Challenges in Developing Models Describing Complex Soil Systems

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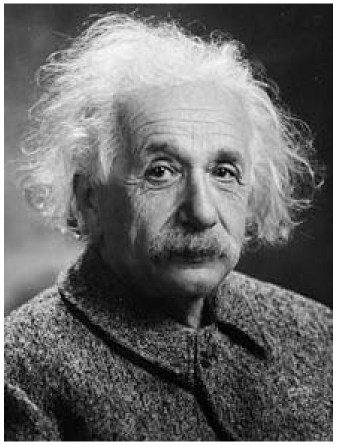
OUTLINE

- How Complex Should Models Be?
- The Use of Complex Models
- Selected HYDRUS-Based Models
  (e.g., HP1, colloid transport)
- Models Verification and Validation
  (model inter-comparisons; benchmarking)
- Documentation of Complex Models
  (technical and user manuals, online help, source code)
- Danger (misuse) of Complex Models

How Complex Should Models Be?



Albert Einstein

"Everything should be made as simple as possible, but no simpler."
or
"Make things as simple as possible, but not simpler."

Adapted by modelers as:

"Models should be
as simple as possible,
but no simpler."

The Use of Complex Models

Is there demand for complex models?

- My experience is that there is not.

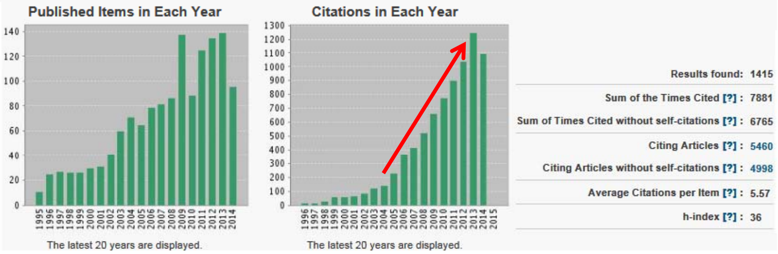
- There are frequent calls for more complex models
- However, once new processes are included in existing models they are often ignored by model users

- While we have hundreds (or even thousands) of users for the basic standard HYDRUS (MODFLOW, PHREEQC) models, we have very few users for specialized modules (e.g., UnsatChem, HP1/2/3, CRide, DualPerm).

The Use of Simpler Models

MODFLOW

ISI, Web of Knowledge



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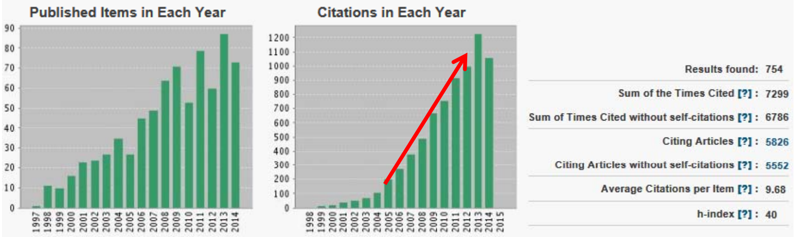
Average Citations per Item [?] : 5.57
h-index [?] : 36

PHREEQC



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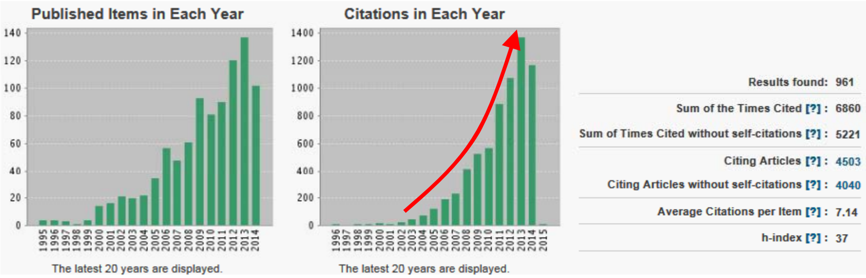
h-index [?] : 40

The Use of Simpler Models

Web of Knowledge

HYDRUS



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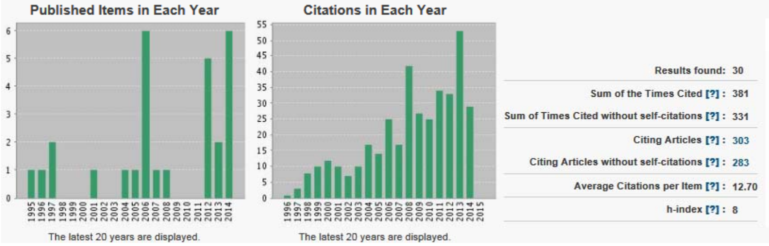
The Use of Complex Models

UnsatChem (Major Ion Chemistry Model)



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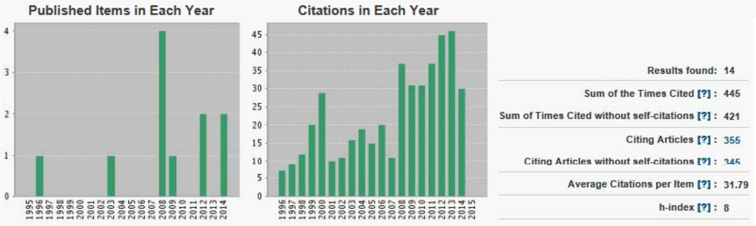
h-index [?] : 8

SOILCO2 (Carbon Dioxide Transport and Production Model)



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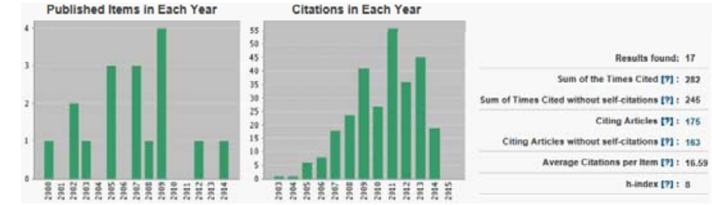
h-index [?] : 8

The Use of Complex Models

CW2D (Wetland Module)



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Citing Articles [?] : 175
Citing Articles without self-citations [?] : 163
Average Citations per Item [?] : 16.59
h-index [?] : 8

HP1 (Coupled HYDRUS + PHREEQC)

1. Jacques, D., J. Šimůnek, D. Mallants, and M. Th. van Genuchten, Operator-splitting errors in coupled reactive transport codes for transient variably saturated flow and contaminant transport in layered soil profiles, *J. Contam. Hydrology*, *88*, 197-218, 2006.
2. Šimůnek, J., D. Jacques, M. Th. van Genuchten, and D. Mallants, Multicomponent geochemical transport modeling using the HYDRUS computer software packages, *J. Am. Water Resour. Assoc.*, *42*(6), 1537-1547, 2006.
3. Jacques, D., J. Šimůnek, D. Mallants, and M. Th. van Genuchten, Modeling coupled hydrological and chemical processes: Long-term uranium transport following mineral phosphorus fertilization, *Vadose Zone Journal*, doi:10.2136/VZJ2007.0084, Special Issue "Vadose Zone Modeling", 7(2), 698-711, 2008.
4. Jacques, D., J. Šimůnek, D. Mallants and M. Th. van Genuchten, Modelling coupled water flow, solute transport and geochemical reactions affecting heavy metal migration in a Podzol soil, *Geoderma*, doi:10.1016/j.geoderma.2008.01.009, *145*, 449-461, 2008.
5. Šimůnek, J., D. Jacques, N. K. C. Twarakavi, and M. Th. van Genuchten, Selected HYDRUS modules for modeling subsurface flow and contaminant transport as influenced by biological processes at various scales, *Biologia*, *64*(3), 465-469, doi: 10.2478/s11756-009-0106-7, 2009.
6. Bessinger, B. A., and C. D. Marks, Treatment of mercury-contaminated soils with activated carbon: A laboratory, field, and modeling study, *Remediation* (The journal of Environmental Cleanup Costs, Technologies, & Techniques), doi: 10.1002/rem.20275, *21*(1), 115-135, 2010.
7. Jacques, D., L. Wang, E. Martens, and D. Mallants, Modelling chemical degradation of concrete during leaching with rain and soil water types, *Cement and Concrete Research*, *40*(8), 1306-1313, 2010.
8. Jacques, D., C. Smith, J. Šimůnek, and D. Smiles, Inverse optimization of hydraulic, solute transport, and cation exchange parameters using HP1 and UCODE to simulate cation exchange, *J. Contaminant Hydrology*, *142-143*, 109-125, 2012.
9. Zhang, H., N. A. Nordin, and M. S. Olson, Evaluating the effects of variable water chemistry on bacterial transport during infiltration, *Journal of Contaminant Hydrology*, *150*, 54–64, 2013.
10. Jacques, D., J. Perko, S.C. Seetharam, and D. Mallants, A cement degradation model for evaluating the evolution of retardation factors in radionuclide leaching models, *Applied Geochemistry*, in press, 2014.
11. Leterme, B., P. Blanc, and D. Jacques, A reactive transport model for mercury fate in soil—application to different anthropogenic pollution sources, *Environmental Science and Pollution Research International*, *21*, 12279–12293, DOI 10.1007/s11356-014-3135-x, 2014.
12. Thaysen, E. M., S. Jessen, D. Postma, R. Jakobsen, D. Jacques, P. Ambus, E. Laloy, and I. Jakobsen, Effects of lime and concrete waste of carbon cycling in the vadose zone, *Environmental Science & Technology*, in press, 2014.
13. Thaysen, E. M., S. Jessen, D. Postma, R. Jakobsen, D. Jacques, P. Ambus, E. Laloy, and I. Jakobsen, Effects of lime and concrete waste of vadose zone carbon cycling, *Vadose Zone Journal*, *13*(11), pp. 11, doi:10.2136/vzj2014.07.0083, 2014.

The Use of Complex Models

- Quantitative mechanistic models that consider basic physical, mechanical, chemical, and biological processes have the potential to be powerful tools to integrate our understanding of complex soil systems.
- The soil science community has often called for models that would include a large number of these diverse processes.
- However, once attempts have been made to develop such models, the response from the community has not always been overwhelming:
  - these models are consequently highly complex
  - requiring a large number of parameters (not all of which can be easily (or at all) measured and/or identified, and which are often associated with large uncertainties),
  - requiring from their users deep knowledge of all/most of these implemented physical, mechanical, chemical and biological processes.
- Real, or perceived, complexity of these models then discourages users from using them (even for relatively simple applications, for which they would be perfectly adequate).
- It is virtually impossible to verify these types of models analytically (or validate them), raising doubts about their applicability.

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  (model inter-comparisons; benchmarking)
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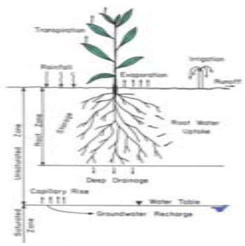
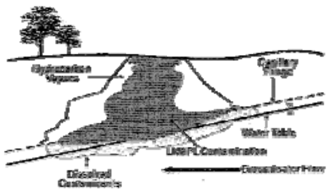
Why to Develop Complex Models?

Environmental Problems:

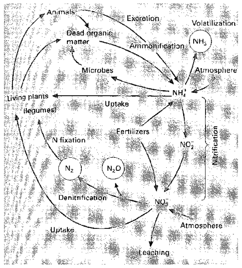
Water Flow



Solute Transport



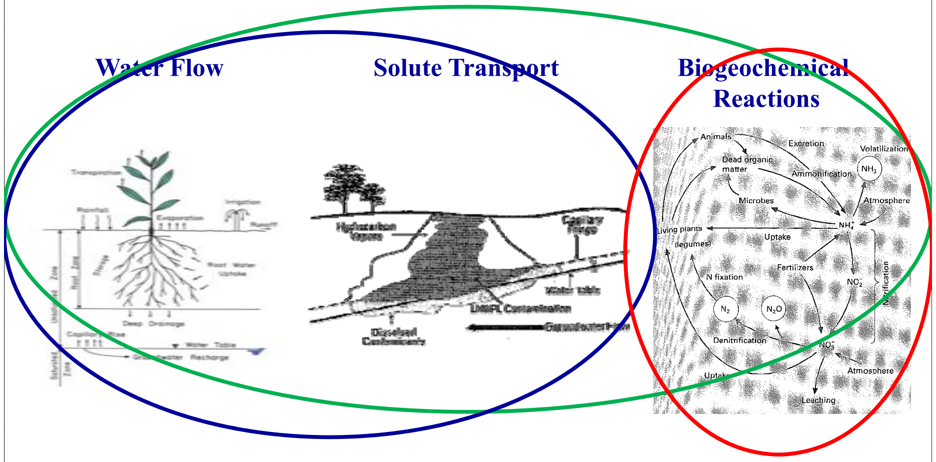
Biogeochemical Reactions



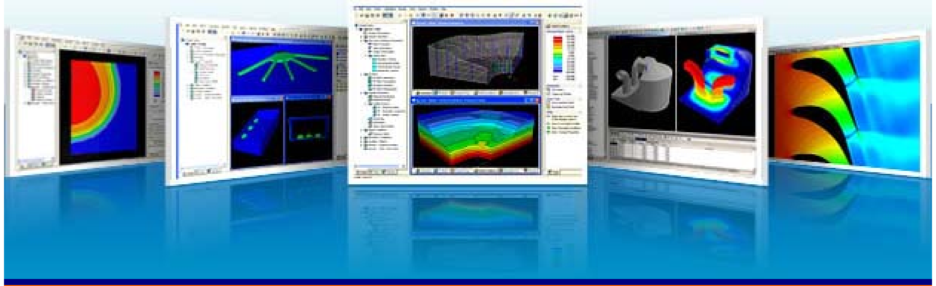
Advanced (complex) mathematical/numerical models are needed to analyse complex environmental problems involving water flow and nutrient/contaminant transport, as well as many biogeochemical reactions in soils

How to Develop Complex Models?

HP1/2/3 models for complex environmental problems:



HYDRUS **HP1/2/3** **PHREEQC**



HYDRUS (1D/2D/3D)

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

- thousands of users around the world
- thousands of applications published
- used by scientists, students, and/or practicing professionals

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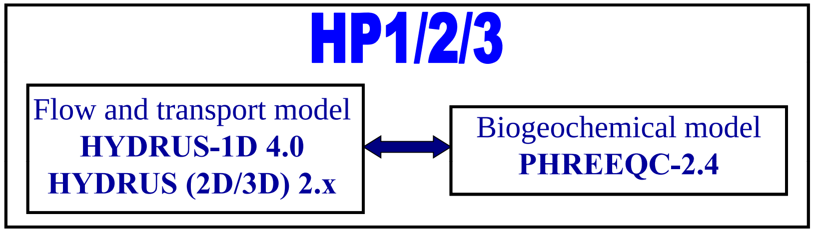
HP1/2/3 (HYDRUS+PHREEQC)

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):

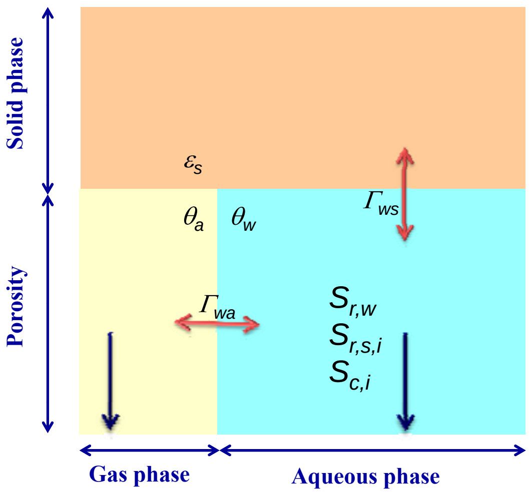
- Variably-Saturated Water Flow
- Solute Transport
- Heat Transport
- Gas Transport
- Root Water Uptake

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

Uniform Flow and Transport Model in HP1



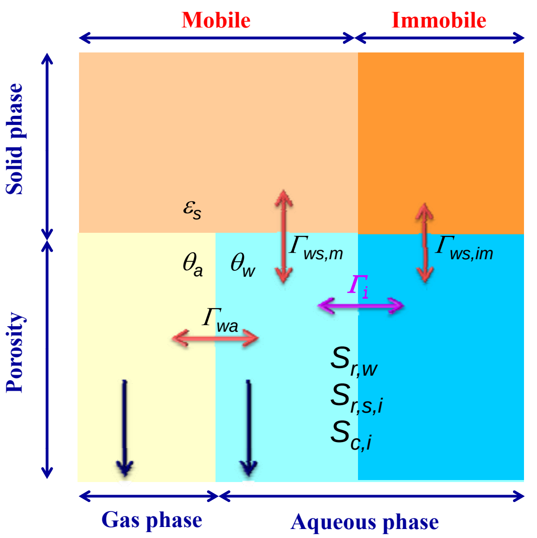
Three phase system
Aqueous, solid and gas phase

Transport
Water flow
Heat transport
Advection-dispersion in water
Diffusion in gas phase

Homogeneous sink/source terms S
Root water uptake $S_{r,w}$
Solute root water uptake $S_{r,s,i}$
Degradation/decay/transform. $S_{c,i}$

Heterogeneous mass exchange Γ
Aqueous – solid phase Γ_{ws}
Aqueous – air phase Γ_{wa}

Uniform Flow and MIM Transport in HP1



Three phase system
Aqueous, solid and gas phase

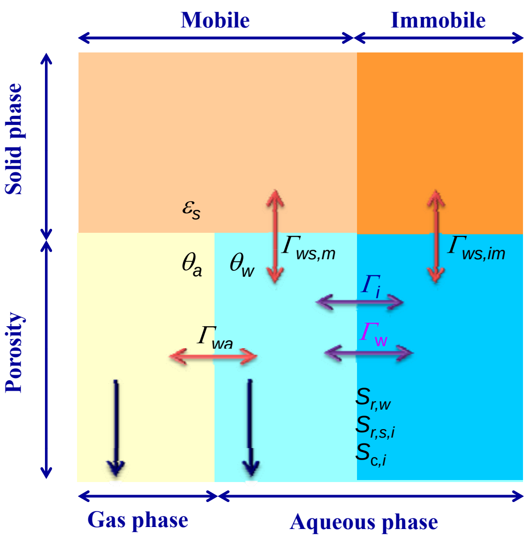
Two liquid-phase domains
Mobile / Immobile

Transport
Water flow
Heat transport
Advection-dispersion in water
Diffusion in gas phase
Solute exchange Γ_i

Homogeneous sink/source terms S
Root water uptake $S_{r,w}$
Solute root water uptake $S_{r,s,i}$
Degradation/decay/transformation $S_{c,i}$

Heterogeneous mass exchange Γ
Aqueous – solid phase Γ_{ws}
(in both mobile/immobile domains)
Aqueous – air phase Γ_{wa}

Dual-Porosity Water Flow and Solute Transport in HP1



Three phase system
Aqueous, solid and gas phase

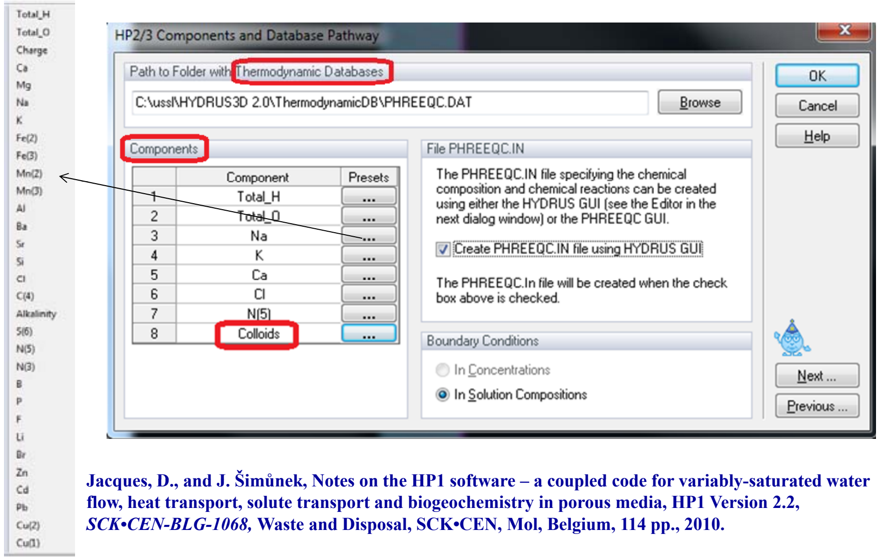
Two domains
Mobile / Immobile

Transport
Water flow
Heat transport
Advection-dispersion in water
Diffusion in gas phase
Water exchange Γ_w
Solute exchange Γ_i

Homogeneous sink/source terms S
Root water uptake $S_{r,w}$
Solute root water uptake $S_{r,s,i}$
Degradation/decay/transformation $S_{c,i}$

Heterogeneous mass exchange Γ
Aqueous – solid phase Γ_{ws}
(in both mobile/immobile domains)
Aqueous – air phase Γ_{wa}

HYDRUS GUI for HP1/2/3



HP2/3 Components and Database Pathway

Path to Folder with Thermodynamic Databases: C:\ussl\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

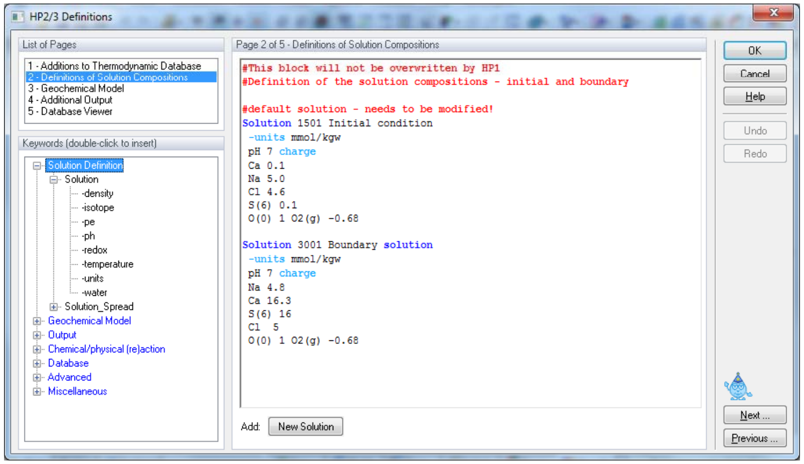
The PHREEQC.In file will be created when the check box above is checked.

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 (2D/3D) GUI for HP2/3



Page 2 of 5 - Definitions of Solution Compositions

```
#This block will not be overwritten by HP1
#Definition of the solution compositions - initial and boundary

#default solution - needs to be modified!
Solution 1501 Initial condition
 -units mmol/kgw
 pH 7 charge
 Ca 0.1
 Na 5.0
 Cl 4.6
 S(6) 0.1
 O(0) 1 O2(g) -0.68

Solution 3001 Boundary solution
 -units mmol/kgw
 pH 7 charge
 Na 4.8
 Ca 16.3
 S(6) 16
 Cl  5
 O(0) 1 O2(g) -0.68
```

Four text editors to define the geochemical model, required output, and solution compositions are fully incorporated into the GUI.

Transport and Cation Exchange Heavy Metals (HP1 Application)

An 8-cm soil column initially contains a solution (with heavy metals) in equilibrium with the cation exchanger. The column is then flushed with three pore volumes of solution w/o heavy metals.

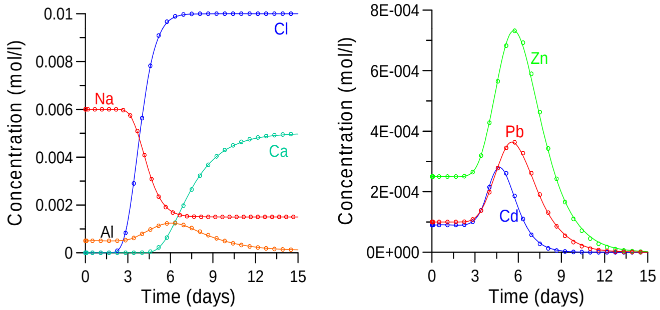
Parameters: *q*=2 cm/d, *l*=0.2 cm, CEC=11 mmol/cell.

Initial concentrations: Al=0.5, Br=11.9, K=2, Na=6, Mg=0.75, **Cd**=0.09, **Pb**=0.1, **Zn**=0.25 mmol/L.

Boundary concentration: Al= 0.1, Br=3.7, Cl=10, **Ca**=5, Mg=1 mmol/L.

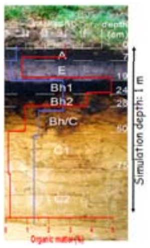
Species and Complexes: Al^{3+}, $Al(OH)^{2+}$, $Al(OH)_2^+$, $Al(OH)_3$, $Al(OH)_4^-$, Br^-, Cl^-, Ca^{2+}, $Ca(OH)^+$, Cd^{2+}, $Cd(OH)^+$, $Cd(OH)_2$, $Cd(OH)_3^-$, $Cd(OH)_4^{2-}$, $CdCl^+$, $CdCl_2$, $CdCl_3^-$, K^+, KOH, Na^+, NaOH, Mg^{2+}, $Mg(OH)^+$, Pb^{2+}, $Pb(OH)^+$, $Pb(OH)_2$, $Pb(OH)_3^-$, $Pb(OH)_4^{2-}$, $PbCl^+$, $PbCl_2$, $PbCl_3^-$, $PbCl_4^{2-}$, Zn^{2+}, $Zn(OH)^+$, $Zn(OH)_2$, $Zn(OH)_3^-$, $Zn(OH)_4^{2-}$, $ZnCl^+$, $ZnCl_2$, $ZnCl_3^-$, $ZnCl_4^2$

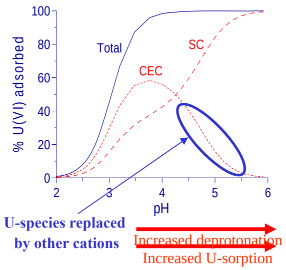
Exchange Species: AlX_3, $AlOHX_2$, CaX_2, CdX_2, KX, NaX, MgX_2, PbX_2, ZnX_2

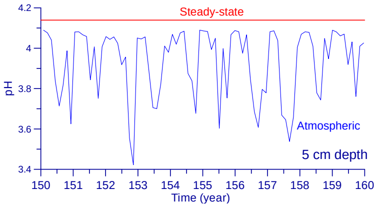


U-Transport in Agricultural Field Soils (HP1 Application)

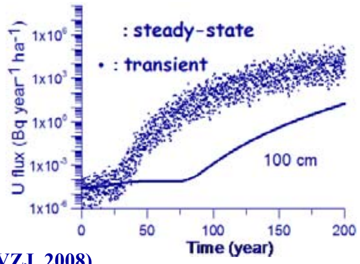
Podzol Soil







- **Water content variations induce *p*H variations (dry soil => low *p*H)**
- **pH variations => variations in sorption potential (low *p*H => low sorption – higher mobility)**



- **Aueous speciation reactions**
  C, Ca, Cl, F, H, K, Mg, N(5), Na, O(0), O(-2), P, S(6), U(6)
- **Multi-site cation exchange reactions**
  - Related to amount of organic matter
  - Increases with increasing pH
  - UO_2^{2+} adsorbs
- **Surface complexation reactions**
  - Specific binding to charged surfaces (≡FeOH)
  - Related to amount of Fe-oxides
- **200-year time series of synthetic meteorological data**
- **P-fertilizer ($Ca(H_2PO_4)_2$): ~3000 Bq ^{238}U/kg, applied each year on May 1 (1 g P/m^2)**

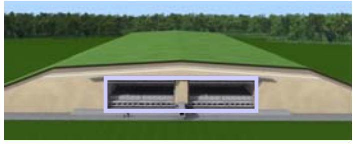
Jacques et al. (VZJ, 2008)

Feedback of Geochemical Changes on Transport Properties

- **HP1 allows dynamic updates of**
  - **porosity**
  - **soil hydraulic properties**
  - **tortuosity in the aqueous and gaseous phase,**
  - **dispersion,**
  - **heat conductivity,**
  - **heat dispersivity**
- **Users have great flexibility in implementing any relationships via BASIC-functions in an input file**

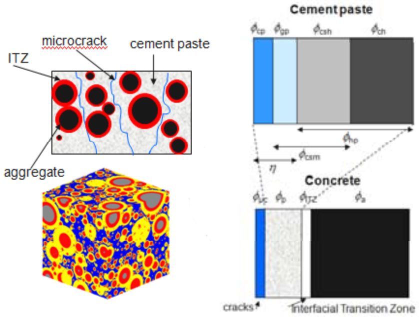
Chemical Degradation of Concrete (HP1 Application)

- **Chemical degradation of concrete in contact with soil water**
- **Disposal site with a low-level radioactive waste**



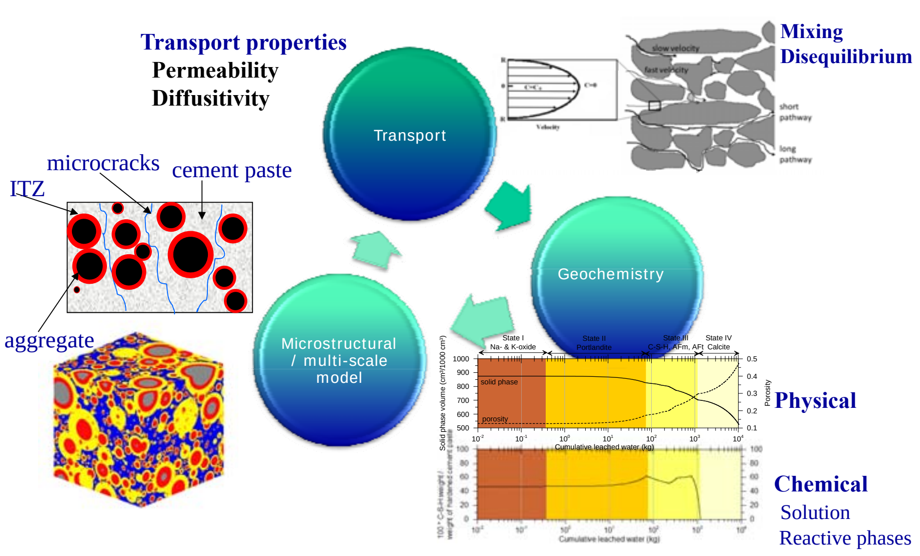
Concrete is multi-scale porous medium

- **Cement Hydrates:**
  portlandite (Port), monocarboaluminate (Mc), strätlingite (Strat), calcite (Cal), OH-hydrotalcite (Ht), CO3-hydrotalcite (Htc), the ideal solid solution between jennite (Jen) and tobermorite (Tob), and the ideal solid solution between ettringite (Ett) and tricarboaluminate (Tca)



- **Model for Cement Phase (ϕ_p):**
  General effective medium homogenization scheme (Oh and Yang, 2004)
  (consist of capillary pores (ϕ_{cp}), gel pores (ϕ_{gp}) incorporated in calcium-silicate hydrates (CSH), solid parts of CSH (ϕ_{csh}), and other cement hydrates (ϕ_{ch}) (mainly portlandite)
- **Updated Transport Properties:**
  - Porosity
  - Tortuosity
  - Permeability (Wissmeier and Barry, 2009)

Coupled Reactive Transport Model



Transport properties
Permeability
Diffusivity

microcracks
cement paste
ITZ
aggregate

Mixing
Disequilibrium

Physical

Chemical
Solution
Reactive phases

Mathematical Model
Link Between Different Processes

Water flow equation (variably-saturated flow)

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

$$\theta(h) = \frac{\theta_s - \theta_r}{\left(1+(\alpha h)^n\right)^m} + \theta_r$$

$$K(S_e) = K_s S_e^L \left[1-\left(1-S_e^{n/(n-1)}\right)^m\right]^2$$

Reactive solute transport equation (# number of components)

$$\frac{\partial \theta C_j}{\partial t} = \frac{\partial}{\partial z}\left(\theta D_{hd}\frac{\partial C_j}{\partial z}\right) - \frac{\partial q C_j}{\partial z} + R_j$$

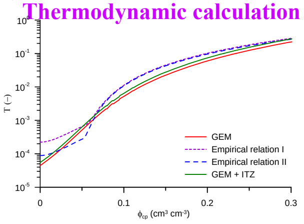
Cement model
Thermodynamic calculation

$$D_{hd} = \lambda \frac{q}{\eta} + D_p$$

$$D_p = \tau D_0 S(\theta) G(T) H(t) M(\varphi)$$

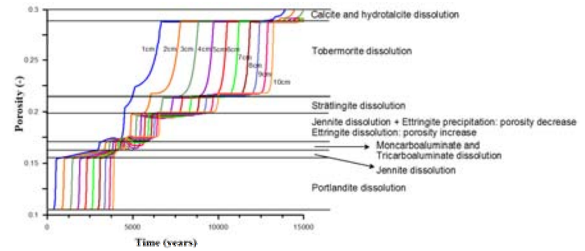
$$T(\phi)$$

τ : tortuosity
D_0 : free water diffusion coefficient
Factors:
  $S(\theta)$ effect of water saturation
  $G(T)$ effect of temperature
  $H(t)$ effect of degree of hydration
  $M(\phi)$ effect of microstructural changes

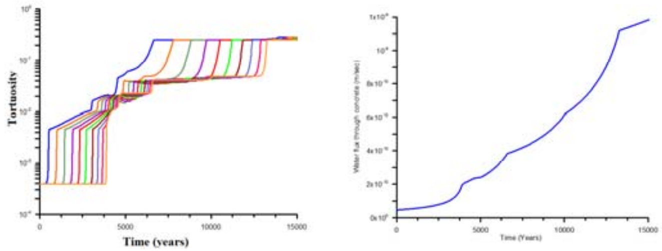


Chemical Degradation of Concrete
(HP1 Application)

Porosity changes during leaching of the concrete core at different depths:

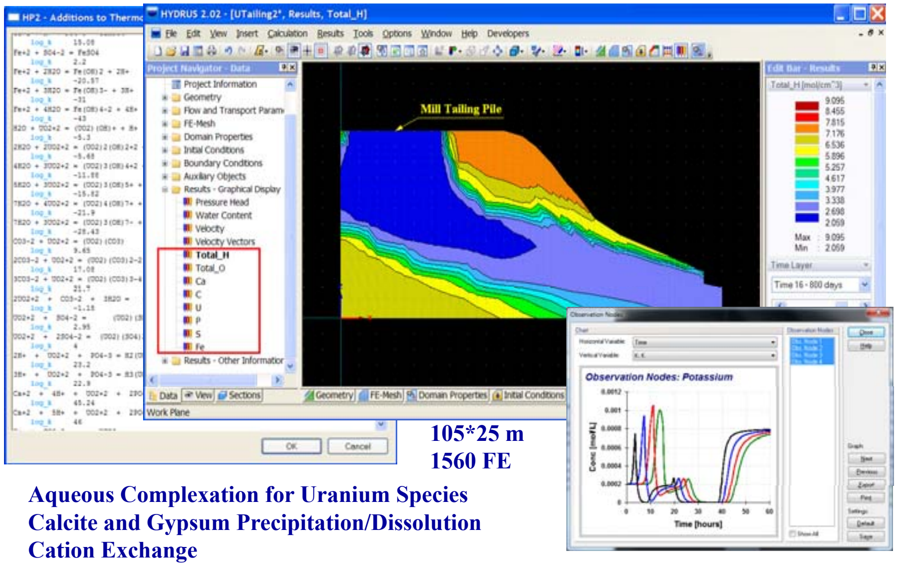


Evolution of tortuosity and water flux:



Jacques et al. (2010)

Uranium Transport from a Mill Tailing Pile



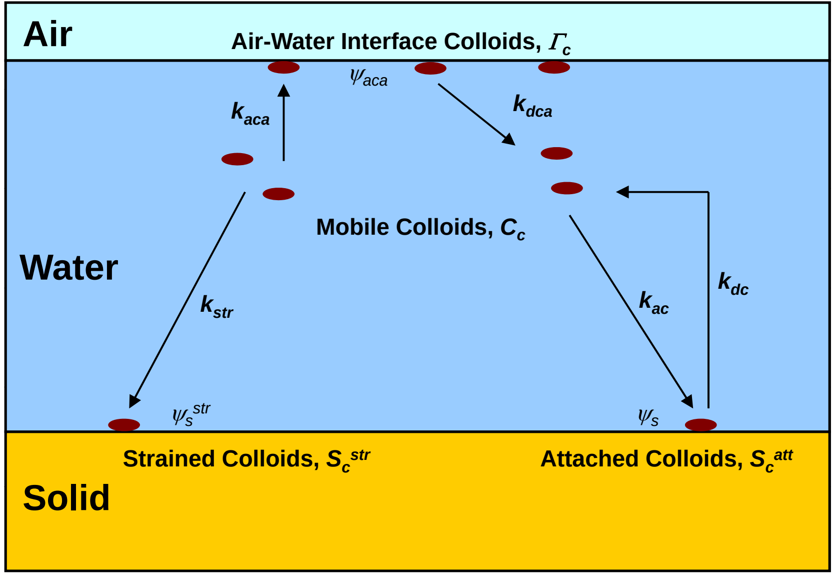
105*25 m
1560 FE

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

HP1/2 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**

Colloid, Virus, and Bacteria Transport


Air
Air-Water Interface Colloids, Γ_c
ψ_{aca}
k_{aca}
k_{dca}
Water
Mobile Colloids, C_c
k_{str}
k_{ac}
k_{dc}
ψ_s^{str}
ψ_s
Solid
Strained Colloids, S_c^{str}
Attached Colloids, S_c^{att}

Particle Transport in Hydrus

$$\frac{\partial \theta_w C_c}{\partial t} + \rho \frac{\partial S_c}{\partial t} + \frac{\partial A_{aw} \Gamma_c}{\partial t} = \frac{\partial}{\partial x}\left(\theta_w D_c \frac{\partial C_c}{\partial x} \right) - \frac{\partial q_c C_c}{\partial x} + R_c$$

Colloid mass-transfer between the aqueous and solid phases:

$$\rho \frac{\partial S_c}{\partial t} = \rho \frac{\partial S_c^{str}}{\partial t} + \rho \frac{\partial S_c^{att}}{\partial t} = \theta_w \psi_s^{str} k_{str} C_c + (\theta_w \psi_s k_{ac} C_c - \rho k_{dc} S_c) - R_{sc}$$

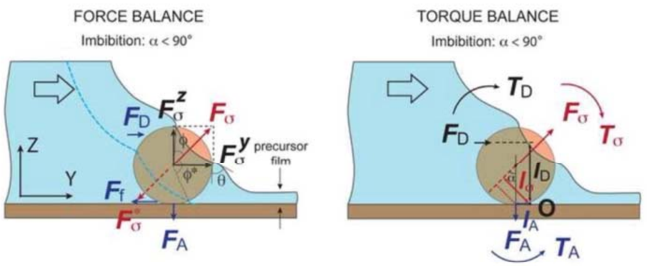
Colloid mass-transfer between the aqueous phase and the air–water interface:

$$\frac{\partial A_{aw} \Gamma_c}{\partial t} = \theta_w \psi_{aca} k_{aca} C_c - A_{aw} k_{dca} \Gamma_c - R_{ac}$$

C_c	**colloid concentration in the aqueous phase [nL^{-3}]**
S_c	**colloid concentrations adsorbed to the solid phase [nM^{-1}]**
S_c^{str}	**solid-phase concentrations of strained colloids [nM^{-1}]**
S_c^{att}	**solid-phase concentrations of attached colloids [nM^{-1}]**
Γ_c	**colloid concentrations adsorbed to the air–water interface [nL^{-2}]**
θ_w	**volumetric water content accessible to colloids [L^3L^{-3}] (due to ion or size exclusion, θ_w may be smaller than the total volumetric water content θ)**
D_c	**dispersion coefficient for colloids [L^2T^{-1}]**
q_c	**volumetric water flux density for colloids [LT^{-1}]**
ρ	**bulk density [ML^{-3}]**

A_{aw}	**air-water interfacial area per unit volume [L^2L^{-3}]**
R_i	**various chemical and biological reactions [$nL^{-3}T^{-1}$]**
k_{str}	**first-order straining coefficient [T^{-1}]**
k_{ac}	**first-order colloid attachment coefficient [T^{-1}]**
k_{dc}	**first-order colloid detachment coefficient [T^{-1}]**
ψ_s	**dimensionless colloid retention function [-]**
ψ_{aca}	**dimensionless colloid retention function for the air–water interface (-)**
k_{aca}	**first-order colloid attachment coefficient to the air–water interface [T^{-1}]**
k_{dca}	**first-order colloid detachment coefficient from the air–water interface [T^{-1}]**

Why is colloid release different under transient from steady-state conditions?



(Lazouskaya et al. 2013; JCIS)

- **Colloid retention and release (at/from SWI) are controlled by forces and torques**
- **Release is a diffusion controlled process under steady-state conditions**
- **Transients conditions alter the adhesive and/or hydrodynamic forces**
- **Imbibition: AWI is destroyed (colloids are released to the water phase)**
- **Draining: Colloids are removed from SWI to AWI and the aqueous phase**

Effects of Imbibition and Draining on Colloids

- **Imbibition**: AWI is destroyed (colloids are released to the water phase)
- **Draining**: Colloids are removed from SWI to AWI and the aqueous phase

$$E_{aw} = \frac{\partial A_{aw}\Gamma}{\partial t} = \theta k_{aaw}\psi_a A_{aw} c - A_{aw} k_{daw}\Gamma - E_{ra} + f_{aw} E_{swa}$$

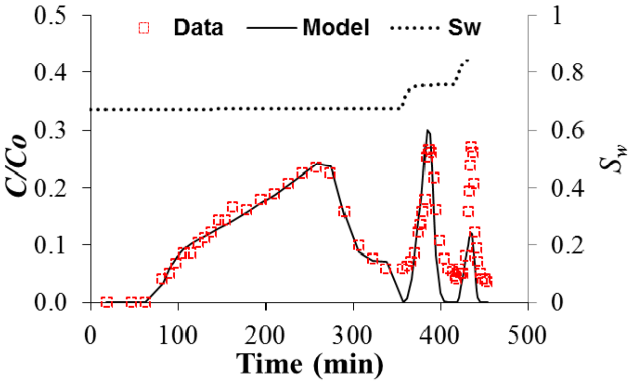
$$E_{ra} = \Gamma \frac{\partial A_{aw}}{\partial t} H_o\left(\frac{\partial \theta}{\partial t}\right) = \Gamma \frac{dA_{aw}}{d\theta}\frac{\partial \theta}{\partial t} H_o\left(\frac{\partial \theta}{\partial t}\right)$$

$$E_{swa} = \rho_b f_{eq} \frac{S_i}{A_s}\frac{dA_{aw}}{d\theta}\frac{\partial \theta}{\partial t} H_o\left(-\frac{\partial \theta}{\partial t}\right) H_o\left(d_c - w_f\right)$$

E_{ra} - destruction of air-water interface during wetting
E_{swa} - colloids removed from the solid phase due to drainage
f_{aw} - a fraction of E_{swa} that is transferred to the air-water interface

Bradford et al. (2014)

Imbibition: Release of Microbes from AWI

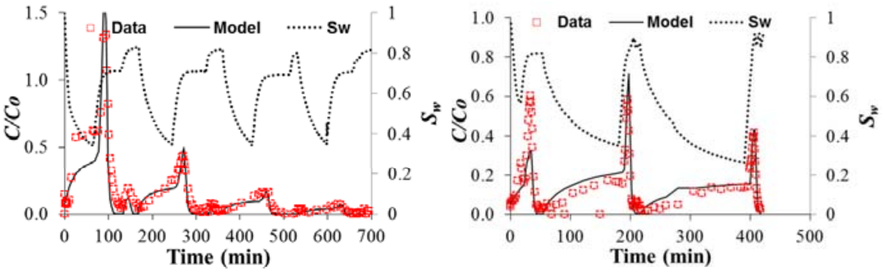


- Cells at the AWI or triple point are released during imbibition due to expansion of water films and destruction of AWI.
- The amount of D21g release is highly dependent on the initial amount and distribution of cells.

Bradford et al. (2014)

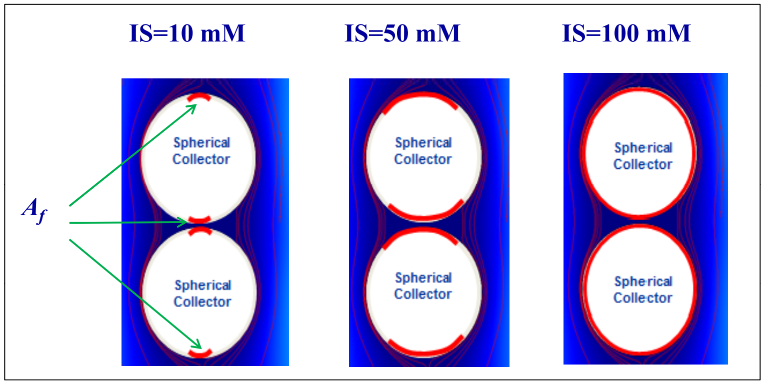
Cycles of Drainage and Imbibition

- Multiple cycles of drainage and imbibition are needed to release D21g from the SWI.
- Release depends on the initial amount of retention on the SWI and the saturation history.



Bradford et al. (2014)

Colloid Release under Transient Chemical Conditions



$$\rho_b \frac{\partial S_{eq}}{\partial t} = E_{IS} = -\rho_b F_{eq} \frac{S_i}{A_{if}}\left|\frac{dA_f}{dC_{IS}}\frac{\partial C_{IS}}{\partial t}\right| H_o\left(-\frac{\partial C_{IS}}{\partial t}\right)$$

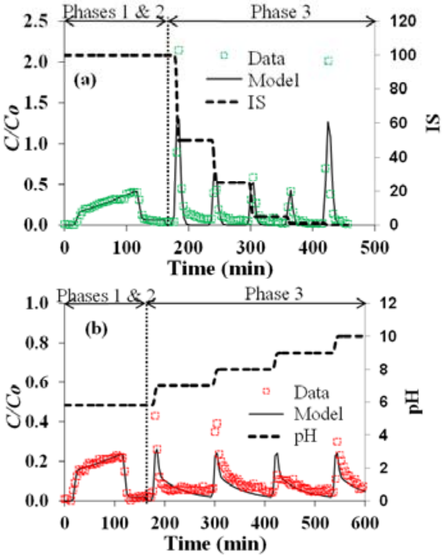
- Values of A_f or S_{max} (denoted in red) change with the physicochemical conditions
- The amount of release is related to changes in A_f or S_{max}

Bradford et al. (2014)

Colloid Release under Transient Chemical Conditions

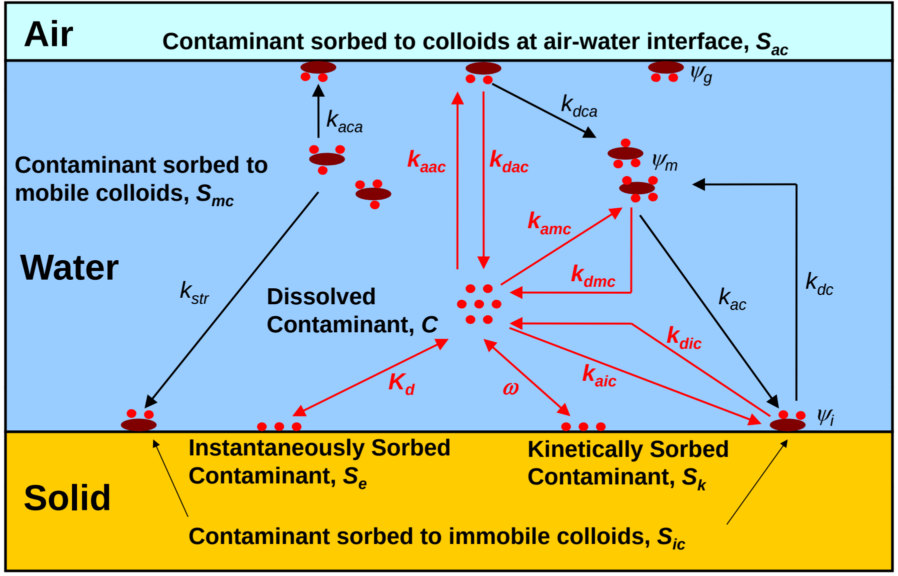
- Release of D21g with a reduction in IS

- Release of D21g with an increase in pH



Bradford et al. (2014)

Colloid-Facilitated Solute Transport



Air

Contaminant sorbed to colloids at air-water interface, S_{ac}

Contaminant sorbed to mobile colloids, S_{mc}

Water

Dissolved Contaminant, C

Solid

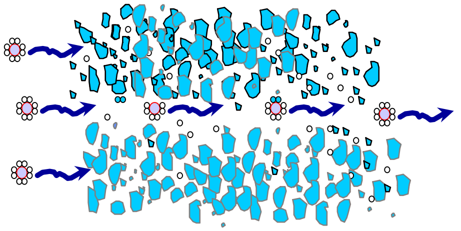
Instantaneously Sorbed Contaminant, S_e

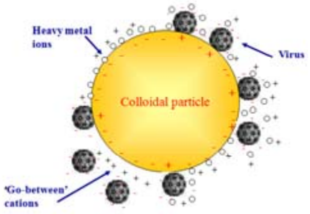
Kinetically Sorbed Contaminant, S_k

Contaminant sorbed to immobile colloids, S_{ic}

Particle-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.

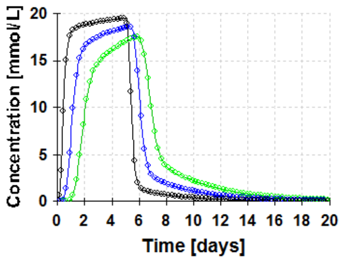
Provide a vehicle for rapid transport of less mobile contaminants.

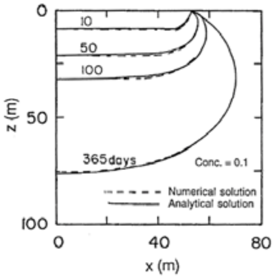
OUTLINE

- How Complex Should Models Be?
- The Use of Complex Models
- Selected HYDRUS-Based Models
  (e.g., HP1, colloid transport)
- Models Verification and Validation
  (model inter-comparisons; benchmarking)
- Documentation of Complex Models
  (technical and user manuals, online help, source code)
- Danger (misuse) of Complex Models

Models Verification

- **Model Verification:** is the process of confirming that the numerical model is correctly implemented with respect to the conceptual (or mathematical) model. During verification the model is tested to find and fix errors in the implementation of the model. The objective of model verification is to ensures that the implementation of the model (i.e., governing equations) is correct.
- **Verification of a numerical code** consists of showing that the results generated by the model for simpler problems are consistent with available analytical solutions.





Models Verification

- Available analytical solutions are often limited to idealized transport domains, homogeneous and isotropic media, and uniform initial and constant boundary conditions.
- The very reason for developing numerical models is to go beyond the range of available analytical solutions, i.e., to allow irregular transport domains, non-homogeneous and anisotropic media, variable boundary conditions, and nonlinear processes, i.e. to use them for situations or conditions for which they can not be directly verified.
- Verification in such conditions is often accomplished using approximate tests of having internal consistency and accuracy, such as:

  - mass conservation
  - global mass-balance errors
  - insensitivity to changes in mesh sizes and time steps
  - insensitivity to changes in units

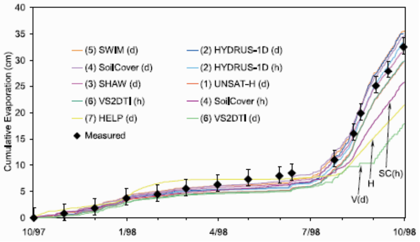
Models Verification (Benchmarking)

- Alternatively, one can show that the results generated by the model are the same, or similar, as results generated with other numerical codes. The latter procedure is often also called *Benchmarking*.
- Code Inter-Comparison is then likely the most suitable method to assess code capabilities and model performance. However, this requires existence of multiple models of similar/overlapping capabilities, which may not always exist.

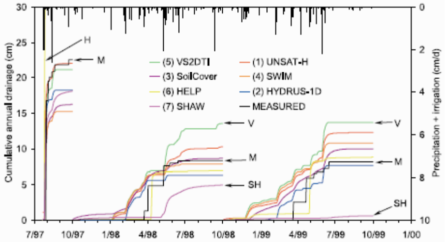
Benchmarking Studies

(Scanlon et al., 2002)

- **Scanlon et al. (WRR, 2002)** compared water balance simulation results from seven different codes (HELP, HYDRUS-1D, SHAW, SoilCover, SWIM, UNSAT-H, and VS2DTI) using three-year water balance monitoring data from non-vegetated engineered covers (3 m deep) in warm (Texas) and cold (Idaho) desert regions.



Time series of cumulative evaporation for the Texas site. The main outliers are VS2DTI with daily precipitation input (V(d)), HELP (H), and SoilCover with hourly precipitation input (SC(h)).



Time series of daily precipitation and measured and simulated drainage at the Idaho Site. Drainage curves were restarted on 1 October each year. The main outliers are HELP (H) for the first few months, SHAW (SH) for 1999, and VS2DTI (V) for 1999 and 2000.

Benchmarking Studies
(Vanderborght et al., 2005)

- **Vanderborght et al. (VZJ, 2005)** developed and used a set of analytical benchmarks (of different complexity) to test numerical models (HYDRUS-1D, MACRO, MARTHE, SWAP, and WAVE) of flow and transport in soils.
- **Analytical Solutions**:
  - Kirchhoff Transform (water flow; Darcy e.)
  - Laplace Transform (solute transport; CDE)
  - Boltzmann Transform (water flow; Richards e.)
  - Traveling Wave Solution (water flow and solute transport)
- **Scenarios**:
  - Steady-state flux in layered profile
  - Steady-state evaporation from a water table
  - Infiltration in an initially dry soil
  - Transient evaporation from a soil profile
  - Steady-state linear solute transport in homogeneous soil profile
  - Steady-state nonlinear solute transport in homogeneous soil profile
  - Steady-state nonequilibrium linear solute transport with flow interruption
  - Steady-state linear solute transport in a dual-porosity medium

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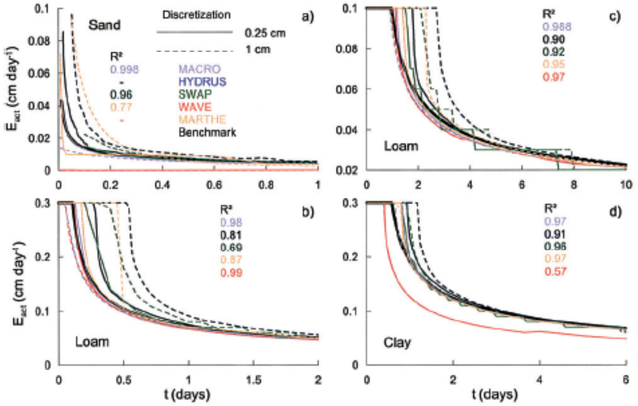
Benchmarking Studies
(Vanderborght et al., 2005)

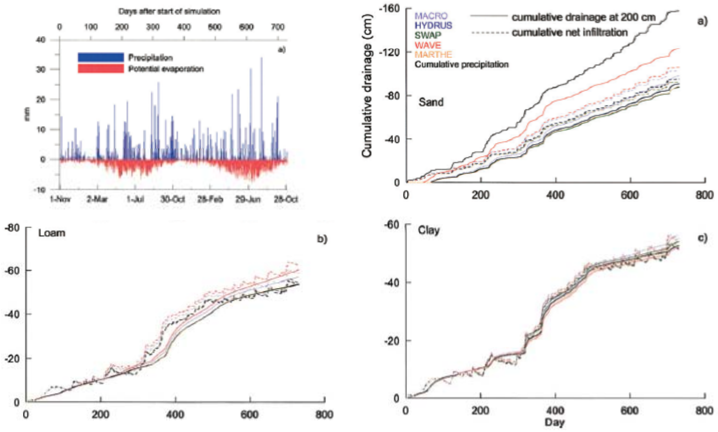
Vanderborght et al. (VZJ, 2005)



Evaporation rate, E_{act}, from initially wet (a) sandy, (b, c) loamy, and (d) clayey soil profiles. Dashed lines are simulated E_{act} using a spatial discretization of 1 cm, full lines using a discretization of 0.25 cm. (Black line is analytical benchmark; R^2 is calculated for simulations with a discretization of 0.25 cm.)

Benchmarking Studies
(Vanderborght et al., 2005)

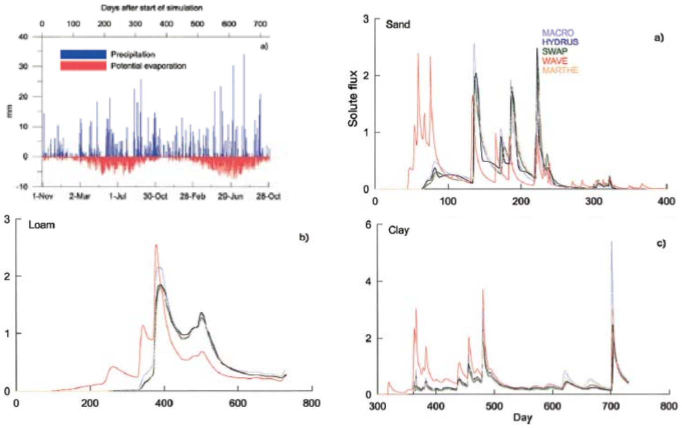
Vanderborght et al. (VZJ, 2005)



Simulated **cumulative drainage** at the 2-m depth (full lines) and cumulative net infiltration (precipitation - actual evaporation) (dashed lines) in (a) sandy, (b) loamy, and (c) clayey soil profiles. (Full black line is the cumulative precipitation)

Benchmarking Studies
(Vanderborght et al., 2005)

Vanderborght et al. (VZJ, 2005)



Simulated **Solute Fluxes** at the 2-m depth in (a) sandy, (b) loamy, and (c) clayey soil profiles for climatic boundary conditions.

Benchmarking Studies
(Reactive Transport Models)

- A set of well-described benchmark problems for complex reactive transport numerical models was developed in the special issue of *Computational Geosciences* (CrunchFlow, HP1, MIN3P, PFlotran, and TOUGHREACT) (e.g., Steefel et al., 2015; Xie et al., 2015).
  - kinetic dissolution
  - clogging in a simple (1D) geochemical system
  - clogging in a complex (2D heterogeneous) geochemical system

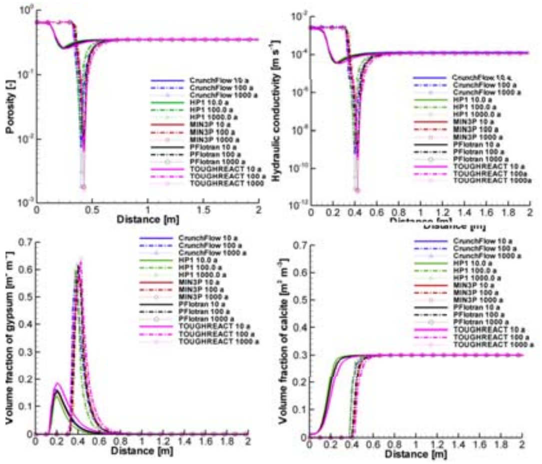
Steefel, C., S. Yabusaki, and U. Mayer, Special Volume on Subsurface Environmental Simulation Benchmarks, *Computational Geosciences*, in press, 2015.

Steefel, C. I., C. A. J. Appelo, B. Arora, D. Jacques[14], T. Kalbacher, O. Kolditz, V. Lagneau, P. C. Lichtner, K. U. Mayer, J. C. L. Meeussen, S. Molins, D. Moulton, H. Shao, J. Šimůnek, N. Spycher, S. B. Yabusaki, and G. T. Yeh, Reactive transport codes for subsurface environmental simulation, *Computational Geosciences*, doi:10.1007/s10596-014-9443-x, in press, 2015.

Xie, M., K. U. Mayer, F. Claret, P. Alt-Epping, D. Jacques, C. Steefel, C. Chiaberge, and J. Šimůnek, Implementation and evaluation of permeability-porosity and tortuosity-porosity relationships linked to mineral dissolution-precipitation, *Computational Geosciences*, in press, 2015.

Benchmarking Studies
(Reactive Transport Models)

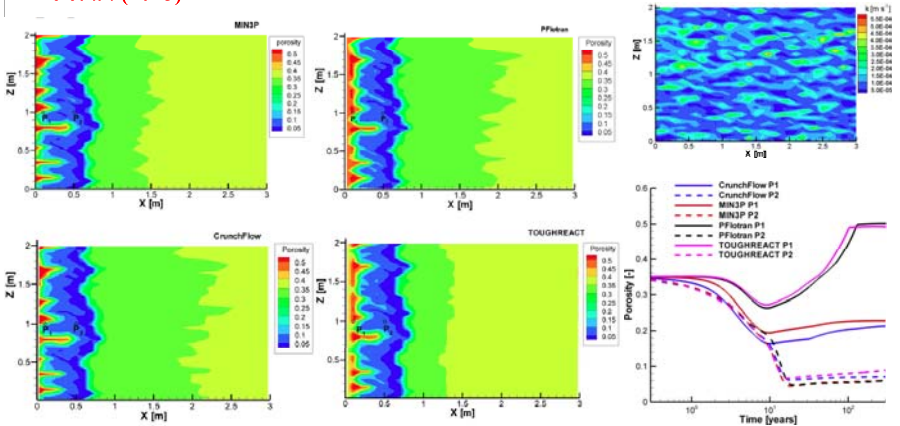
Xie et al. (2015)



Profiles (B2) of porosity, hydraulic conductivity, and volume fraction of gypsum and calcite, h (d) at 10, 100, and 120 years by CrunchFlow, HP1, MIN3P, PFlotran, and TOUGHREACT.

Benchmarking Studies
(Reactive Transport Models)

Xie et al. (2015)



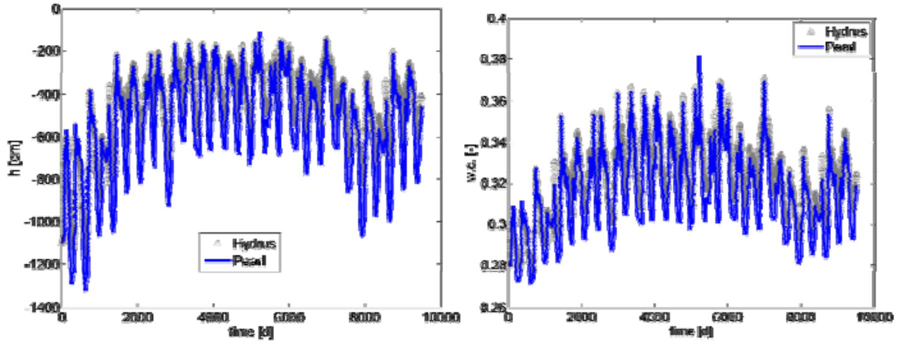
Hydraulic conductivity initial distribution, and distribution of porosity simulated by MIN3P, PFlotran, CrunchFlow, and TOUGHREACT at 300 years.

Benchmarking Studies
(Focus Scenarios)

- **FOCUS Scenarios**: standardized scenario's have been developed for 9 locations and approximately 14 crops per location.
- **Scenario's** are a combination of crop, location, the long-term application schedule (i.e. annual, biennial or triennial applications) and agronomic parameters (particularly irrigation data).
- **Scenarios** collectively represent agriculture across Europe for the purpose of Tier 1 EU-level assessment of leaching potential.
- In the initial assessments of **pesticide registration**, models are used to get a first indication of the leaching potential of a pesticide.
- **Models**: PEARL, PELMO, PRZM (and Macro for one location)
- **FOCUS**: Forum for International Co-ordination of pesticide fate models and their Use (FOCUS).

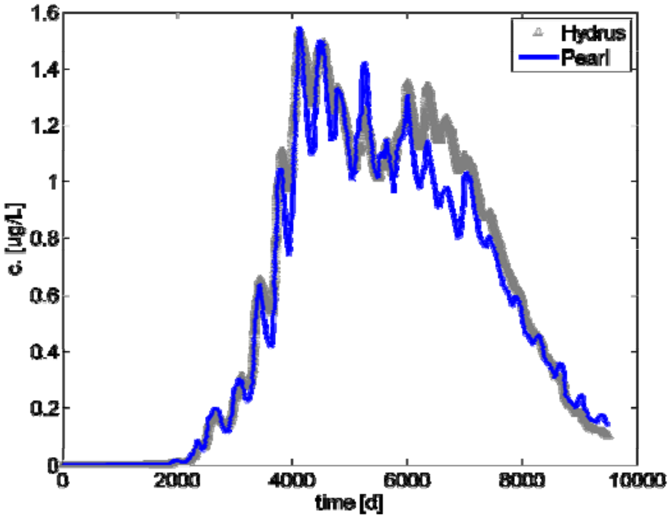
Benchmarking Studies
(Focus Scenarios)

Location: Chateaudun, Fr.
Domain: 450 cm, 7 layers
Time: 26 years, atmospheric daily meteo
Solute: multiple substances with different K_d and half-life
Plants: Root growth
Models: Pearl and HYDRUS
Carried out by: Stathis Diamantopoulos



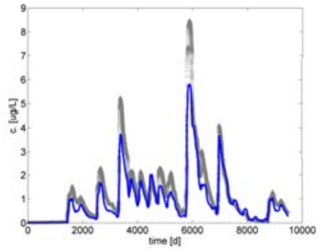
Benchmarking Studies
(Focus Scenarios)

Substance A

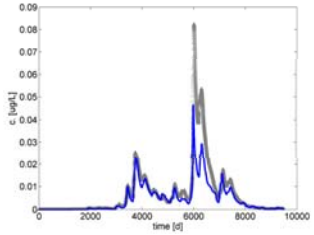


Benchmarking Studies
(Focus Scenarios)

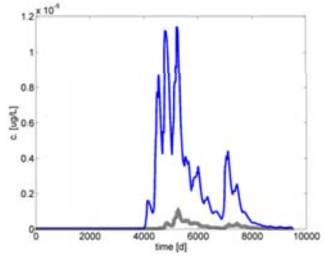
Substance B



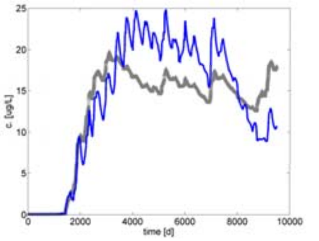
Substance D



Substance C



Substance C's daughter product



Additional Benchmarking Studies

- ◆ Oster et al. (AWM, 2012) compared the simulated crop yields grown under production practices and (transient) conditions (involving pressure head and osmotic stresses) in the western San Joaquin Valley of California using the ENVIRO-GRO, HYDRUS-1D, SALTMED, SWAP, and UNSATCHEM models.
- ◆ Hanson et al. (2004) evaluated 13 models varying in their spatial, mechanistic, and temporal complexity for their ability to capture intra- and inter-annual components of the water and carbon cycle for an upland, oak-dominated forest of eastern Tennessee.
- ◆ Rosenzweig et al. (2013) described the Agricultural Model Intercomparison and Improvement Project (AgMIP), which is a major international effort linking the climate, crop, and economic modeling communities with cutting-edge information technology to produce improved crop and economic models and the next generation of climate impact projections for the agricultural sector.
- ◆ WCRP (World Climate Research Programme) Working Group on Coupled Modeling catalogues a large number of Model Intercomparison Projects (MIPs) related to various climate related models.

Model Validation - Definitions

Narasimhan (1987):

- **Model Verification** is related to the accuracy of the invoked numerical solution schemes and the coding of a model, and
- **Model Validation** to the inherent capability (or the degree of validity) of a model in describing a set of processes (in our case subsurface flow and transport processes).

- **International Atomic Energy Agency:** a validated model gives 'a good representation of the actual processes occurring in a real system' (IAEA, 1982)
- **U.S. Department of Energy:** a validated model 'reflects the behavior of the real world' (US DOE, 1986)
- **OECD/NEA:** 'validation is a process of obtaining assurance that a model is a correct representation of the process or system for which it is intended' (OECD/NEA, 1990)

International Validation Projects

- **INTRACOIN** (International Nuclide Transport Code Intercomparison Study, SNPI, 1986)
- **INTRAVAL** (International Project to Study Validation of Geosphere/Transport Models, SNPI, 1987)
- **HYDROCOIN** (Hydrologic Code Intercomparison Study, OECD/NEA, 1990)
- **Advances in Water Resources** - two special issues to the topic of 'Validation of geo-hydrological models' (Hassanizadeh & Carrera, 1992)

Validation of Geo-Hydrological Models

- **Konikow & Bredehoeft (1992): Ground-water models cannot be validated.** Since groundwater models are embodiment of scientific hypothesis they cannot be proven or validated, similarly as any scientific hypothesis or theory, but only tested and invalidated. The terms validation and verification are misleading and their use in groundwater science should be abandoned in favor of more meaningful model-assessment descriptors.
- **de Marsily et al. (1992):** We do not validate our models, but we try to show that they are not invalidated by the data!
- **Anderson & Woessner (1992):** the issue of model validation is mainly a regulatory one, not a scientific one. A model can never be proven valid from a scientific standpoint because our understanding of a system will always be incomplete.
- **Oreskes et al. (1994):** Verification and validation of numerical models of natural systems is impossible since such systems are never closed and model results are always non-unique.

OUTLINE

- How Complex Should Models Be?
- The Use of Complex Models
- Selected HYDRUS-Based Models
  (e.g., HP1, colloid transport)
- Models Verification and Validation
  (model inter-comparisons; benchmarking)
- **Documentation of Complex Models**
  (technical and user manuals, online help, source code)
- Danger (misuse) of Complex Models

Documentation of Complex Models

Important Factors for Acceptance of Complex Models:

- Detailed description of all processes in Technical and User Manuals
  - HYDRUS-1D (342 pages)
  - HYDRUS (2D/3D) (260 pp. Technical manual, 301 pp. User manual, over 1000 pages of online help, + documentation of modules)
  - SWAP (284 pages)
- Availability of the source code
- Availability of examples/tutorials
- Verification/validation
- Training (short courses) (Hydrus short courses, currently annually in Europe (Prague), US (Golden, Colorado), China (Beijing), and Brazil, and semiannually in Israel (Sede Boqer) and Australia (Adelaide))
- Numerical robustness
- …

OUTLINE

- How Complex Should Models Be?
- The Use of Complex Models
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  (e.g., HP1, colloid transport)
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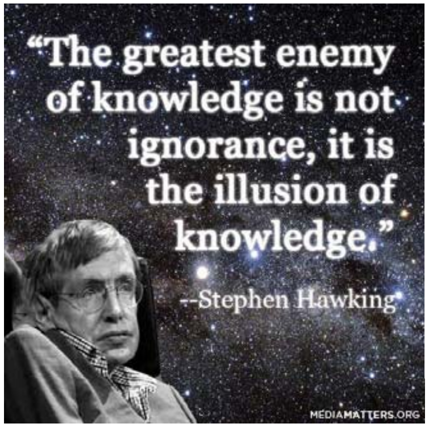
Danger (misuse) of Complex Models



By developing and making available powerful numerical models, we are providing people with tools, which they are sometimes applying without fully understanding the theories underlying these tools and in conditions, for which they are not always appropriate.

Conclusions

- It is a challenge, not only to develop complex models describing complex soil systems, but also to persuade the soil science community in using them.
- As a result, complex quantitative mechanistic models are still an underutilized tool in soil science research.