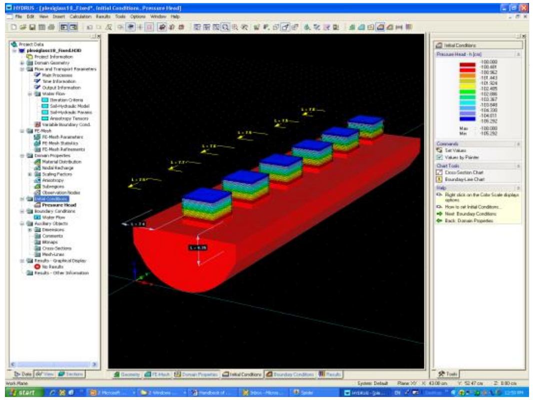
77


Plume Movement in
a Transect with Stream

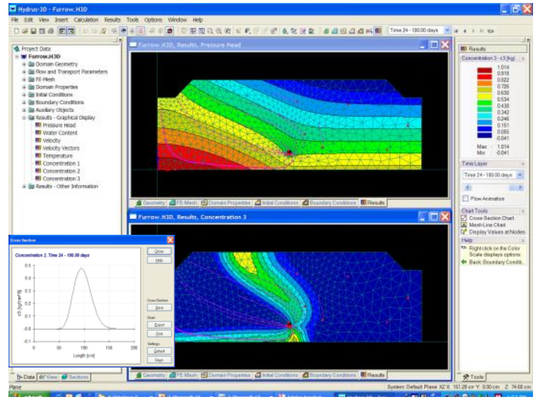
78



79



80



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Geochemical Modeling

1. HYDRUS-UNSATCHEM Approach

HYDRUS-1D

2. HYDRUS-PHREEQC Approach

HP1

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HYDRUS-1D + UNSATCHEM

- **HYDRUS-1D** (Šimůnek et al., 1998)
  - variably saturated water flow
  - heat transport
  - root water uptake
  - solute transport
- **UNSATCHEM** (Šimůnek et al., 1996)
  - carbon dioxide transport
  - major ion chemistry
    - cation exchange
    - precipitation-dissolution (instantaneous and kinetic)
    - complexation

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Carbon Dioxide Transport

Šimůnek and Suarez [1993]:

$$\frac{\partial(c_a\theta_a + c_w\theta)}{\partial t} = \frac{\partial}{\partial x_i}\theta_a D_{ij}^a \frac{\partial c_a}{\partial x_j} + \frac{\partial}{\partial x_i}\theta D_{ij}^w \frac{\partial c_w}{\partial x_j} - \frac{\partial}{\partial x_i} q_i c_w - Sc_w + P$$

- c_w — **volumetric concentrations of CO_2 in the dissolved phase [L^3L^{-3}]**
- c_a — **volumetric concentrations of CO_2 in the gas phase [L^3L^{-3}]**
- D_{ij}^a — **effective soil matrix diffusion coefficient of CO_2 in the gas phase [L^2T^{-1}]**
- D_{ij}^w — **effective soil matrix dispersion coefficient of CO_2 in the dissolved phase [L^2T^{-1}]**
- q_i — **soil water flux [LT^{-1}]**
- q_a — **volumetric air content [L^3L^{-3}]**
- P — **CO_2 production rate [$L^3L^{-3}T^{-1}$]**
- Sc_w — **dissolved CO_2 removed from the soil by root water uptake**

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HYDRUS-1D + UNSATCHEM

1	Aqueous components	7	Ca^{2+}, Mg^{2+}, Na^+, K^+, SO_4^{2-}, Cl^-, NO_3^-
2	Complexed species	10	$CaCO_3^o$, $CaHCO_3^+$, $CaSO_4^o$, $MgCO_3^o$, $MgHCO_3^+$, $MgSO_4^o$, $NaCO_3^-$, $NaHCO_3^o$, $NaSO_4^-$, KSO_4^-
3	Precipitated species	6	$CaCO_3$, $CaSO_4 \cdot 2H_2O$, $MgCO_3 \cdot 3H_2O$, $Mg_5(CO_3)_4(OH)_2 \cdot 4H_2O$, $Mg_2Si_3O_{7.5}(OH) \cdot 3H_2O$, $CaMg(CO_3)_2$
4	Sorbed species (exchangeable)	4	Ca, Mg, Na, K
5	CO_2-H_2O species	7	P_{CO2}, $H_2CO_3^*$, CO_3^{2-}, HCO_3^-, H^+, OH^-, H_2O
6	Silica species	3	H_4SiO_4, $H_3SiO_4^-$, $H_2SiO_4^{2-}$

Kinetic reactions: calcite precipitation/dissolution, dolomite dissolution
Activity coefficients: extended Debye-Hückel equations, Pitzer expressions

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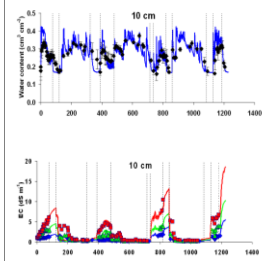
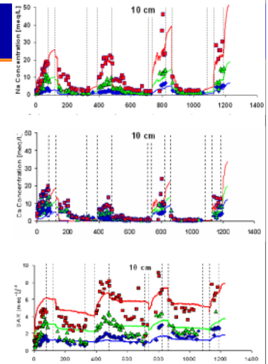
Lysimeter Study



Gonçalves et al. (2006)



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HP1 - Coupled HYDRUS-1D and PHREEQC

HYDRUS-1D [Šimůnek et al., 1998]:
- Variably Saturated Water Flow
- Solute Transport
- Heat transport
- Root water uptake

PHREEQC [Parkhurst and Appelo, 1999]:

Available chemical reactions:
- Aqueous complexation
- Redox reactions
- Ion exchange (Gains-Thomas)
- Surface complexation – diffuse double-layer model and non-electrostatic surface complexation model
- Precipitation/dissolution
- Chemical kinetics
- Biological reactions

HP1

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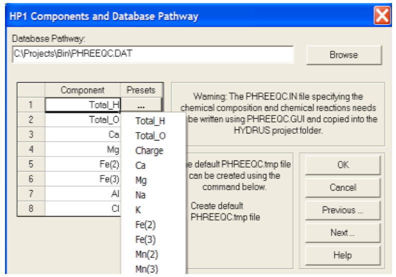
HYDRUS-1D GUI for HP1



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HP1 Examples

- Transport of heavy metals (Zn^{2+}, Pb^{2+}, and Cd^{2+}) subject to multiple cation exchange
- Transport with mineral dissolution of amorphous SiO_2 and gibbsite ($Al(OH)_3$)
- Heavy metal transport in a medium with a pH-dependent cation exchange complex
- Infiltration of a hyperalkaline solution in a clay sample (this example considers kinetic precipitation-dissolution of kaolinite, illite, quartz, calcite, dolomite, gypsum, hydrotalcite, and sepiolite)
- Long-term transient flow and transport of major cations (Na^{+}, K^{+}, Ca^{2+}, and Mg^{2+}) and heavy metals (Cd^{2+}, Zn^{2+}, and Pb^{2+}) in a soil profile.
- Kinetic biodegradation of NTA (biomass, cobalt)

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HYDRUS Package for Modflow

The Unsaturated Flow Package for Modflow-2000

Hyeyoung Sophia Seo, Navin Twarakavi, Jirka Šimůnek, and Eileen P. Poeter

Seo, H. S., J. Šimůnek, and E. P. Poeter, Documentation of the HYDRUS Package for MODFLOW-2000, the U.S. Geological Survey Modular Ground-Water Model, *GWMI 2007-01*, International Ground Water Modeling Center, Colorado School of Mines, Golden, Colorado, 96 pp., 2007.

Twarakavi, N. K. C., J. Šimůnek, and H. S. Seo, Evaluating interactions between groundwater and vadose zone using HYDRUS-based flow package for MODFLOW, *Vadose Zone Journal*, doi:10.2136/VZJ2007.0082, Special Issue "Vadose Zone Modeling", *7*(2), 757-768, 2008.

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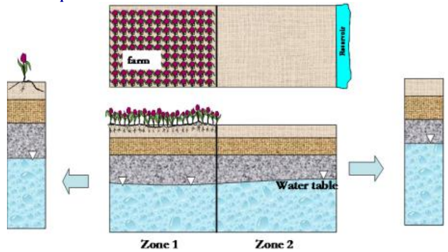
HYDRUS Package: Zoning

MODFLOW model domain is grouped in to zones based on similarities in soil hydraulic characteristics, hydrogeology and meteorology.
A HYDRUS vertical profile is assigned to each of the zones on which the 1D Richards equation is used.



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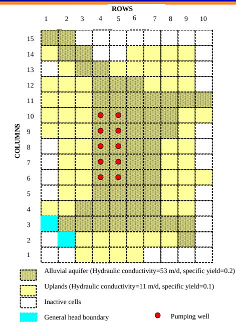
HYDRUS - MODFLOW - Case Study

Hypothetical regional-scale ground water flow problem:

Model domain, spatial distribution of hydraulic conductivities and specific yields, wells (red circles) and general head boundaries.



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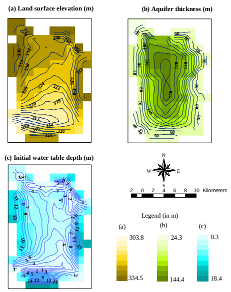
HYDRUS - MODFLOW - Case Study

Hypothetical regional-scale ground water flow problem:

a) Land surface elevation
b) depth to bedrock
c) water table depth at the beginning of the simulation



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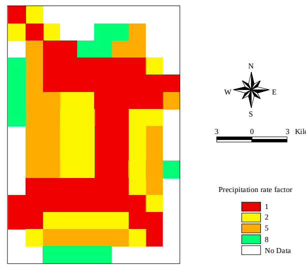
HYDRUS - MODFLOW - Case Study

Hypothetical regional-scale ground water flow problem:

Zonation showing the spatial distribution of precipitation



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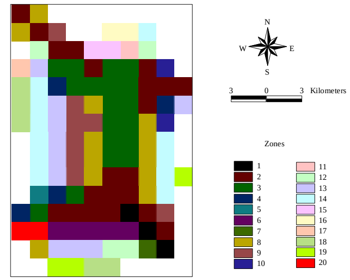
HYDRUS - MODFLOW - Case Study

Hypothetical regional-scale ground water flow problem:

MODFLOW zones used to define HYDRUS soil profiles



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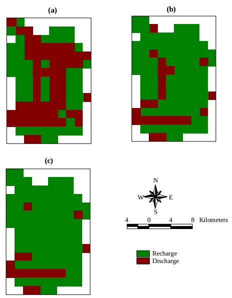
HYDRUS - MODFLOW - Case Study

Hypothetical regional-scale ground water flow problem:

Ground water table fluxes (recharge vs discharge) as predicted by the HYDRUS package at the end of stress periods (a) 3, (b) 6 and (c) 12.



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New HYDRUS Web Site

www.pc-progress.com/en/default.aspx

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New HYDRUS Web Site: Public Libraries

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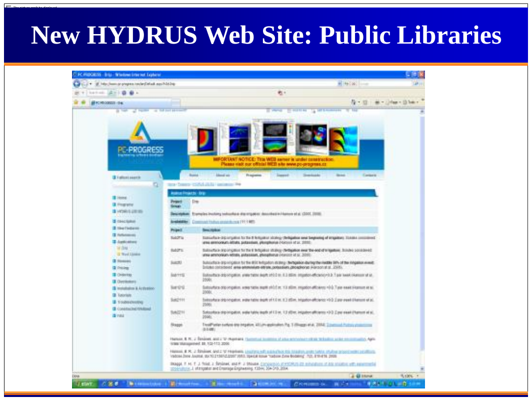
New HYDRUS Web Site: Public Libraries

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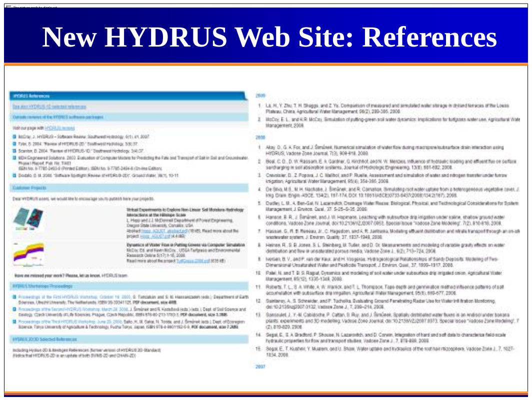
New HYDRUS Web Site: References

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Short Courses

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