Modeling Water Flow and Transport of Particle-Like Substances in Soils and Groundwater Using the HYDRUS Software Packages

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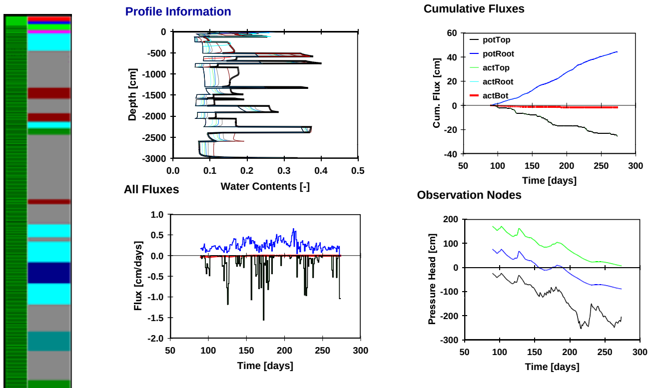
OUTLINE

- Introduction – Background on HYDRUS
- Historical Development (models of increasing complexity)
- Preferential Flow and Transport
- Spatial Heterogeneity
- Effects of Chemical Conditions – HP1/2/3
- Colloid-Facilitated Solute Transport
- Miscellaneous Other Options

HYDRUS-1D



Software for Simulating Water Flow and Solute Transport in One-Dimensional Variably-Saturated Soils Using Numerical Solutions

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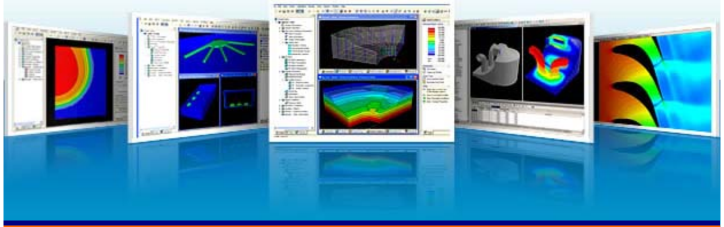

HYDRUS (2D/3D)

Software for Simulating Water Flow and Solute Transport in Two/Three-Dimensional Variably-Saturated Soils Using Numerical Solutions

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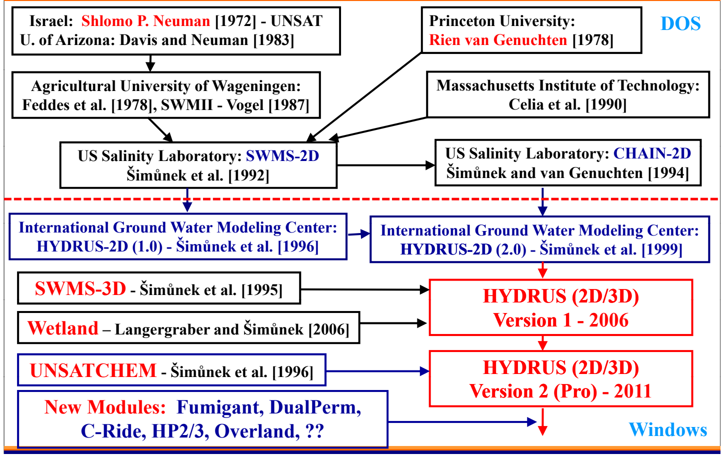
History of HYDRUS (2D/3D)



DOS

Israel: Shlomo P. Neuman [1972] - UNSAT
U. of Arizona: Davis and Neuman [1983]

Princeton University:
Rien van Genuchten [1978]

Agricultural University of Wageningen:
Feddes et al. [1978], SWMII - Vogel [1987]

Massachusetts Institute of Technology:
Celia et al. [1990]

US Salinity Laboratory: SWMS-2D
Šimůnek et al. [1992]

US Salinity Laboratory: CHAIN-2D
Šimůnek and van Genuchten [1994]

International Ground Water Modeling Center:
HYDRUS-2D (1.0) - Šimůnek et al. [1996]

International Ground Water Modeling Center:
HYDRUS-2D (2.0) - Šimůnek et al. [1999]

SWMS-3D - Šimůnek et al. [1995]

Wetland – Langergraber and Šimůnek [2006]

HYDRUS (2D/3D)
Version 1 - 2006

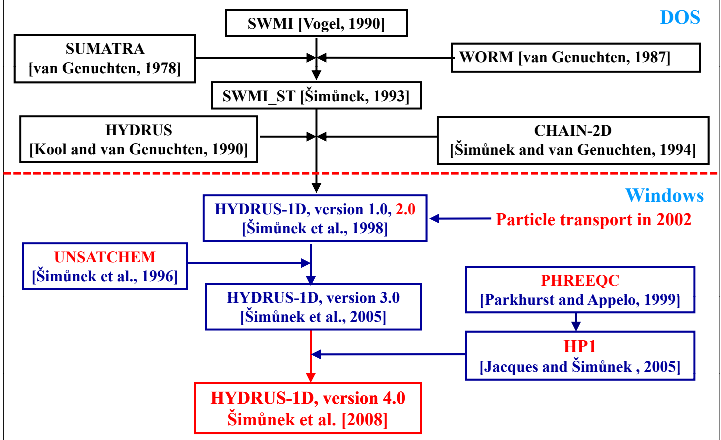
UNSATCHEM - Šimůnek et al. [1996]

HYDRUS (2D/3D)
Version 2 (Pro) - 2011

New Modules: Fumigant, DualPerm,
C-Ride, HP2/3, Overland, ??

Windows

History of HYDRUS-1D



DOS

SWMI [Vogel, 1990]

SUMATRA
[van Genuchten, 1978]

WORM [van Genuchten, 1987]

SWMI_ST [Šimůnek, 1993]

HYDRUS
[Kool and van Genuchten, 1990]

CHAIN-2D
[Šimůnek and van Genuchten, 1994]

Windows

HYDRUS-1D, version 1.0, 2.0
[Šimůnek et al., 1998]

Particle transport in 2002

UNSATCHEM
[Šimůnek et al., 1996]

HYDRUS-1D, version 3.0
[Šimůnek et al., 2005]

PHREEQC
[Parkhurst and Appelo, 1999]

HP1
[Jacques and Šimůnek , 2005]

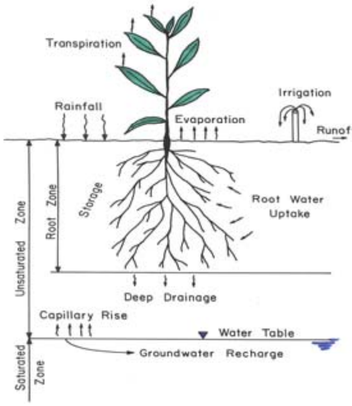
HYDRUS-1D, version 4.0
Šimůnek et al. [2008]

Agricultural Applications

- Precipitation
- Irrigation
- Runoff
- Evaporation
- Transpiration
- Root Water Uptake
- Capillary Rise
- Deep Drainage

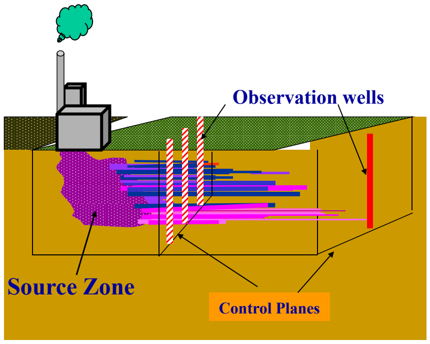
- Fertilizers, nutrients
- Pesticides
- Fumigants
- Emerging Pollutants (steroids and hormones, pharmaceuticals)

- Colloids
- Pathogens
- Nanoparticles



Industrial Applications

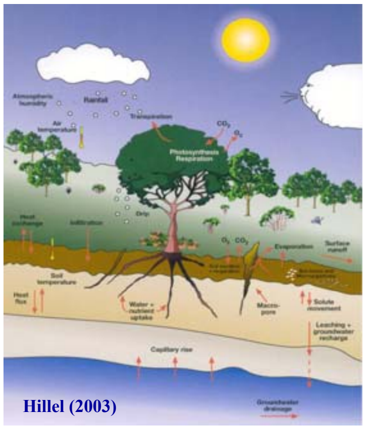
- Industrial Pollution
- Municipal Pollution
- Landfill Covers
- Waste Repositories
- Radioactive Waste Disposal Sites
- Remediation
- Brine Releases
- Contaminant Plumes
- Seepage of Wastewater from Land Treatment Systems
- Emerging Pollutants (gasoline additives, industrial additives, personal hygiene products, flame retardants, explosives, surfactants)



- Colloids,
- Pathogens
- Nanoparticles

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)

Governing Equations

Variably-Saturated Water Flow (Richards Equation)

$$\frac{\partial\theta(h)}{\partial t}=\frac{\partial}{\partial z}\left[K(h)\left(\frac{\partial h}{\partial z}-1\right)\right]-S(h)$$

Solute Transport (Convection-Dispersion Equation)

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

Heat Movement

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

HYDRUS – Main Processes

Water Flow:

- Richards equation for variably-saturated water flow
- Various models of soil hydraulic properties, Hysteresis
- Sink term, accounting for water uptake by plant roots (uncompensated and compensated; reduced due to osmotic and pressure stress)
- Preferential flow
- Isothermal and thermal liquid and vapor flow

Solute Transport:

- Convective-dispersive transport in water, Diffusion in gas
- Linear and nonlinear reactions between the solid and liquid phases
- Zero-order production, First-order degradation
- Physical and chemical nonequilibrium solute transport
- Sink term, accounting for nutrient uptake by plant roots (active and passive)

Heat Transport:

- Conduction and convection with flowing water (transport of latent heat)

Inverse Parameter Optimization:

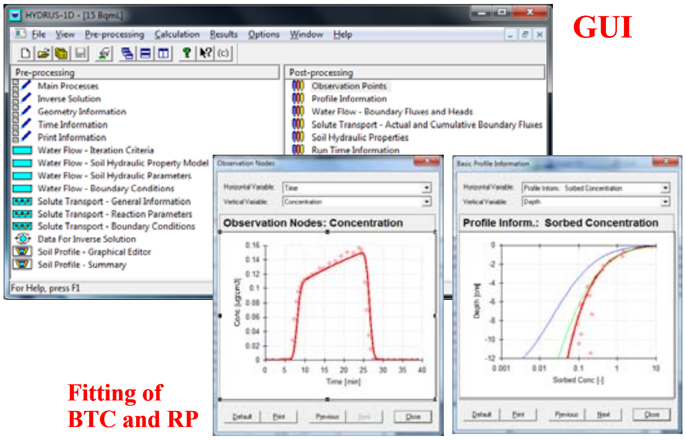
- Marquardt-Levenberg method
- Optimize soil hydraulic and solute transport parameters

HYDRUS – Solute Transport

- Transport of Single Ions or Particles (colloids, viruses, bacteria)
- 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

- General BioGeoChemical Reactions (the HP1/2/3 module)
- Colloid-Facilitated Solute Transport (the C-Ride module)
- Processes in Wetlands (the CW2D and CWM1 modules)
- Transport/Reactions of Major Ions (the UNSATCHEM module)

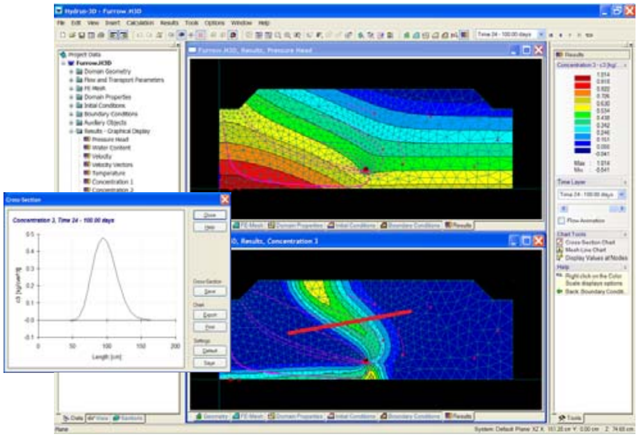
HYDRUS-1D



GUI

Fitting of BTC and RP

HYDRUS (2D/3D)



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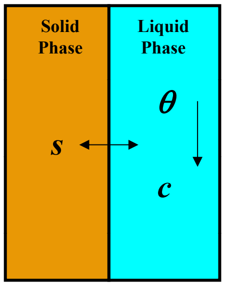
One-Site Equilibrium Sorption Model



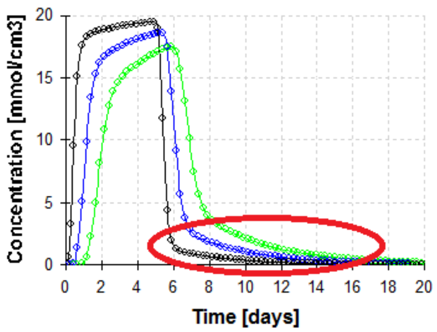
$$\frac{\partial \theta c}{\partial t}+\rho\frac{\partial s}{\partial t}=\frac{\partial}{\partial z}\left(\theta D\frac{\partial c}{\partial z}\right)-\frac{\partial qc}{\partial z}-\phi$$

Adsorption Isotherms:

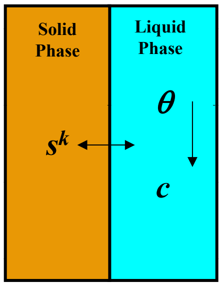
Linear :	$s=K_d c$
Freundlich :	$s=K_f c^{\beta}$
Langmuir :	$s=\frac{K_l c}{1+\eta c}$
F - L Combined :	$s=\frac{K_d c^{\beta}}{1+\eta c^{\beta}}$

Retardation Factor: $R=1+\frac{\rho}{\theta}\frac{\partial s}{\partial c}=1+\frac{\rho K_d}{\theta}$

Breakthrough Curves with Tailing



One-Site Kinetic Sorption Model



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

- **Transport of Single Ions**

$$\rho\frac{\partial s^k}{\partial t}=\rho\alpha\left[K_d c - s^k\right]-\phi_k$$

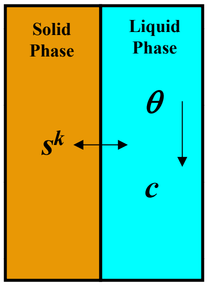
α – first-order mass transfer (sorption rate) [T^{-1}]

- **Transport of Particles (colloids, viruses, bacteria)**

$$\rho\frac{\partial s^k}{\partial t}=k_a\theta c-k_d\rho s^k-\phi_k$$

k_a – attachment rate coefficient [T^{-1}]
k_d – detachment rate coefficient [T^{-1}]

One-Site Kinetic Sorption Model



The formulation based on attachment-detachment coefficients is mathematically identical to the formulation using first-order mass transfer coefficients

$$\theta k_a c - k_d \rho s^k = \rho\alpha\left(K_d c - s^k\right)$$

$$k_d = \alpha$$

$$k_a = \alpha\frac{\rho}{\theta}K_d$$

$$K_d = \frac{\theta k_a}{\rho k_d}$$

Filtration Theory

Rajagopalan and Tien [1976], Logan et al. [1995]:

$$k_a = \frac{3(1-\theta)}{2d_c}\eta\alpha v$$

d_c	diameter of the sand grains [L]
α	sticking efficiency [-]
v	pore water velocity [LT^{-1}]
η	single-collector efficiency [-]

$$\eta = 4A_s^{1/3}N_{Pe}^{-2/3} + A_s N_{Lo}^{1/8} N_R^{15/8} + 0.00338 A_s N_G^{1.2} N_R^{-0.4}$$

The first, second, and third terms represent removal by diffusion, interception, and gravitational sedimentation

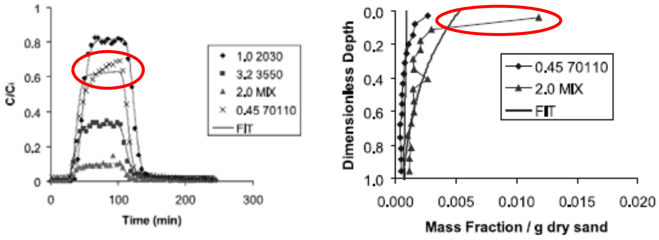
N_{Pe}	- Peclet number [-]
N_R	- interception number [-]
N_G	- gravitation number [-]
N_{Lo}	- accounts for London-van der Walls attractive forces [-]
A_s	- correction factor [-]

Application to Transport of Colloids

Transport of fluorescent latex colloids in columns with glass beads and Ottawa sands

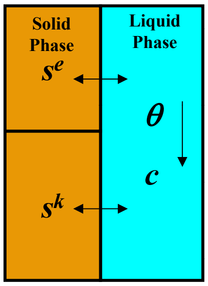
Colloids: d_p=0.45, 1, 2, 3.2 mm

Sands: d_{50}=0.7, 0.36, 0.15, 0.24 (mix), 0.26 (GB)



Bradford, S. A., S. R. Yates, M. Bettehar, and J. Šimůnek, Physical factors affecting the transport and fate of colloids in saturated porous media, *Water Resources Research*, 38(12), 1327, 63.1-63.12, 2002.

Two-Site Sorption Model



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

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

- Solute Transport

$$s^e = f_e K_d c$$

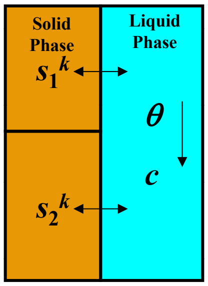
$$\rho\frac{\partial s^k}{\partial t} = \alpha_k\rho\left[(1-f_e)K_d c - s^k\right] - \phi_k$$

f_e - fraction of exchange sites in equilibrium with the liquid phase [-]

α_k – first-order mass transfer (sorption rate) [T^{-1}]

Selim et al. [1976], van Genuchten and Wagenet [1989]

Two Kinetic Sorption Sites Model



$$s = s_1^k + s_2^k$$

$$\frac{\partial\theta c}{\partial t} + \rho\frac{\partial s_1^k}{\partial t} + \rho\frac{\partial s_2^k}{\partial t} = \frac{\partial}{\partial z}\left(\theta D\frac{\partial c}{\partial z}\right) - \frac{\partial qc}{\partial z} - \phi$$

- Transport of Particles

$$\rho\frac{\partial s_1^k}{\partial t} = k_{a1}\theta c - k_{d1}\rho s_1^k - \phi_{k1}$$

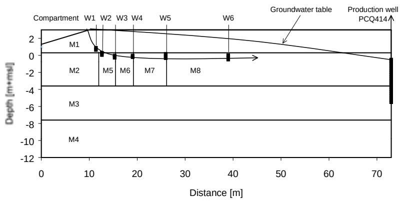
$$\rho\frac{\partial s_2^k}{\partial t} = k_{a2}\theta c - k_{d2}\rho s_2^k - \phi_{k2}$$

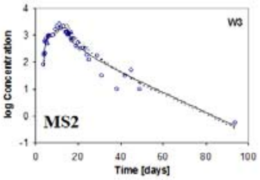
The two kinetic sites model can be used to describe different processes. While the first kinetic process could be used for chemical attachment, the second kinetic process could represent physical straining.

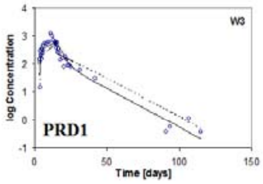
Two Applications with Jack Schijven

Dune Recharge

(a field site with a source compartment, and monitoring (W) and production wells)







MS2 and PRD1 viruses

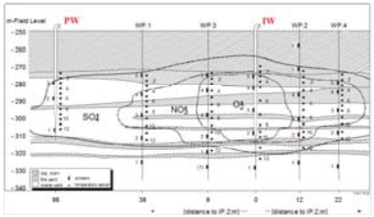
2D one- and two-site sorption models

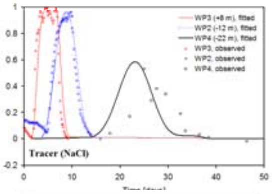
Schijven, J., and J. Šimůnek, Kinetic modeling of virus transport at field scale, *J. of Contaminant Hydrology*, *55*(1-2), 113-135, 2002.

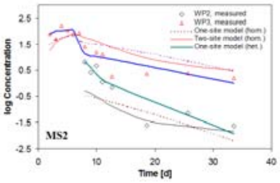
Two Applications with Jack Schijven

Deep Well Injection

A field site with injection (IW), monitoring (WP), and production wells (PW)







MS2
2D one- and two-site sorption models
Homogeneous or heterogeneous profile

Schijven, J., and J. Šimůnek, Kinetic modeling of virus transport at field scale, *J. of Contaminant Hydrology*, *55*(1-2), 113-135, 2002.

Retention Functions

$$\rho \frac{\partial s^k}{\partial t} = k_a \psi \theta c$$

◆ **Time-dependent retention function [Adamczyk et al., 1994]**

$$\psi = \left(1 - \frac{s}{s_{\max}}\right)$$

◆ **Depth-dependent retention function [Bradford et al., 2003]**

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

Retention Functions

◆ **Time- and depth-dependent retention function [Bradford et al., 2005]**

$$\psi = \left(1 - \frac{s}{s_{\max}}\right)\left(\frac{d_c + x}{d_c}\right)^{-\beta}$$

◆ **Random sequential adsorption model [Johnson and Elimelech, 1995]**

$$\psi = 1 - 4a + 3.308a^2 + 1.4069a^3 \qquad \text{for} \quad s < 0.8 s_{\max}$$

$$\psi = \frac{(1 - bs)^3}{2 {d_{50}}^2 b^3} \qquad \text{for} \quad s > 0.8 s_{\max}$$

$$a = 0.546 \frac{s}{s_{\max}} \qquad b = \frac{1}{s_{\max}}$$

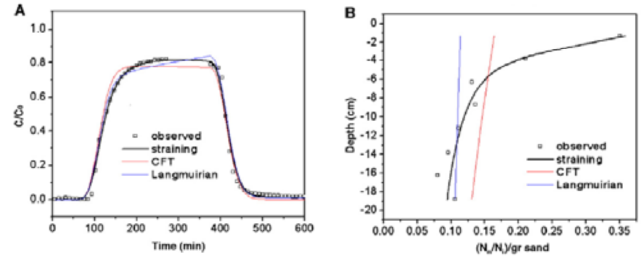
◆ **Ripening**

$$\psi = \max\left(1, s^{s_{\max}}\right) \qquad \rho \frac{\partial s^k}{\partial t} = k_a \psi (\theta c) + k_{\mathrm{int}} \left(\rho s^k\right)(\theta c) - k_d \left(\rho s^k\right) = k_a \psi^* (\theta c) - k_d \left(\rho s^k\right)$$

$$\psi^* = \psi + \frac{k_{\mathrm{int}}}{k_a}\left(\rho s^k\right)$$

k_{int} - the particle interaction rate coefficient [T^{-1}] [Wang et al., 2012]

Application to Bacteria Transport

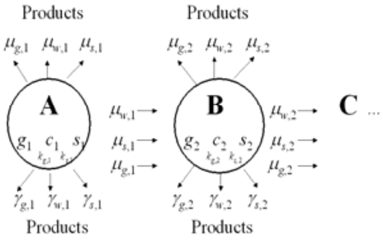


***Rhodococcus rhodochrous* breakthrough curves (A) and retention profile (B) in 567 µm sand and a water saturation of 80%. Fitted curves were obtained using the Classical filtration theory (CFT) (red), Langmuirian blocking (blue), and straining (black) models.**

Gargiulo et al. (JCH, 2007)

Transport of Multiple Species

General structure of the system of solutes considered in HYDRUS



After neglecting the gas phase and simplifying:

$$\frac{\partial \theta c_1}{\partial t} + \frac{\partial \rho s_1}{\partial t} = \frac{\partial}{\partial z}\left(\theta D_1 \frac{\partial c_1}{\partial z}\right) - \frac{\partial q c_1}{\partial z} - \mu_1 (\theta c_1 + \rho s_1)$$

$$\frac{\partial \theta c_2}{\partial t} + \frac{\partial \rho s_2}{\partial t} = \frac{\partial}{\partial z}\left(\theta D_2 \frac{\partial c_2}{\partial z}\right) - \frac{\partial q c_2}{\partial z} + \mu_1 (\theta c_1 + \rho s_1) - \mu_2 (\theta c_2 + \rho s_2)$$

Transport of *E. coli* [Bradford et al., 2006]

Hypothesis: When a critical value of S_{crit} is reached, *E. coli* can be released into the aqueous phase as an aggregated species

Species 1: mono-dispersed *E. coli*

$$\frac{\partial \theta c_1}{\partial t} + \rho \frac{\partial s_1^k}{\partial t} = \frac{\partial}{\partial z}\left(\theta D \frac{\partial c_1}{\partial z}\right) - \frac{\partial q c_1}{\partial z}$$

$$\rho \frac{\partial s_1^k}{\partial t} = \theta k_{a1} \psi_1 c_1 - \rho k_{d1} s_1^k - \rho k_{12} F_p$$

$$F_p = \max\left(s_1^k - s_{crit}, 0\right)$$

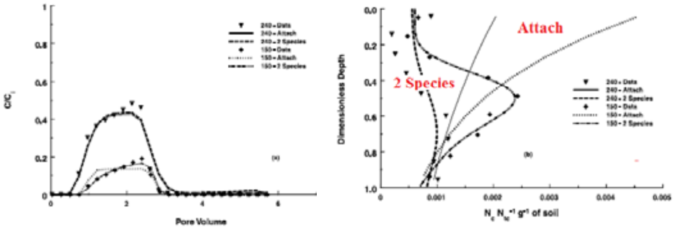
Species 2: aggregated *E. coli*

$$\frac{\partial \theta c_2}{\partial t} + \rho \frac{\partial s_2^k}{\partial t} = \frac{\partial}{\partial z}\left(\theta D \frac{\partial c_2}{\partial z}\right) - \frac{\partial q c_2}{\partial z} + \rho k_{12} F_p$$

$$\rho \frac{\partial s_2^k}{\partial t} = \theta k_{a2} \psi_2 c_2 - \rho k_{d2} s_2^k$$

Transport of *E. coli* [Bradford et al. 2006]

Non-monotonic deposition profiles:



Effluent concentration curves (left) and deposition profiles (right) for *E. coli* in the 240 and 150 mm Ottawa sands.

Attach - attachment and detachment
2 Species - straining and both mono-dispersed and aggregated *E. coli*

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Preferential Flow and Transport

Fractured Rock

Heterogeneous Sediments

Macroporous Soil

The DualPerm Module

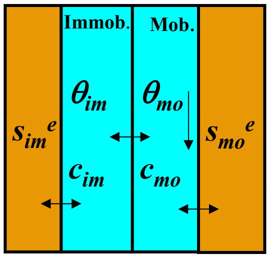
Preferential Flow and Transport Approaches

Approaches commonly used in Soil Physics and Subsurface Hydrology assume that there are two pore systems:

- **Dual-Porosity Models** – while water in the macropore domain is mobile, water in the micropore domain is immobile; dissolved solutes move into and out of immobile domain by molecular diffusion (e.g., van Genuchten and Wierenga, 1976)
- **Dual-Permeability Models** – while water is mobile in both domains, it moves slower in the micropores and faster in the macropores (e.g., Gerke and van Genuchten, 1992).

Alternative Terms:
Matrix – Fracture
Micropores – Macropores
Intra-porosity – Inter-porosity

Dual-Porosity Model
(with Equilibrium Sorption)



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

$$s = s^e_{mo} + s^e_{im}$$

- Solute Transport
[van Genuchten and Wierenga, 1976]

$$\frac{\partial \theta_{mo} c_{mo}}{\partial t} + f_{mo}\rho \frac{\partial s_{mo}}{\partial t} = \frac{\partial}{\partial z}\left(\theta_{mo} D_{mo} \frac{\partial c_{mo}}{\partial z}\right) - \frac{\partial q_{mo} c_{mo}}{\partial z} - \omega_{ph}(c_{mo} - c_{im}) - \phi_{mo}$$

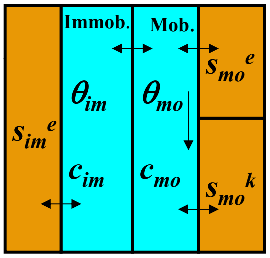
$$\frac{\partial \theta_{im} c_{im}}{\partial t} + (1 - f_{mo})\rho \frac{\partial s_{im}}{\partial t} = \omega_{ph}(c_{mo} - c_{im}) - \phi_{im}$$

$$s_{mo} = K_{d1} c_{mo} \qquad s_{im} = K_{d2} c_{im}$$

f_{mo} – fraction of exchange sites in contact with the mobile region [-]

ω_{ph} – mass transfer between mobile and immobile regions (physical process) [T^{-1}]

Dual-Porosity Model
(with Equilibrium and Kinetic Sorption)



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

$$s = s^e_{mo} + s^k_{mo} + s^e_{im}$$

- Solute Transport
[Šimůnek et al., 2008]

$$\frac{\partial \theta_{mo} c_{mo}}{\partial t} + f_{mo}\rho \frac{\partial s^e_{mo}}{\partial t} = \frac{\partial}{\partial z}\left(\theta_{mo} D_{mo} \frac{\partial c_{mo}}{\partial z}\right) - \frac{\partial q_{mo} c_{mo}}{\partial z} - \phi_{mo} - \omega_{ph}(c_{mo} - c_{im}) - \alpha_{ch}\left(s^k_{mo,e} - s^k_{mo}\right)$$

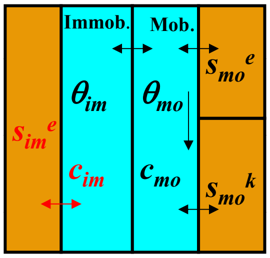
$$\frac{\partial \theta_{im} c_{im}}{\partial t} + (1 - f_{mo})\rho \frac{\partial s_{im}}{\partial t} = \omega_{ph}(c_{mo} - c_{im}) - \phi_{im}$$

$$f_{mo}\rho \frac{\partial s^k_{mo}}{\partial t} = \alpha_{ch}\left(s^k_{mo,e} - s^k_{mo}\right) - \phi_{mo,k}$$

$$s^e_{mo} = f_{em} K_d c_{mo} \qquad s^k_{mo,e} = (1 - f_{em}) K_d c_{mo}$$

f_{mo} – fraction of exchange sites in contact with the mobile region [-]
f_{em} – fraction of exchange sites in mobile region in equilibrium with the liquid phase [-]
ω_{ph} – mass transfer between mobile and immobile regions (physical process) [T^{-1}]
α_{ch} – first-order mass transfer (sorption rate; chemical process) [T^{-1}]

Dual-Porosity Model
(with Equilibrium and Kinetic Sorption and Size Exclusion)



- **Particle Transport with Size Exclusion**

$$\frac{\partial \theta_{mo} c_{mo}}{\partial t} + f_{mo}\rho \frac{\partial s_{mo}^{e}}{\partial t} = \frac{\partial}{\partial z}\left(\theta_{mo} D_{mo} \frac{\partial c_{mo}}{\partial z}\right) - \frac{\partial q_{mo} c_{mo}}{\partial z} - \phi_{mo} - \omega_{ph}(c_{mo} - c_{im}) \cancel{- \alpha_{ch}\left(s_{mo,e}^{k} - s_{mo}^{k}\right)}$$

$$\cancel{\frac{\partial \theta_{im} c_{im}}{\partial t} + (1 - f_{mo})\rho \frac{\partial s_{im}}{\partial t} = \omega_{ph}(c_{mo} - c_{im}) - \phi_{im}}$$

$$f_{mo}\rho \frac{\partial s_{mo}^{k}}{\partial t} = \alpha_{ch}\left(s_{mo,e}^{k} - s_{mo}^{k}\right) - \phi_{mo,k}$$

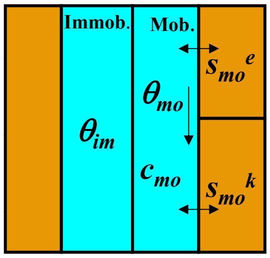
$$s_{mo}^{e} = f_{em} K_d c_{mo} \qquad s_{mo,e}^{k} = (1 - f_{em}) K_d c_{mo}$$

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

$$s = s_{mo}^{e} + s_{mo}^{k} + s_{im}^{e}$$

f_{mo} – fraction of exchange sites in contact with the mobile region [-]
f_{em} – fraction of exchange sites in mobile region in equilibrium with the liquid phase [-]
ω_{ph} – mass transfer between mobile and immobile regions (physical process) [T^{-1}]
α_{ch}– first-order mass transfer (sorption rate; chemical process) [T^{-1}]

Dual-Porosity Model
(with Equilibrium and Kinetic Sorption and Size Exclusion)



- **Particle Transport with Size Exclusion**

$$\frac{\partial \theta_{mo} c_{mo}}{\partial t} + f_{mo}\rho \frac{\partial s_{mo}^{e}}{\partial t} = \frac{\partial}{\partial z}\left(\theta_{mo} D_{mo} \frac{\partial c_{mo}}{\partial z}\right) - \frac{\partial q_{mo} c_{mo}}{\partial z} - \phi_{mo} - \alpha_{ch}\left(s_{mo,e}^{k} - s_{mo}^{k}\right)$$

$$f_{mo}\rho \frac{\partial s_{mo}^{k}}{\partial t} = \alpha_{ch}\left(s_{mo,e}^{k} - s_{mo}^{k}\right) - \phi_{mo,k}$$

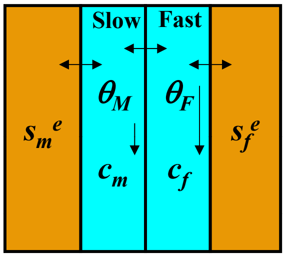
$$s_{mo}^{e} = f_{em} K_d c_{mo} \qquad s_{mo,e}^{k} = (1 - f_{em}) K_d c_{mo}$$

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

$$s = s_{mo}^{e} + s_{mo}^{k}$$

f_{mo} – fraction of exchange sites in contact with the mobile region [-]
f_{em} – fraction of exchange sites in mobile region in equilibrium with the liquid phase [-]
ω_{ph} – mass transfer between mobile and immobile regions (physical process) [T^{-1}]

Dual-Permeability Model
(with Equilibrium Sorption)



- **Solute Transport**

[Gerke and van Genuchten, 1992]

$$\theta = \theta_M + \theta_F = w\theta_f + (1 - w)\theta_m$$

$$s = w s_f^{e} + (1 - w) s_m^{e}$$

w – the ratio of the volumes of the macropore/fracture domain and the total soil system

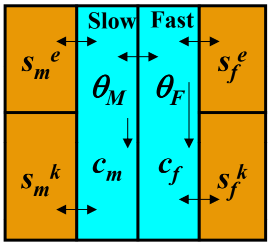
ω_{dp} – mass transfer between fracture and matrix domains (physical process) [T^{-1}]

$$\frac{\partial \theta_f c_f}{\partial t} + \rho \frac{\partial s_f^{e}}{\partial t} = \frac{\partial}{\partial z}\left(\theta_f D_f \frac{\partial c_f}{\partial z}\right) - \frac{\partial q c_f}{\partial z} - \phi_f - \frac{\Gamma_s}{w}$$

$$\frac{\partial \theta_m c_m}{\partial t} + \rho \frac{\partial s_m^{e}}{\partial t} = \frac{\partial}{\partial z}\left(\theta_m D_m \frac{\partial c_m}{\partial z}\right) - \frac{\partial q c_m}{\partial z} - \phi_m - \frac{\Gamma_s}{1 - w}$$

$$\Gamma_s = \omega_{dp}(1 - w)\theta_m (c_f - c_m) + \Gamma_w c^*$$

Dual-Permeability Model
(with Two Kinetic and Two Equil. Sorption Sites)



- **Solute Transport** [Šimůnek et al., 2008]

$$\theta = \theta_M + \theta_F = w\theta_f + (1 - w)\theta_m$$

$$s = w\left(s_f^{e} + s_f^{k}\right) + (1 - w)\left(s_m^{e} + s_m^{k}\right)$$

$$\rho \frac{\partial s_f^{k}}{\partial t} = \rho_f \alpha_{ch,f}\left[(1 - f_f) K_{df} c_f - s_f^{k}\right] - \phi_{f,k}$$

$$\rho \frac{\partial s_m^{k}}{\partial t} = \rho_m \alpha_{ch,m}\left[(1 - f_m) K_{dm} c_m - s_m^{k}\right] - \phi_{m,k}$$

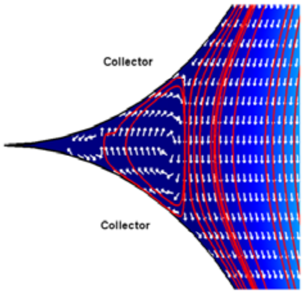
$$\frac{\partial \theta_f c_f}{\partial t} + \rho \frac{\partial s_f^{e}}{\partial t} = \frac{\partial}{\partial z}\left(\theta_f D_f \frac{\partial c_f}{\partial z}\right) - \frac{\partial q c_f}{\partial z} - \phi_f - \frac{\Gamma_s}{w} - \Gamma_f$$

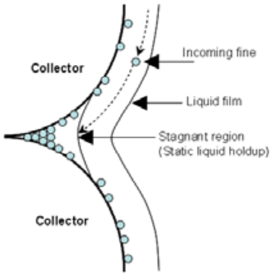
$$\frac{\partial \theta_m c_m}{\partial t} + \rho \frac{\partial s_m^{e}}{\partial t} = \frac{\partial}{\partial z}\left(\theta_m D_m \frac{\partial c_m}{\partial z}\right) - \frac{\partial q c_m}{\partial z} - \phi_m - \frac{\Gamma_s}{1 - w} - \Gamma_m$$

$$\Gamma_s = \omega_{dp}(1 - w)\theta_m (c_f - c_m) + \Gamma_w c^*$$

Pore-Scale Flow Field

- Navier Stokes and continuity equations
- Incompressible fluid and negligible inertial terms

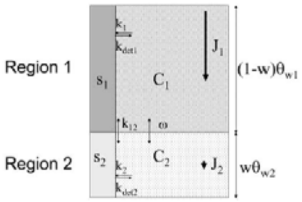




Rolling of particles into stagnant regions

Colloid Transport in Dual-Permeability Media

Bradford et al. [2009]



$$\rho \frac{\partial s_1}{\partial t} = k_{a1}\theta_1 c_1 - k_{d1}\rho s_1 - \frac{\rho k_{12} s_1}{1 - w}$$

$$\rho \frac{\partial s_2}{\partial t} = k_{a2}\theta_2 c_2 - k_{d2}\rho s_2 + \frac{\rho k_{12} s_1}{w}$$

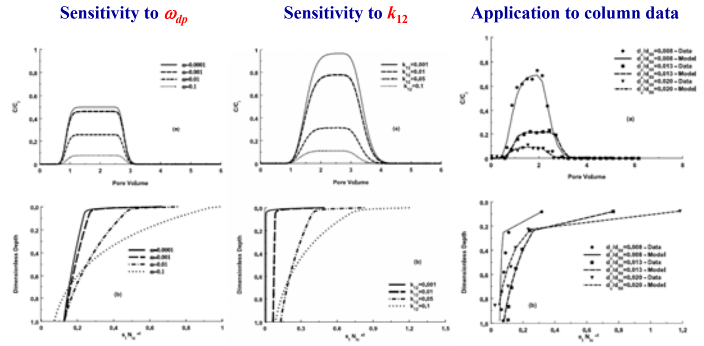
$$\Gamma_s = \omega_{dp}(1 - w)\theta_1 (c_2 - c_1)$$

k_{12} – transfer of colloids from solid phase region 1 to 2 [T^{-1}]
ω_{dp} – colloid exchange between liquids in regions 1 to 2 [T^{-1}]

Hypothesis:

- Colloids colliding with solid surfaces in fast regions of the pore space experience different hydrodynamic forces than colloids in slow regions.
- The higher hydrodynamic forces in the fast region act to remove colloids from the solid surface, thus causing the fast region to be associated with lower rates of colloid retention.
- Colloid exchange occurs between the two regions in the aqueous phase.
- Colloid exchange may also occur on the solid phase from fast to slow regions due to either rolling or sliding of colloids on the solid surface.

Colloid Transport in Dual-Permeability Media



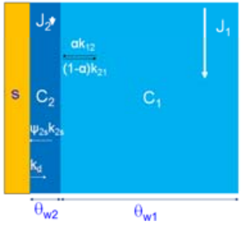
ω_{dp} – colloid exchange between liquid regions 1 to 2 [T^{-1}]
k_{12} – transfer of colloids from solid phase region 1 to 2 [T^{-1}]

3 µm colloids, q=0.1 cm/min, IS=6 mM, pH=10, and d_{50}=360, 240, and 150 mm.

Bradford et al. [2009]

Colloid Transport in Dual-Permeability Media

Bradford et al. [2011]



$$\frac{\partial \theta_1 c_1}{\partial t} = \frac{\partial}{\partial z}\left(\theta_1 D_1 \frac{\partial c_1}{\partial z}\right) - \frac{\partial q_1 c_1}{\partial z} - \Gamma_s$$

$$\frac{\partial \theta_2 c_2}{\partial t} + \rho \frac{\partial s}{\partial t} = \frac{\partial}{\partial z}\left(\theta_2 D_2 \frac{\partial c_2}{\partial z}\right) - \frac{\partial q_2 c_2}{\partial z} + \Gamma_s$$

$$\Gamma_s = \theta_1 \alpha k_{12} c_1 - \theta_2 (1-\alpha) k_{21} c_2$$

$$\rho \frac{\partial s}{\partial t} = \theta \psi_{2s} k_{2s} c_2 - \rho k_d (s - f_c s_i)$$

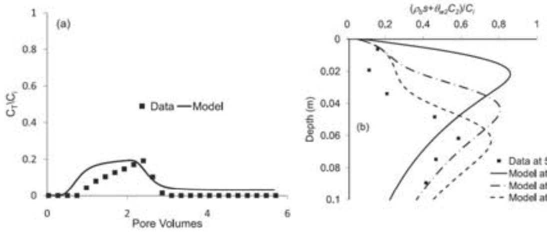
Hypothesis:

- Colloids are transported through the bulk aqueous phase by advection and dispersion in **Region 1**.
- **Region 2** is associated with the zone of colloid interaction with the SWI. The thickness of this region is very small. Colloids may be transported by advection and dispersion, but with much lower velocity than in Region 1.
- **Mass transfer** of colloids to and from regions 1 to 2 is quantified using first-order kinetic expressions (αk_{12}; $(1-\alpha)k_{21}$).
- Colloids in Region 2 interacts with SWI (**kinetic retention and release, k_{2s} and k_d**). Immobilized colloids on the solid phase may fill up retention locations over time (**blocking, ψ**).

Bradford et al. [2011] provide initial estimates of various model parameters.

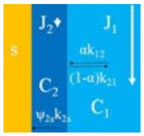
Application to the Transport of *E. coli*

Non-monotonic deposition profiles [Bradford et al. 2006, 2011]:

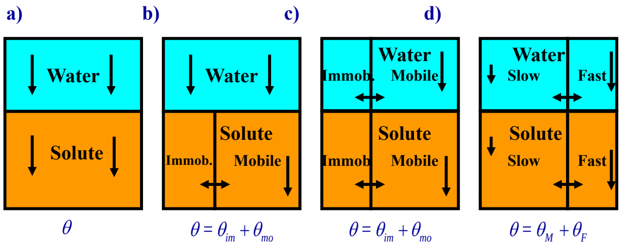


Effluent concentration curves (left) and deposition profiles (right) for *E. coli* in the Ottawa sand (q_T=0.1 cm/min; d_{50}=150 mm; r_c=250 nm).

- Fitted values of α, s_{max}, k_{2s}, and k_{21}.
- Nonmonotonic profile that slowly move with time reflect a decrease in the rates of release (k_{21}) and immobilization (k_{2s})



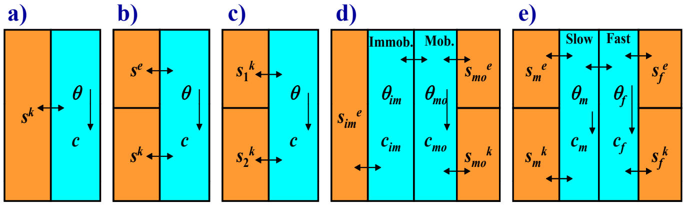
Physical Nonequilibrium Solute Transport Models in HYDRUS



a) Uniform Flow
b) **Mobile-Immobile Water**
c) **Dual-Porosity** (Šimůnek et al., 2003)
d) **Dual-Permeability** (Gerke and van Genuchten, 1993)

Chemical Nonequilibrium Solute Transport Models in HYDRUS

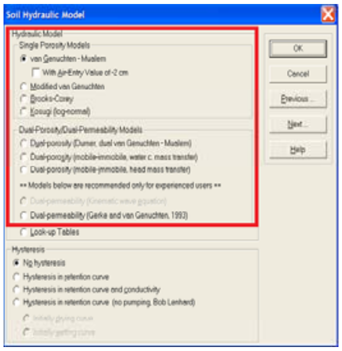
Šimůnek and van Genuchten (2008):



a) One-Site Kinetic Model
b) **Two-Site Model** (kinetic and instantaneous sorption)
c) **Two Kinetic Sites** Model
(particle transport, e.g., colloids, viruses, bacteria)
d) **Dual-Porosity** with One Kinetic Site Model
e) **Dual-permeability** with Two-Site Model

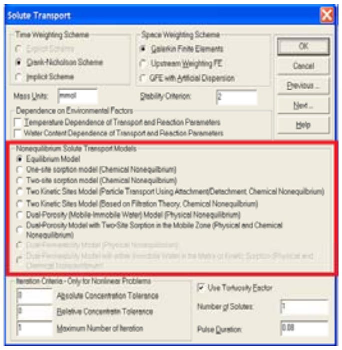
Nonequilibrium Models in the HYDRUS GUI

Variably-Saturated Water Flow



Hydraulic Model
Single Porosity Models
● van Genuchten - Mualem
☐ With Air-Entry Value of -2 cm
○ Modified van Genuchten
○ Brooks-Corey
○ Kosugi (log-normal)
Dual-Porosity/Dual-Permeability Models
○ Dual-porosity (Durner, dual van Genuchten - Mualem)
○ Dual-porosity (mobile-immobile, water c. mass transfer)
○ Dual-porosity (mobile-immobile, head mass transfer)
** Models below are recommended only for experienced users **
○ Dual-permeability (Kinematic wave equation)
○ Dual-permeability (Gerke and van Genuchten, 1993)
○ Look-up Tables
Hysteresis
● No hysteresis
○ Hysteresis in retention curve
○ Hysteresis in retention curve and conductivity
○ Hysteresis in retention curve (no pumping, Bob Lenhard)
○ Initially drying curve
○ Initially wetting curve

Solute Transport



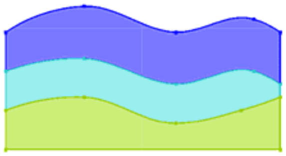
Time Weighting Scheme
○ Explicit Scheme
● Crank-Nicholson Scheme
○ Implicit Scheme
Space Weighting Scheme
● Galerkin Finite Elements
○ Upstream Weighting FE
○ GFE with Artificial Dispersion
Mass Units: mmol
Stability Criterion: 2
Dependence on Environmental Factors
☐ Temperature Dependence of Transport and Reaction Parameters
☐ Water Content Dependence of Transport and Reaction Parameters
Nonequilibrium Solute Transport Models
● Equilibrium Model
○ One-site sorption model (Chemical Nonequilibrium)
○ Two-site sorption model (Chemical Nonequilibrium)
○ Two Kinetic Sites Model (Particle Transport Using Attachment/Detachment, Chemical Nonequilibrium)
○ Two Kinetic Sites Model (Based on Filtration Theory, Chemical Nonequilibrium)
○ Dual-Porosity (Mobile-Immobile Water) Model (Physical Nonequilibrium)
○ Dual-Porosity Model with Two-Site Sorption in the Mobile Zone (Physical and Chemical Nonequilibrium)
○ Dual-Permeability Model (Physical Nonequilibrium)
○ Dual-Permeability Model with either Immobile Water in the Matrix or Kinetic Sorption (Physical and Chemical Nonequilibrium)
Iteration Criteria - Only for Nonlinear Problems
0 Absolute Concentration Tolerance
0 Relative Concentratn Tolerance
1 Maximum Number of Iteration
☑ Use Tortuosity Factor
Number of Solutes: 1
Pulse Duration: 0.08

OUTLINE

- ◆ Introduction – Background on HYDRUS
- ◆ Historical Development (models of increasing complexity)
- ◆ Preferential Flow and Transport
- ◆ **Spatial Heterogeneity**
- ◆ Effects of Chemical Conditions – HP1/2/3
- ◆ Colloid-Facilitated Solute Transport
- ◆ Miscellaneous Other Options

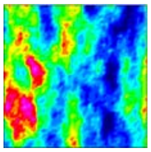
Spatial Heterogeneity

Deterministic

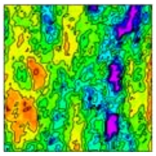


Explicit definition of material layers

Stochastic



Conductivities



Water Contents

Randomly generated fields of various parameters, such as scaling factors (for the pressure heads, water contents and hydraulic conductivities)

Stochastic Spatial Heterogeneity

HYDRUS: The spatial variability of hydraulic properties can be approximated by means of a set of linear scaling transformations, which relate the individual soil hydraulic characteristics [$\theta(h)$ and $K(h)$] to reference characteristics [$\theta^*(h^*)$ and $K^*(h^*)$]:

$$K(h) = \alpha_K K^*(h^*)$$

$$\theta(h) = \theta_r + \alpha_\theta [\theta^*(h^*) - \theta_r^*]$$

$$h = \alpha_h h^*$$

HYDRUS GUI can generate random fields for α_K, α_h, and α_θ.

- Normally or log-normally distributed
- Correlation lengths in *x* and *z* direction
- Miller-Miller geometrical similitude ($a_K = a_h^{-2}$)

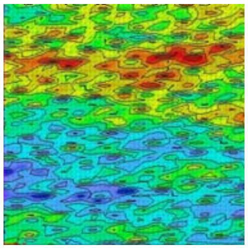
Transport in Heterogeneous Soils

Miller-Miller Similitude: generate scaling factors for pressure heads (a_h) and calculate scaling factors for hydraulic conductivities ($a_K = a_h^{-2}$)

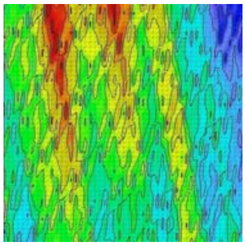
Standard Deviation of log10(a_h) = 0.5

Correlation length in the horizontal direction = 50 (left) and 10 (right) cm

Correlation length in the vertical direction = 10 (left) and 50 (right) cm



Horizontal Layering



Vertical Preferential Pathways

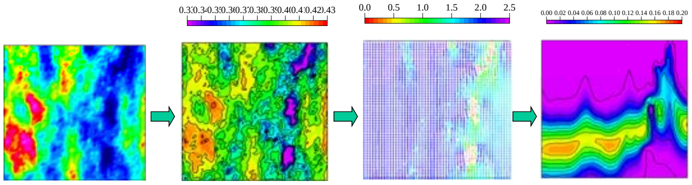
Transport in Heterogeneous Soils

Miller-Miller Similitude: generate scaling factors for pressure heads (a_h) and calculate scaling factors for hydraulic conductivities ($a_K = a_h^{-2}$)

Standard Deviation of log10(a_h) = 0.5

Correlation length in the horizontal direction = 20 cm

Correlation length in the vertical direction = 50 cm



Stochastic Conductivity Field

Water Content Field

Velocity Field

Concentration Field

I II III

Column Studies with Artificial Macropore and Different Solution Chemistry Conditions

Yusong Wang (PhD student) (submitted to WRR):

- ◆ Homogeneous columns (fine/coarse sand, 120/710 µm; *L*=13 cm, *r*=4.8 cm)
- ◆ Columns (*L*=20 cm, *r*=13.2 cm) with an artificial macropore (*r*= 1.14 cm)
- ◆ Saturated flow
- ◆ Bromide, microorganisms *E.coli* D21g (1.84 µm) and coliphage ϕX174 (27 nm)
- ◆ Ionic Strength *IS*=0, 1, 5, 20, and 100 mM

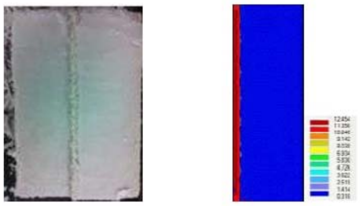
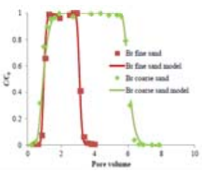


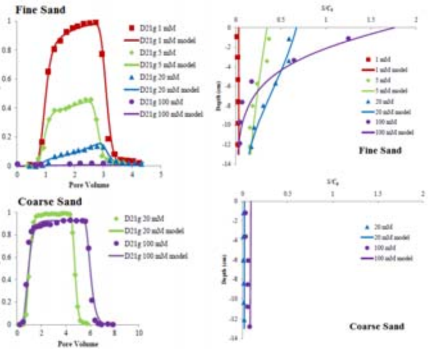
Photo of a heterogeneous soil column with a lens in the middle and simulated flow field.

Column Studies with Artificial Macropore and Different Solution Chemistry Conditions

Homogeneous Columns:



Measured and fitted Br breakthrough curves

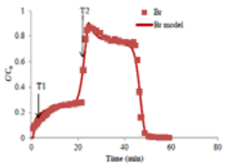


Measured and fitted breakthrough curves and retention profiles of *E.coli*

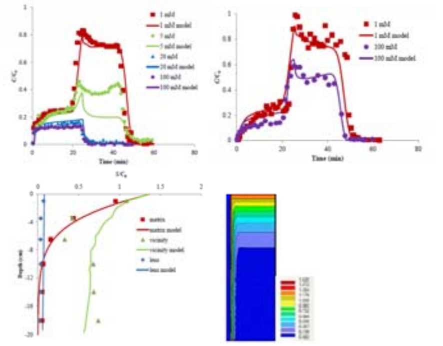
Yusong Wang et al. (submitted to WRR)

Column Studies with Artificial Macropore and Different Solution Chemistry Conditions

Heterogeneous Columns:



Measured and predicted Br breakthrough curves



Measured and predicted breakthrough curves and retention profiles of *E.coli and ϕ*X174

Yusong Wang et al. (submitted to WRR)

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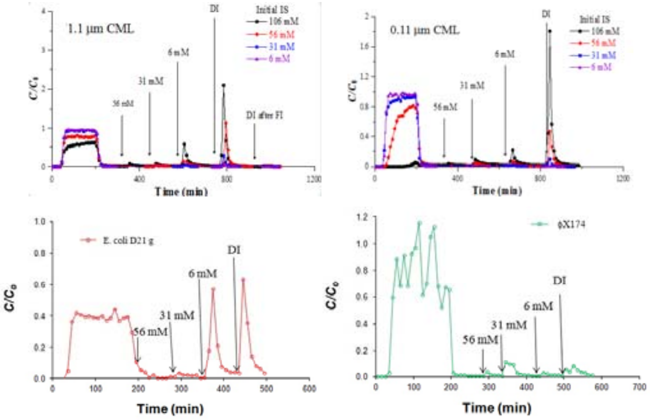
- Miscellaneous Other Options

Transients in Solution IS



HP1/2/3 (HYDRUS+PHREEQC)

Simulating water flow, transport and bio-geochemical reactions in environmental soil quality problems

HPx

A Coupled Numerical Code for Variably Saturated Water Flow, Solute Transport and BioGeoChemistry in Soil Systems

HP1/2/3

Flow and transport model
HYDRUS-1D 4.0
HYDRUS (2D/3D) 2.x

Biogeochemical model
PHREEQC-2.4

HP1/2/3 (HYDRUS+PHREEQC)

HYDRUS-1D or HYDRUS (2D/3D):

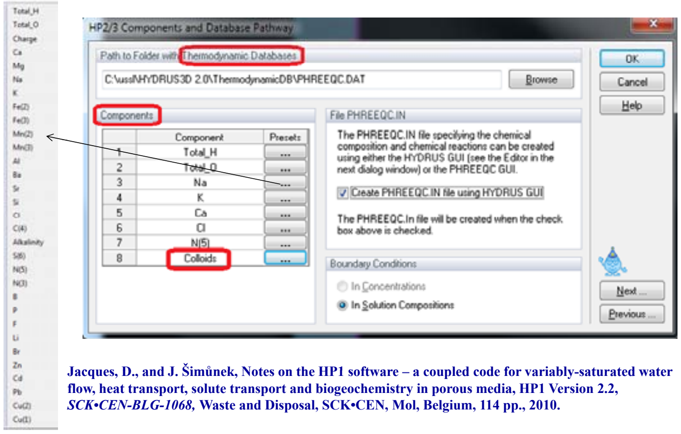
- Variably-Saturated Water Flow
- Solute Transport
- Heat transport
- Root water uptake

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

HYDRUS GUI for HP1/2/3



Path to Folder with Thermodynamic Databases: C:\uss\HYDRUS3D 2.0\ThermodynamicDB\PHREEQC.DAT

Components

	Component	Presets
1	Total_H	...
2	Total_O	...
3	Na	...
4	K	...
5	Ca	...
6	Cl	...
7	N(5)	...
8	Colloids	...

File PHREEQC.IN

The PHREEQC.IN file specifying the chemical composition and chemical reactions can be created using either the HYDRUS GUI (see the Editor in the next dialog window) or the PHREEQC GUI.

☑ Create PHREEQC.IN file using HYDRUS GUI

The PHREEQC.In file will be created when the check box above is checked.

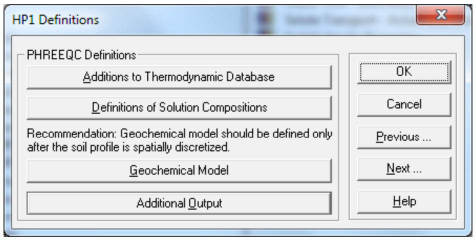
Boundary Conditions

○ In Concentrations

● In Solution Compositions

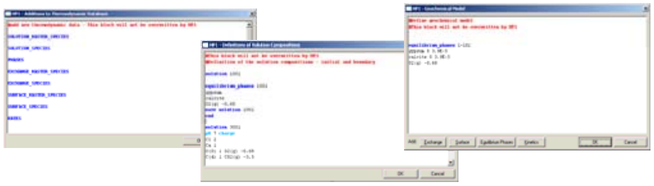
Jacques, D., and J. Šimůnek, Notes on the HP1 software – a coupled code for variably-saturated water flow, heat transport, solute transport and biogeochemistry in porous media, HP1 Version 2.2, *SCK•CEN-BLG-1068,* Waste and Disposal, SCK•CEN, Mol, Belgium, 114 pp., 2010.

HYDRUS GUI for HP1/2/3



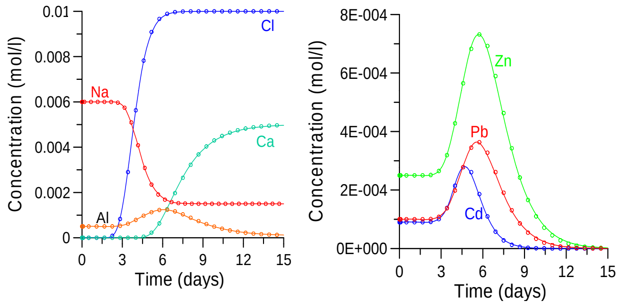
Recommendation: Geochemical model should be defined only after the soil profile is spatially discretized.

Four text editors to define the geochemical model



Transport and Cation Exchange Heavy Metals

Major ions (Ca, Na, Al, Cl) and Heavy Metals (Zn, Pb, Cd)

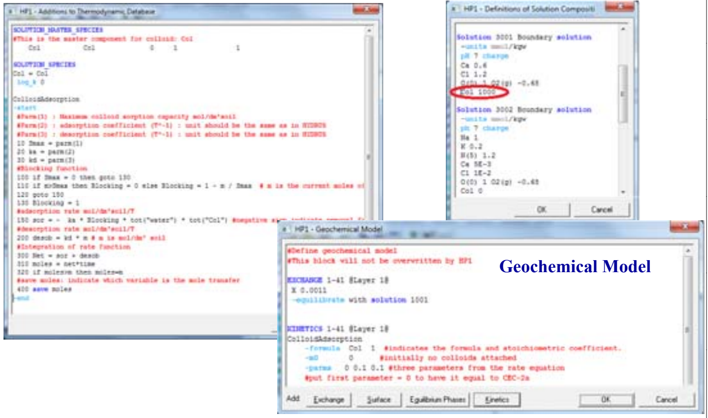


8-cm column is initially contaminated with heavy metals (in equilibrium with the cation exchanger). The column is then flushed with a solution ($CaCl_2$) without heavy metals.

HP1/2/3 for Colloid Transport

Additions to Thermodynamic Database

Definition of Solution Compositions



```
SOLUTION_MASTER_SPECIES
#This is the master component for colloid: Col
   Col        Col           0    1           1

SOLUTION_SPECIES
Col = Col
 log_k 0

ColloidAdsorption
-start
 #Parm(1) : Maximum colloid sorption capacity mol/dm³soil
 #Parm(2) : adsorption coefficient (T^-1) : unit should be the same as in HYDRUS
 #Parm(3) : desorption coefficient (T^-1) : unit should be the same as in HYDRUS
 10 Smax = parm(1)
 20 ka = parm(2)
 30 kd = parm(3)
 #Blocking function
 100 if Smax = 0 then goto 130
 110 if m>Smax then Blocking = 0 else Blocking = 1 - m / Smax  # m is the current moles o
 120 goto 150
 130 Blocking = 1
 #adsorption rate mol/dm³soil/T
 150 sor = -  ka * Blocking * tot("water") * tot("Col") #negative
 #desorption rate mol/dm³soil/T
 200 desob = kd * m # m is mol/dm³ soil
 #Integration of rate function
 300 Net = sor + desob
 310 moles = net*time
 320 if moles>m then moles=m
 #save moles: indicate which variable is the mole transfer
 400 save moles
-end
```

```
Solution 3001 Boundary solution
 -units mmol/kgw
 pH 7 charge
 Ca 0.6
 Cl 1.2
 O(0) 1 O2(g) -0.68
 Col 1000

Solution 3002 Boundary solution
 -units mmol/kgw
 pH 7 charge
 Na 1
 K 0.2
 N(5) 1.2
 Ca 5E-3
 Cl 1E-2
 O(0) 1 O2(g) -0.68
 Col 0
```

Geochemical Model

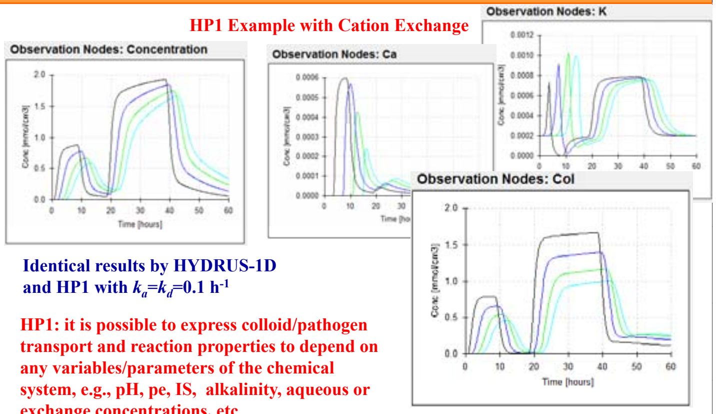
```
#Define geochemical model
#This block will not be overwritten by HP1

EXCHANGE 1-41 @Layer 1@
 X 0.0011
 -equilibrate with solution 1001


KINETICS 1-41 @Layer 1@
ColloidAdsorption
    -formula  Col  1  #indicates the formula and stoichiometric coefficient.
    -m0       0       #initially no colloids attached
    -parms   0 0.1 0.1 #three parameters from the rate equation
    #put first parameter = 0 to have it equal to CEC-2a
```

HP1/2/3 for Colloid Transport

HP1 Example with Cation Exchange

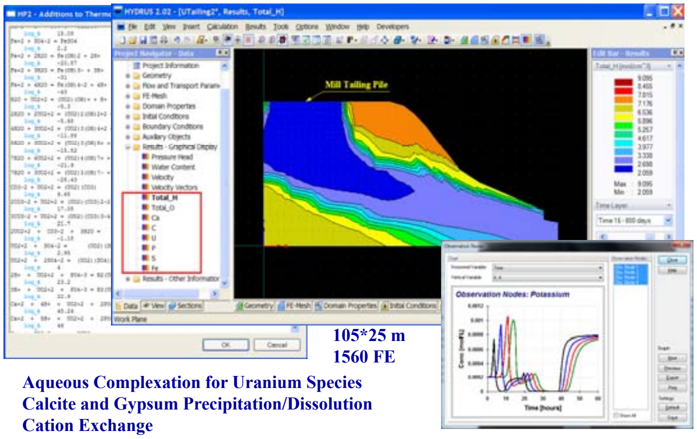


Identical results by HYDRUS-1D and HP1 with k_a=k_d=0.1 h^{-1}

HP1: it is possible to express colloid/pathogen transport and reaction properties to depend on any variables/parameters of the chemical system, e.g., pH, pe, IS, alkalinity, aqueous or exchange concentrations, etc.

HP1 with $k_d^*= k_d^*$(NaX/CEC)

Uranium Transport from Mill Tailing Pile



105*25 m
1560 FE

Aqueous Complexation for Uranium Species
Calcite and Gypsum Precipitation/Dissolution
Cation Exchange

HP1 Examples

- Transport of **Heavy Metals** (Zn^{2+}, Pb^{2+}, and Cd^{2+}) subject to a multiple **pH-dependent Cation Exchange**
- Transport and mineral dissolution of **Amorphous SiO_2** and **Gibbsite**
- Infiltration of a **Hyperalkaline Solution** in a clay sample (kinetic precipitation-dissolution of kaolinite, illite, quartz, calcite, dolomite, gypsum, hydrotalcite, and sepiolite)
- Kinetic biodegradation of **NTA** (biomass, cobalt)
- Long-term **Uranium** transport following mineral phosphorus fertilization (pH-dependent surface complexation and cation exchange)
- Transport of **Explosives**, such as TNT and RDX
- **Property Changes** (porosity/conductivity) due to precipitation/ dissolution reactions

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OUTLINE

- Introduction – Background on HYDRUS
- Historical Development (models of increasing complexity)
- Preferential Flow
- Spatial Heterogeneity
- Effects of Chemical Conditions – HP1/2/3
- **Colloid-Facilitated Solute Transport (C-Ride)**
- Miscellaneous Other Options

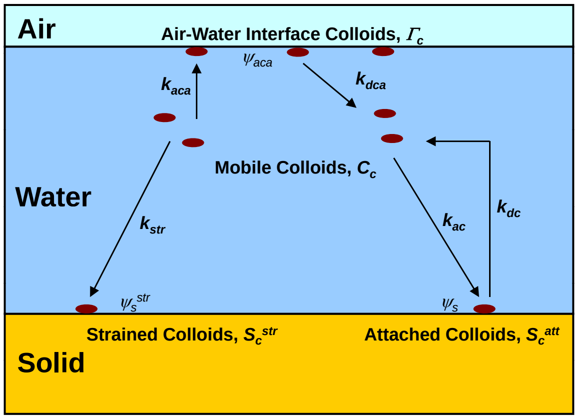
Colloid-Facilitated Solute Transport

- Many contaminants should be relatively immobile in the subsurface since under normal conditions they are strongly sorbed to soil.
- They can also sorb to colloids, which often move at rates similar or faster as non-sorbing tracers.
- Experimental evidence exists that many contaminants are transported not only in a dissolved state by water, but also sorbed to moving colloids.
- Examples: **heavy metals**, **radionuclides**, pesticides, **viruses**, pharmaceuticals, hormones, and other contaminants.

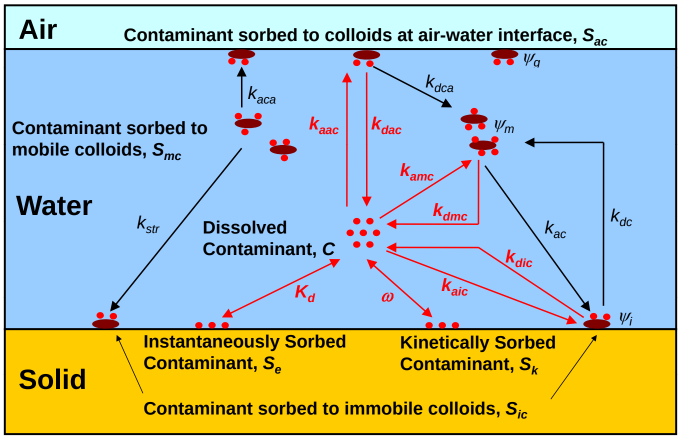
HYDRUS + add-on Module C-Ride

- **HYDRUS** and **HYDRUS (2D/3D)**
  - variably saturated water flow
  - heat transport
  - root water uptake
  - solute transport
- **C-Ride** (Šimůnek et al., 2006, 2012)
  - **Particle Transport**
    - colloids, bacteria, viruses, nanoparticles
    - attachment/detachment, straining, blocking
  - **Colloid-Facilitated Solute Transport**
    - transport of solutes attached to particles

Colloid, Virus, and Bacteria Transport

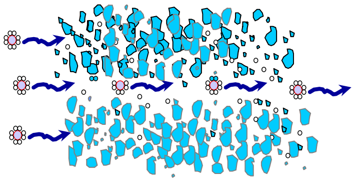


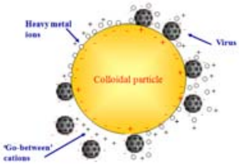
Colloid-Facilitated Solute Transport



Colloid-Facilitated Solute Transport

Pang et al. [2005]: Bacteria act as carriers for heavy metals in gravel aquifers





Since bacteria may be excluded from small pores, they move through interconnected larger pores and cracks where water moves quicker.

Provide a vehicle for rapid transport of less mobile contaminants.

Colloid-Facilitated Solute Transport

Mass Balance of Total Contaminant:

$$\frac{\partial \theta C}{\partial t}+\rho\frac{\partial S_e}{\partial t}+\rho\frac{\partial S_k}{\partial t}+\frac{\partial \theta_w C_c S_{mc}}{\partial t}+\rho\frac{\partial S_c S_{ic}}{\partial t}=$$

$$=\frac{\partial}{\partial x}\left(\theta D\frac{\partial C}{\partial x}\right)-\frac{\partial qC}{\partial x}+\frac{\partial}{\partial x}\left(\theta_w S_{mc} D_c\frac{\partial C_c}{\partial x}\right)-\frac{\partial q_c C_c S_{mc}}{\partial x}+R$$

Left-hand side sums the Mass of Contaminant:

- **in the liquid phase**
- **sorbed instantaneously and kinetically to the solid phase**
- **sorbed to mobile and immobile colloids**

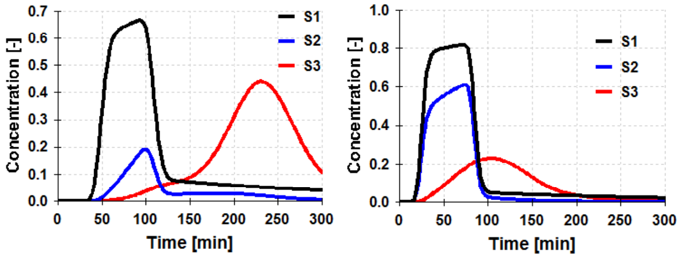
Right-hand side considers various Mass Fluxes

- **dispersive and advective transport of the dissolved contaminant**
- **dispersive and advective transport of contaminant sorbed to mobile colloids**

and Transformation/Reaction (e.g., degradation).

Colloid-Facilitated Solute Transport

C-Ride Module



Breakthrough curves for colloids (black line), solute sorbed to colloids (blue line), and dissolved solute (red line):

Left: solute and colloids are applied independently

Right: solute is attached initially to colloids

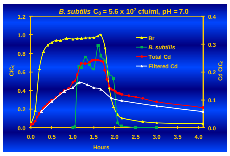
The Retardation Factor for colloids is equal to 1 and for solute to 4

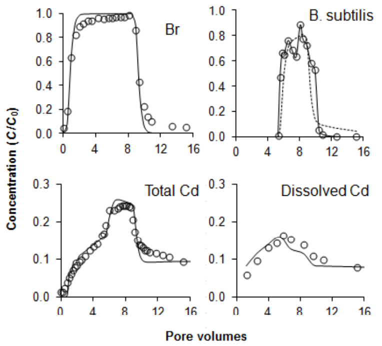
Unit input concentrations.

Bacteria-Facilitated Cadmium Transport

Column Experiments [Pang et al., 2005; Pang and Šimůnek, 2006]

- **Column: 18 cm long and 10 cm internal diameter.**
- **Bulk density = 1.9 g/cm³**
- **Effective porosity = 0.27**
- **Pore-water velocity = 22 m/d**
- **5 PV of a solution containing Cd of about 4 mg/L and bromide (Br) of about 2 mg/L before injection of bacteria**
- **The *Bacillus subtilis* spores were then introduced to the column with Cd and Br for next 3.4 PV**
- **Column was then flushed with tap water (no bacteria, Cd, or Br)**





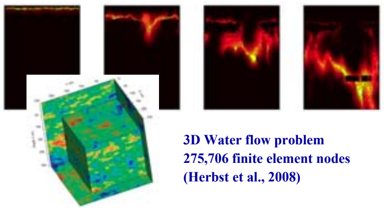
OUTLINE

- Introduction – Background on HYDRUS
- Historical Development (models of increasing complexity)
- Preferential Flow
- Spatial Heterogeneity
- Effects of Chemical Conditions – HP1/2/3
- Colloid-Facilitated Solute Transport
- **Miscellaneous Other Options (e.g., parallel computing, other HYDRUS modules, HYDRUS web)**

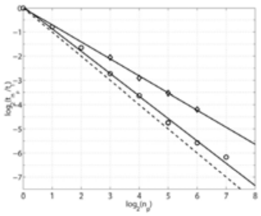
ParSWMS – Parallelized Version of HYDRUS

- **ParSWMS** (Hardelauf et al., 2007) **- Parallelized version of SWMS_3D**, an earlier and simpler version of HYDRUS-3D.
- **Developed by** *Forschungszentrum Jülich, Germany*.
- **MPI (Message-Passing Interface)**. LINUX or UNIX OSs.
- **Test** - Supercomputer with 41 SMP nodes with 32 processors each (total 1312 processors)

2D Water flow and solute transport (Hardelauf et al., 2007)
492,264 finite element nodes



3D Water flow problem
275,706 finite element nodes
(Herbst et al., 2008)



HYDRUS and its Modules

- HYDRUS + PHREEQC = HP1/2/3
  (hydrological + biogeochemical processes)
- HYDRUS + C-Ride
  (colloid-facilitated solute transport)
- HYDRUS + DualPerm
  (preferential water flow and solute transport)
- HYDRUS + Wetland (CW2D/CWM1)
  (processes in constructed wetlands)
- HYDRUS + UNSATCHEM
  (hydrological + CO_2 + geochemical processes)
- HYDRUS + MODFLOW
  (hydrological processes at the large scale)

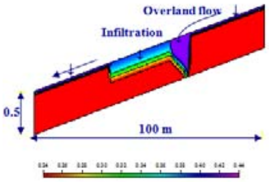
Overland Flow Module

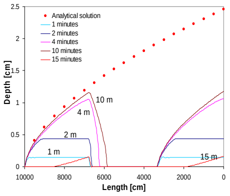
Kinematic Wave Equation (with Manning hydraulic resistance law):

$$\frac{\partial h}{\partial t}+\frac{\partial Q}{\partial x}=q(x,t) \qquad Q=\alpha h^m$$

$$\alpha=1.49\frac{S^{1/2}}{n} \quad \text{and} \quad m=5/3$$

h	- unit storage of water (or mean depth) [L]
Q	- discharge per unit width [L^2T^{-1}],
***q*(*x*,*t*)**	- rate of local input, or lateral inflows (precipitation - infiltration) [LT^{-1}]
n	- Manning's roughness coefficient for overland flow
S	- slope





High intensity rainfall of 0.00666 cm/s (i.e., 24 cm/hour) of 10 minutes duration.
Loamy soils with K_s= 25 cm/d, and K_s= 25 m/d in the middle of the transect.
Soil transect is 100 m long, with a slope of 0.01. Roughness coefficient n = 0.01.

HYDRUS Web Site

Over 3 thousand downloads in 2008, over 5 thousand in 2009, and over 10 thousand downloads annually in 2010 and after; over 13 thousand registered members.

http://www.pc-progress.com/en/Default.aspx

Welcome to PC-Progress

PC-Progress specializes in the development of GUI (Graphical User Interfaces) for FEM/CFD software packages for Windows. We have more than fourteen years of experience in developing programs for numerical modeling in Fluid Mechanics and Structural Engineering. Our software helps thousands of scientists and engineers from around the world.
Read more about us...

Our core products

HYDRUS 2D/3D - software package for simulating water, heat, and solute transport in variably saturated porous media.

MESHGEN Plus - open modeling environment for Finite-Element and Finite-Volume applications. Includes 2D/3D geometry modeller, FE-mesh generator and customizable modules for pre- and post-processing.

Hydrus-1D - one-dimensional public-domain version of HYDRUS. This program has been developed and maintained in cooperation with University of California, Riverside, USA.

News

News
Information about upcomming HYDRUS courses and workshops. A list of newly released programs and updates, publications and remarkable events...

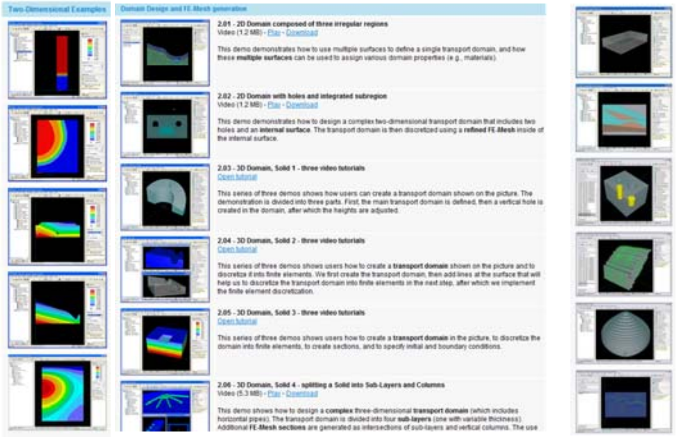
Online Ordering System
Now you can purchase our products or create quotations and pro-forma invoices online...

Services

HYDRUS Services
Extended support of the standard version of HYDRUS and/or modifications of the graphical user interface or computational modules based on clients' specification.

Programming
Rapid development of FEM applications based on the MESHGEN Plus software package.

HYDRUS Tutorials



2.01 - 2D Domain composed of three irregular regions
Video (1.2 MB) - Play - Download

This demo demonstrates how to use multiple surfaces to define a single transport domain, and how these **multiple surfaces** can be used to assign various domain properties (e.g., materials).

2.02 - 2D Domain with holes and integrated subregion
Video (1.2 MB) - Play - Download

This demo demonstrates how to design a complex two-dimensional transport domain that includes two holes and an **internal surface**. The transport domain is then discretized using a **refined FE-Mesh** inside of the internal surface.

2.03 - 3D Domain, Solid 1 - three video tutorials
Open tutorial

This series of three demos shows how users can create a transport domain shown on the picture. The demonstration is divided into three parts. First, the main transport domain is defined, then a vertical hole is created in the domain, after which the heights are adjusted.

2.04 - 3D Domain, Solid 2 - three video tutorials
Open tutorial

This series of three demos shows users how to create a **transport domain** shown on the picture and to discretize it into finite elements. We first create the transport domain, then add lines at the surface that will help us to discretize the transport domain into finite elements in the next step, after which we implement the finite element discretization.

2.05 - 3D Domain, Solid 3 - three video tutorials
Open tutorial

This series of three demos shows users how to create a **transport domain** in the picture, to discretize the domain into finite elements, to create sections, and to specify initial and boundary conditions.

2.06 - 3D Domain, Solid 4 - splitting a Solid into Sub-Layers and Columns
Video (5.3 MB) - Play - Download

This demo shows how to design a **complex** three-dimensional **transport domain** (which includes horizontal pipes). The transport domain is divided into four **sub-layers** (one with variable thickness). Additional **FE-Mesh sections** are generated as intersections of sub-layers and vertical columns. The use

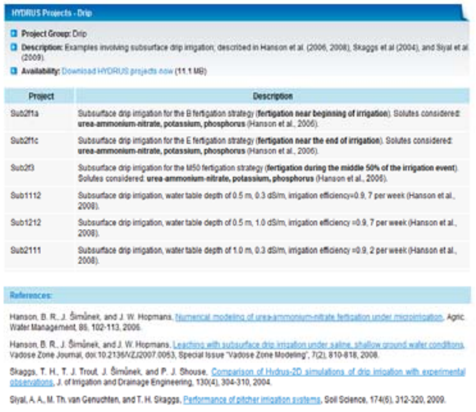
---

Public Library of HYDRUS-1D Projects

Examples demonstrating the use of HYDRUS-1D to simulate:

Bacteria	transport of bacteria in soils (from Gargiulo et al., 2007, 2008)
CFTr	colloid-facilitated solute transport (Šimůnek et al., 2006)
Centrifuge	flow and transport in centrifuge (Šimůnek and Nimmo, 2005)

Public Library of HYDRUS (2D/3D) Projects



HYDRUS Projects - Drip

- **Project Group:** Drip
- **Description:** Examples involving subsurface drip irrigation, described in Hanson et al. (2006, 2008), Skaggs et al (2004), and Siyal et al (2009).
- **Availability:** Download HYDRUS projects now (11.1 MB)

Project	Description
Sub2f1a	Subsurface drip irrigation for the B fertigation strategy (**fertigation near beginning of irrigation**). Solutes considered: **urea-ammonium-nitrate, potassium, phosphorus** (Hanson et al., 2006).
Sub2f1c	Subsurface drip irrigation for the E fertigation strategy (**fertigation near the end of irrigation**). Solutes considered: **urea-ammonium-nitrate, potassium, phosphorus** (Hanson et al., 2006).
Sub2f3	Subsurface drip irrigation for the M50 fertigation strategy (**fertigation during the middle 50% of the irrigation event**). Solutes considered: **urea-ammonium-nitrate, potassium, phosphorus** (Hanson et al., 2006).
Sub1112	Subsurface drip irrigation, water table depth of 0.5 m, 0.3 dS/m, irrigation efficiency=0.9, 7 per week (Hanson et al., 2008).
Sub1212	Subsurface drip irrigation, water table depth of 0.5 m, 1.0 dS/m, irrigation efficiency =0.9, 7 per week (Hanson et al., 2008).
Sub2111	Subsurface drip irrigation, water table depth of 1.0 m, 0.3 dS/m, irrigation efficiency =0.9, 2 per week (Hanson et al., 2008).

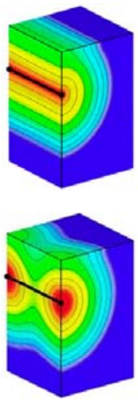
References:

Hanson, B. R., J. Šimůnek, and J. W. Hopmans, Numerical modeling of urea-ammonium-nitrate fertigation under microirrigation, Agric. Water Management, 85, 102-113, 2006.

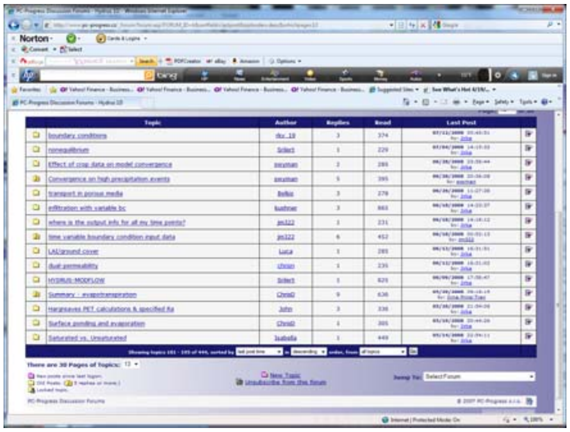
Hanson, B. R., J. Šimůnek, and J. W. Hopmans, Leaching with subsurface drip irrigation under saline, shallow ground water conditions, Vadose Zone Journal, doi:10.2136/VZJ2007.0053, Special Issue "Vadose Zone Modeling", 7(2), 810-818, 2008.

Skaggs, T. H., T. J. Trout, J. Šimůnek, and P. J. Shouse, Comparison of Hydrus-2D simulations of drip irrigation with experimental observations, J. of Irrigation and Drainage Engineering, 130(4), 304-310, 2004.

Siyal, A. A., M. Th. van Genuchten, and T. H. Skaggs, Performance of pitcher irrigation systems, Soil Science, 174(6), 312-320, 2009.



HYDRUS Discussion Forums



	Topic	Author	Replies	Read	Last Post
	boundary conditions	dkr_19	3	374	by: Jirka
	nonequilibrium	Srilert	1	229	by: Jirka
	Effect of crop data on model convergence	peyman	2	285	by: Jirka
	Convergence on high precipitation events	peyman	5	395	by: peyman
	transport in porous media	Beibit	3	278	by: Jirka
	exfiltration with variable bc	kushner	3	883	by: Jirka
	where is the output info for all my time points?	jm122	1	231	by: Jirka
	time variable boundary condition input data	jm122	6	452	by: jm122
	LAI/ground cover	Luca	1	285	by: Jirka
	dual permeability	chrisn	1	235	by: Jirka
	HYDRUS-MODFLOW	Srilert	1	825	by: Jirka
	Summary - evapotranspiration	ChrisD	9	636	by: Jirka Pimp Tsai
	Hargreaves PET calculations & specified Ra	John	3	338	by: Jirka
	Surface ponding and evaporation	ChrisD	1	305	by: Jirka
	Saturated vs. Unsaturated	Isabella	1	449	by: Jirka

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PC-Progress Discussion Forums

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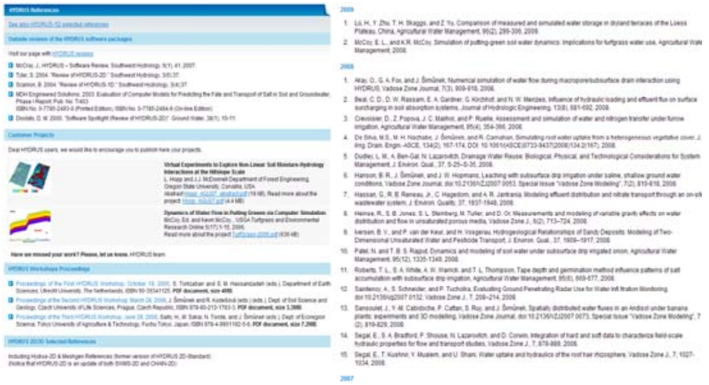
HYDRUS Web Site: References



HYDRUS References

See also HYDRUS-1D selected references

Outside reviews of the HYDRUS software packages

Visit our page with HYDRUS reviews

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- Tyler, S. 2004. "Review of HYDRUS-2D." Southwest Hydrology, 3(6):37.
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- Diodato, D. M. 2000. "Software Spotlight (Review of HYDRUS-2D)". Ground Water, 38(1), 10-11.

Customer Projects

Dear HYDRUS users, we would like to encourage you to publish here your projects.

Virtual Experiments to Explore Non-Linear Soil Moisture-Hydrology Interactions at the Hillslope Scale
L. Hopp and J.J. McDonnell Department of Forest Engineering, Oregon State University, Corvallis, USA
Abstract: Hopp_HGU07_abstract.pdf (19 kB), Read more about the project: Hopp_HGU07.pdf (4.4 MB)

Dynamics of Water Flow in Putting Greens via Computer Simulation
McCoy, Ed. and Kevin McCoy, , USGA Turfgrass and Environmental Research Online 5(17):1-15, 2006.
Read more about the project: Turfgrass 2006.pdf (638 kB)

Have we missed your work? Please, let us know. HYDRUS team.

HYDRUS Workshops Proceedings

- Proceedings of the First HYDRUS Workshop, October 18, 2005, S. Torkzaban and S. M. Hassanizadeh (eds.), Department of Earth Sciences, Utrecht University, The Netherlands, ISBN 90-39341125. **PDF document, size 4MB**
- Proceedings of the Second HYDRUS Workshop, March 28, 2008, J. Šimůnek and R. Kodešová (eds.), Dept. of Soil Science and Geology, Czech University of Life Sciences, Prague, Czech Republic, ISBN 978-80-213-1783-3. **PDF document, size 3.3MB**
- Proceedings of the Third HYDRUS Workshop, June 28, 2008, Saito, H., M. Sakai, N. Toride, and J. Šimůnek (eds.), Dept. of Ecoregion Science, Tokyo University of Agriculture & Technology, Fuchu Tokyo, Japan, ISBN 978-4-9901192-5-6. **PDF document, size 7.2MB**

HYDRUS 2D/3D Selected References

Including Hydrus-2D & Meshgen References (former version of HYDRUS 2D-Standard)
(Notice that HYDRUS-2D is an update of both SWMS-2D and CHAIN-2D)

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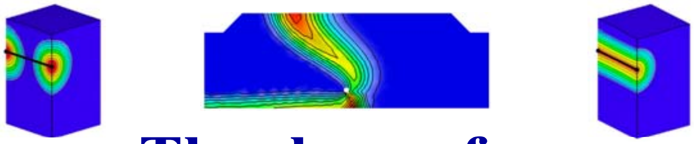
Over one thousand applications of HYDRUS-1D and HYDRUS (2D/3D) published in peer-reviewed journal articles, and many more unpublished.

Questions and Suggestions?



Thank you for your attention