Coupling of COMSOL and the Geochemical Modelling Framework PHREEQC

COMSOL Conference
26th October 2011
Stuttgart, Germany

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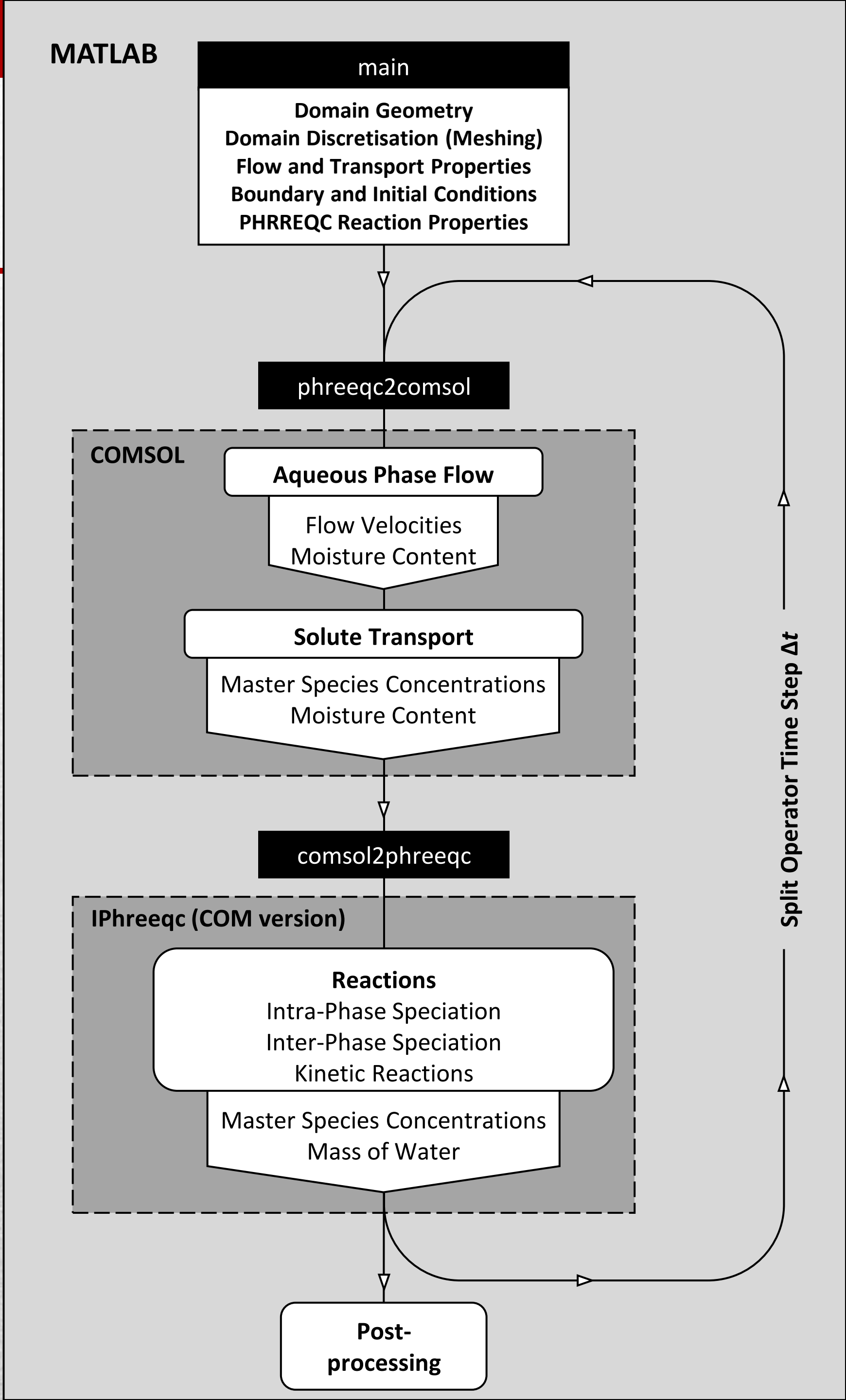
Fields of Application

- Water resource management and pollution control (e.g., pesticide behaviour)
- Agricultural management (e.g., drip irrigation, fertigation)
- Remediation designs and contaminated site clean-up (e.g., bauxite residue management)
- Risk assessment for hazardous waste disposal (e.g., nuclear waste disposal)
- Scientific tool to investigate coupled geophysical, geomecanical and geochemical processes (e.g., CO_2-sequestration)

PHREEQC

Open source geochemical modelling framework developed by USGS

- Activity corrected solution speciation
- Surface complexation and ion exchange adsorption models
- Kinetic and equilibrium mineral reactions
- Redox reactions
- Gas phase exchange
- Kinetic organic and biotic processes
- Comprehensive geochemical databases



Component-Based Aqueous Phase Flow

Flow, transport and reactions

Richards' equation: Phase mass balance

$$\frac{\partial \rho\theta}{\partial t} = -\nabla\cdot(\rho\theta\boldsymbol{v})$$

$$\frac{\partial}{\partial t}\left(\sum_i n_i m_i\right) - \nabla\cdot\left[\frac{\bar{\bar{\boldsymbol{k}}}}{\mu}\nabla\left(p + \sum_i \rho g z m_i\right)\right] = \nabla\cdot\left(\sum_i \boldsymbol{j}_i\right)$$

Advection-dispersion equation: Component mass balance

$$\frac{\partial \theta c_i}{\partial t} = -\nabla\cdot(\boldsymbol{v}\theta c_i) + \nabla\cdot\left(\theta\bar{\bar{\boldsymbol{D}}}\nabla c_i\right)$$

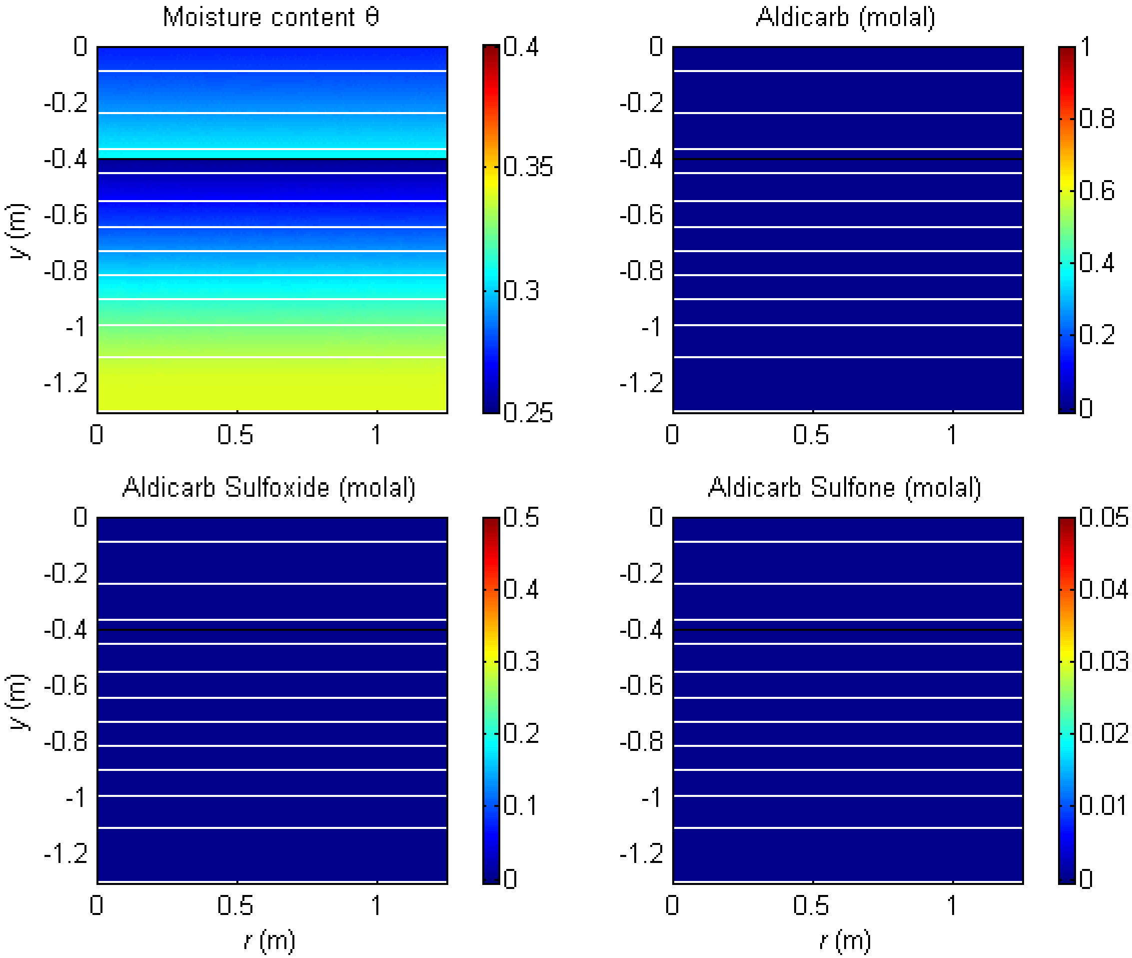
$$m_i\frac{\partial n_i}{\partial t} = -\nabla\cdot(\boldsymbol{v} n_i m_i) + \nabla\cdot(\boldsymbol{j}_i)$$

Equilibrium solution speciation: Mass action

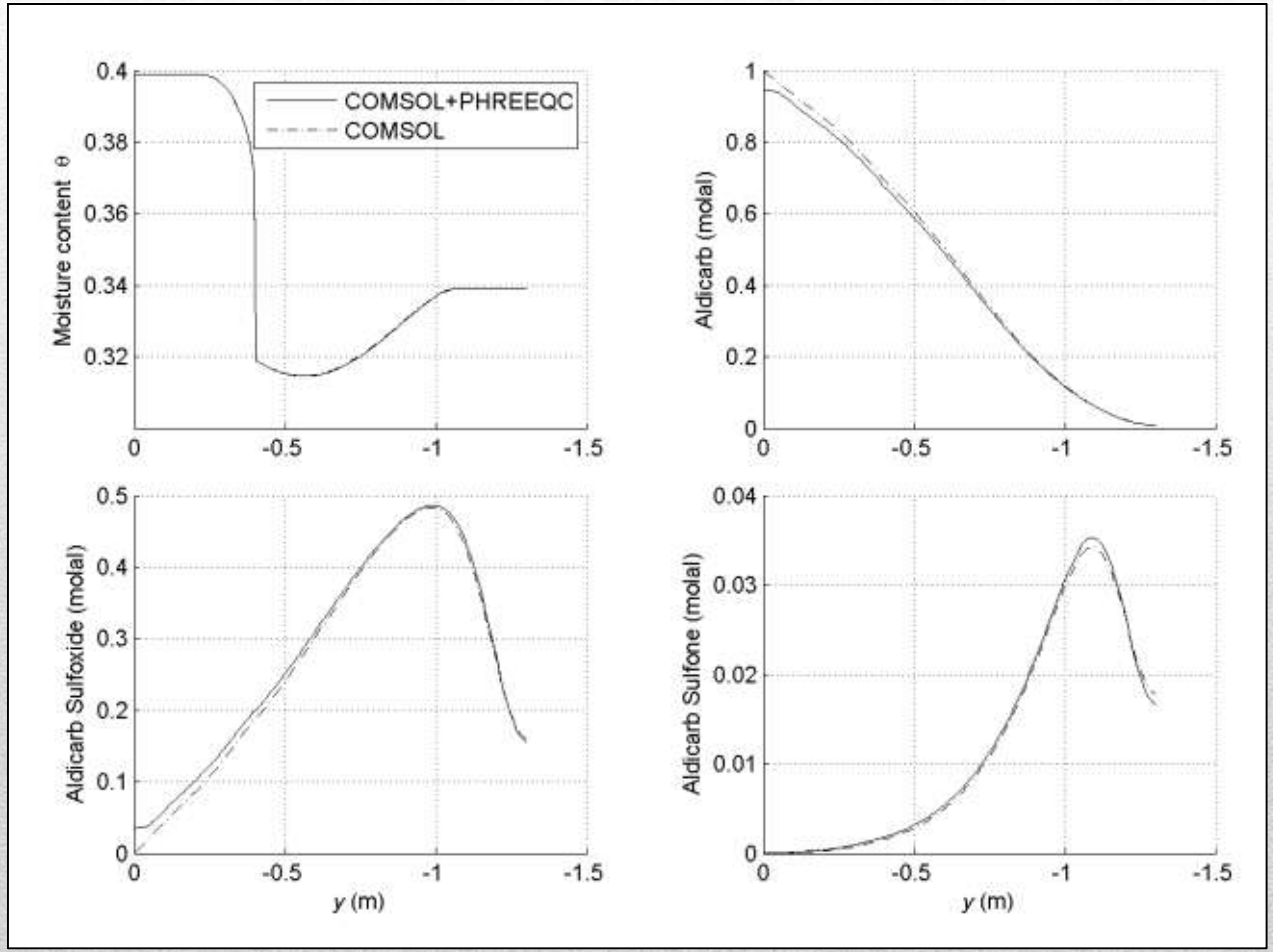
$$n_i = \frac{K_i W_{aq}}{\gamma_i}\prod_e \mathcal{A}_e^{-s_{e,i}}$$

Model Verification

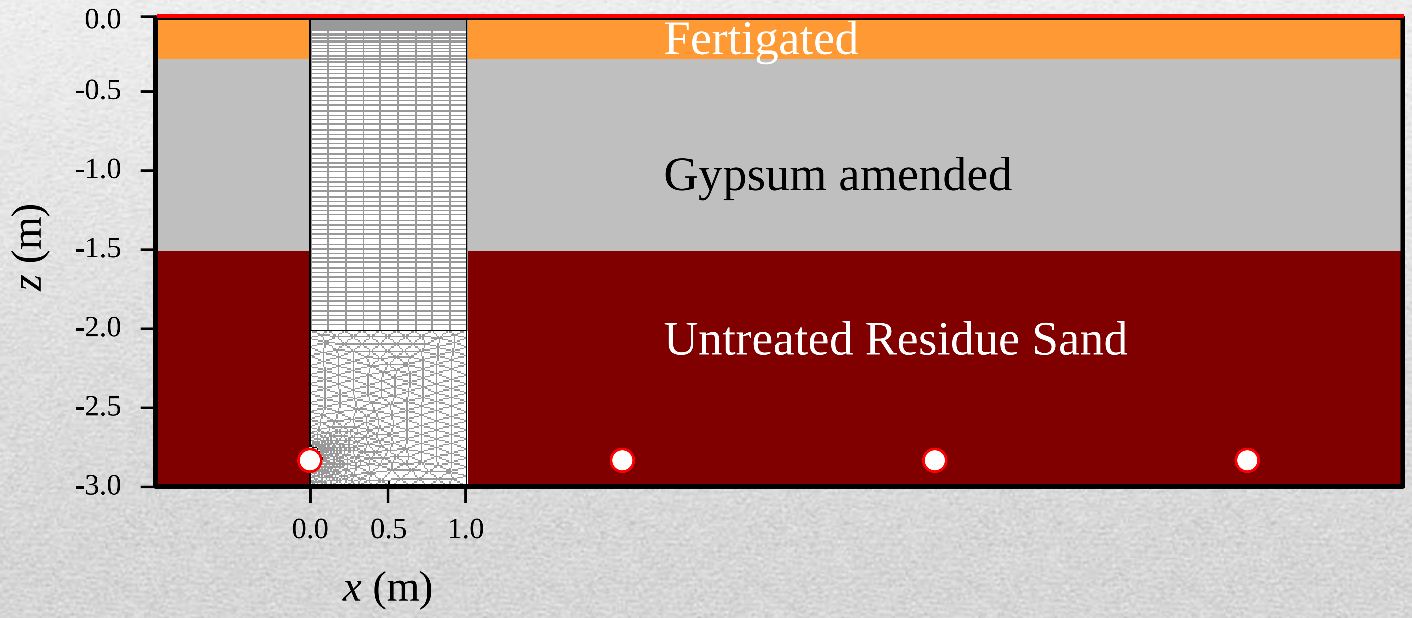
Simulation time (d)



Model Verification



Simulation of Bauxite Residue in Field Conditions



Geochemical Model

Mineral composition

Mineral	Equilibrium constant	Rate constant (mol m^{-2} s^{-1})	Relative amount (mol kg_{solid}^{-1})
Calcite	$10^{-8.48}$ [a]	-	2.53×10^{-2}
Natron	$10^{-1.31}$ [a]	-	3.99×10^{-2}
Muscovite	10^{14} [b]	-	2.51×10^{-2}
Analcime	$10^{6.72}$ [a]	-	3.05×10^{-2}
Sodalite	$10^{-55.89}$ [c]	3.41×10^{-9}	4.24×10^{-3}
TCA	10^{74} [d]	7.48×10^{-10}	5.57×10^{-3}

Fertilizer minerals

Mineral	Relative amount (mol l_{soil}^{-1})
DAP	5.67×10^{-3}
Arcanite	2.41×10^{-3}
$CuSO_4$	1.50×10^{-4}
Zincosite	1.41×10^{-4}
$MnSO_4$	1.55×10^{-5}
$MgSO_4$	1.10×10^{-3}
Borax	2.62×10^{-5}

Adsorption model

Cation exchanger	Relative amount (eq kg_{solid}^{-1})
X-	8.6×10^{-3}

[a] minteq.dat (distributed with PHREEQC)
[b] sit.dat (distributed with PHREEQC)
[c] calculated from thermodynamic data in Komada et al.
[d] from Khaitan et al.

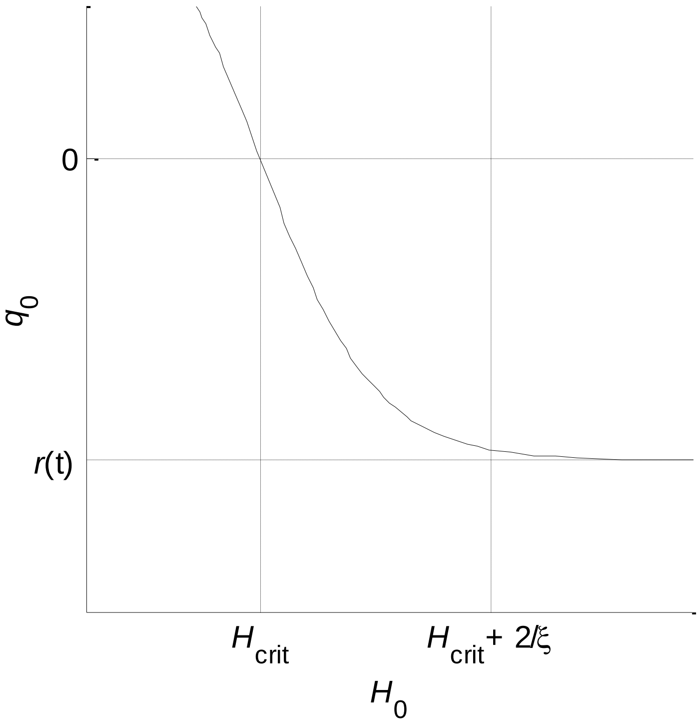
Amendment

Mineral	Relative amount (mol l_{soil}^{-1})
Gypsum	1.10×10^{-1}

Boundary Conditions

Recharge:

$$q_0 = \begin{cases} r(t), & H_0 \le H_{po} \\ r(t) - k_{po}\,(H_0 - H_{po}), & H_0 > H_{po} \end{cases}$$



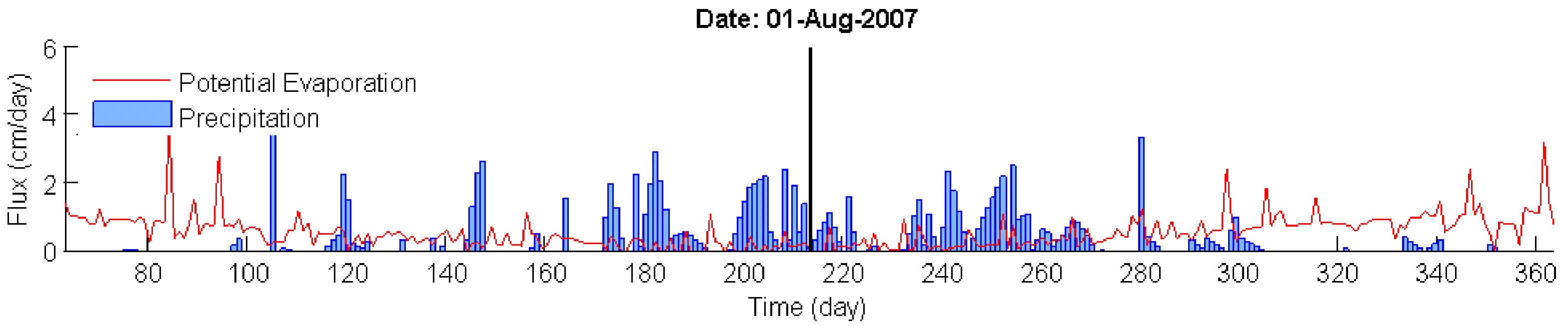
Evaporation:

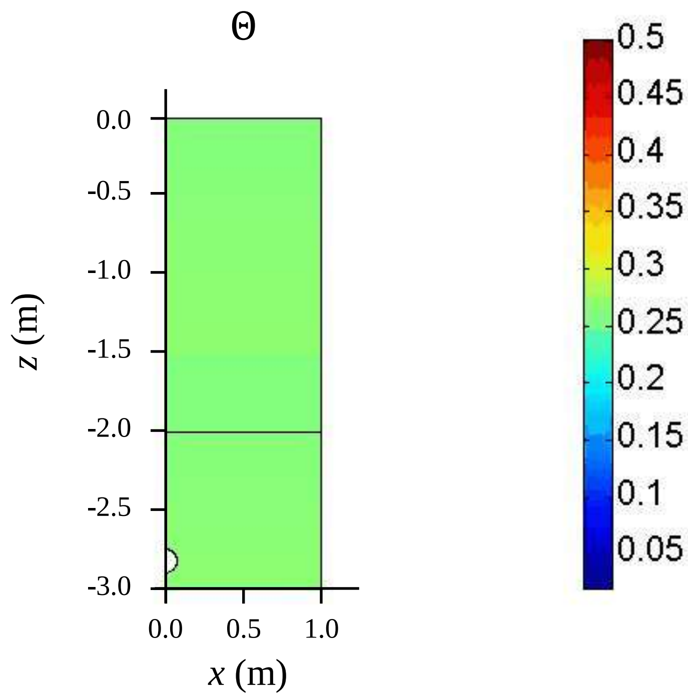
$$q_0 = -r(t)\tanh\left[\frac{\xi}{r(t)}(H_0 - H_{crit})\right]$$

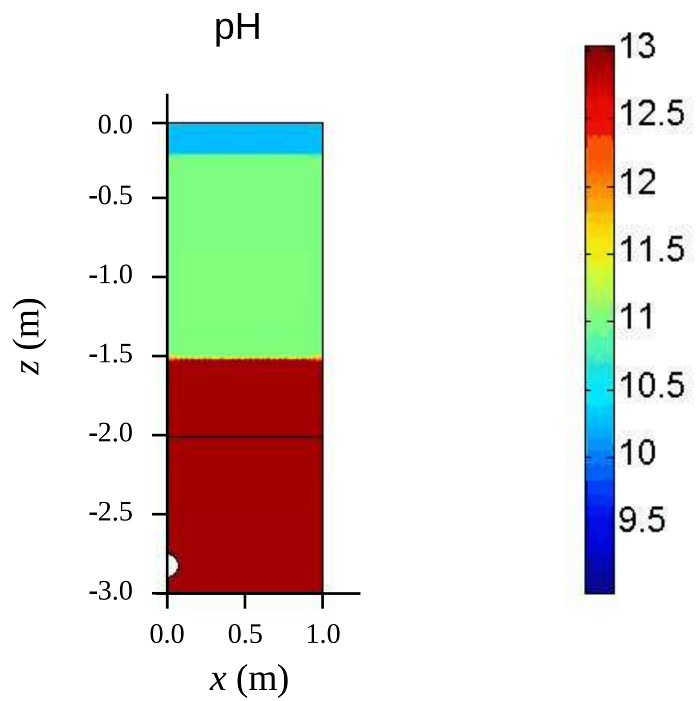
Atmospheric boundary including evaporation and recharge:

$$q_0 = \begin{cases} -r(t)\tanh\left[\frac{\xi}{r(t)}(H_0 - H_{crit})\right] & r(t) < 0 \\ r(t)\mathcal{H}\left(H_{po} - H_0\right) + \left[r(t) - k_{po}\,(H_0 - H_{po})\right]\mathcal{H}\left(H_0 - H_{po}\right) & r(t) \ge 0 \end{cases}$$

Lysimeter Simulation







Thank you for your attention!

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Literature

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