Models of root growth, water and solute uptake: System of equations aimed for DuMux implementation

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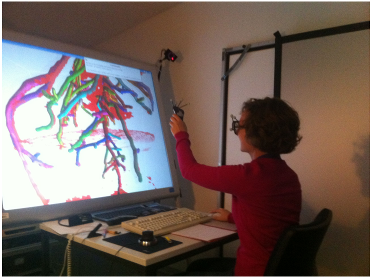
Background

Research group

Root-soil interactions modelling

Scientific questions

Nutrient efficiency of crops
Phosphate scarcity
Water efficiency of crops
Water management
Pesticides in the soil-plant system



Manual root tracking in the holobench, JSC

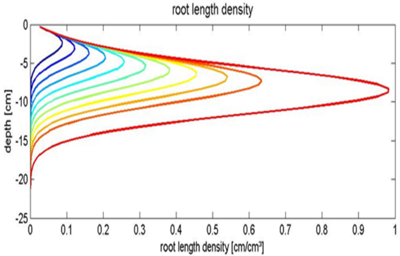
Motivation to use DuMux

- We currently use different codes, e.g. R-SWMS, Matlab, Comsol
- Originating from two groups: Javaux and Schnepf
- Limitations in terms of memory, grids, computation time
- We see DuMux as a software enviroment that facilitates "merging" of the different model approaches
- Allows flexibility for model development/adaptation

Should we transfer to DuMux?

Root growth models

Density-based root models: pde's that could probably be implemented in Dumux



Discrete root architecture models: connected line segments

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Nutrient uptake model

$$\frac{\partial}{\partial t}\left[(b+\theta)c\right] + \nabla \cdot \left[D\theta f \nabla c - \mathbf{uc}\right] - F(c,\theta,t) = 0 \qquad (1)$$

Depending on the specific problem, the geometry may be 1D, 2D or 3D.

t time, c concentration of solute in solution, b buffer power, D diffusion coefficient in free solution, f impedance factor, θ volumetric water content, $\mathbf{u}$ water flux, $F(c,\theta,t)$ sink term for nutrient uptake.

Example Roose et al. (2001): 1D soil profile

$$-D\theta f \frac{\partial c}{\partial z} + W_{top} c = \zeta \qquad \text{at } z = 0 \tag{2}$$

$$-D\theta f \frac{\partial c}{\partial z} + W_{bottom} c = 0 \qquad \text{at } z = L \tag{3}$$

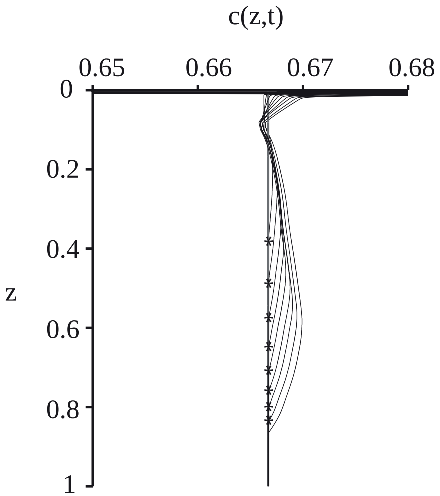
$$c = c_0 \qquad att = 0 \tag{4}$$

W water flux at top/bottom of soil profile, ζ fertilizer application rate, L depth of soil profile

$$F(c, \theta, t) = \frac{1}{V} \int_{\#roots} 2r\pi l F_{analytical,single}(age, z) \tag{5}$$

V representative soil volume, age $= t - t_{\text{creation}}$

Output



Interacting ions

3D soil domain with homogeneous initial and zero-flux boundary conditions

$$\left[\theta + \rho \frac{k_{L,p} k_{L,ex} s_{max,p} c_{ex} - k_{L,p} s_{max,p}}{(1 + k_{L,p} c_p + k_{L,ex} c_{ex})^2}\right] \frac{\partial c_p}{\partial t} - \rho \frac{k_{L,p} k_{L,ex} s_{max,p} c_p}{(1 + k_{L,p} c_p + k_{L,ex} c_{ex})^2} \frac{\partial c_{ex}}{\partial t} = \nabla \cdot \left(D_{lp} \theta f \nabla c_p\right) - F_p \quad (6)$$

$$\left[\theta + \rho \frac{k_{L,p} k_{L,ex} s_{max,ex} c_p - k_{L,ex} s_{max,ex}}{(1 + k_{L,p} c_p + k_{L,ex} c_{ex})^2}\right] \frac{\partial c_{ex}}{\partial t} - \rho \frac{k_{L,p} k_{L,ex} s_{max,ex} c_{ex}}{(1 + k_{L,p} c_p + k_{L,ex} c_{ex})^2} \frac{\partial c_p}{\partial t} = \nabla \cdot \left(D_{lex} \theta f \nabla c_{ex}\right) - k_{dec} \theta c_{ex} + F_{ex} \quad (7)$$

p Phosphate, ex exudate, ρ bulk density, k_L and s_{max} Langmuir sorption parameters, k_{dec} decomposition rate constant

Sink terms based on discrete root architecture model

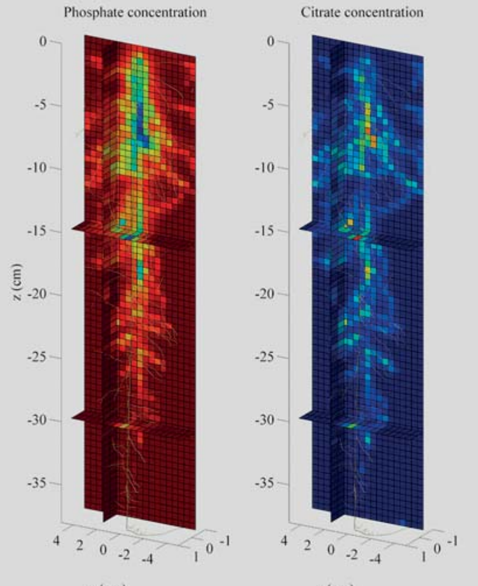
$$F_{p,V}(t) = \frac{1}{V} \sum_{s=1}^{N(t)} 2 r_s \pi l_s F_{p,s}(age) \tag{8}$$

$$F_{ex,V}(t) = \frac{1}{V} \sum_{s=1}^{N(t)} 2 r_s \pi l_s F_{ex,s}(age) \tag{9}$$

s segment index in V, $N(t)$ number of segements in V, F_{ex} efflux rate of exudate, $F_{p,s}$, F_p P influx into root segment, determined from an axisymmetric 1D model on single root scale, l_s segment length

$N(t)$ and l_s are results from a dynamic root architecture model.

Output


Phosphate concentration
Citrate concentration
z (cm)
0
-5
-10
-15
-20
-25
-30
-35
4
2
0
-2
-4
1
0
-1

Water flow in a 3D soil domain

$$\frac{\partial \theta}{\partial t} = \nabla \cdot \left(\frac{K}{\rho g} (\nabla \psi_m - \rho g e_z) - S \right) \tag{10}$$

$$S(t, V) = \frac{1}{V} \sum_{s=1}^{N(t)} q_{r,s} l_s \tag{11}$$

No-flux boundary conditions at top and bottom, homogeneous initial condition

ψ_m soil matric potential, K hydraulic conductivity tensor, ρ density of water, $\mathbf{e_z}$ unit vector pointing in z direction, S sink term for root water uptake

Water flow in a 1D root branching structure

$$\frac{\partial}{\delta\zeta} J_a = q_r \tag{12}$$

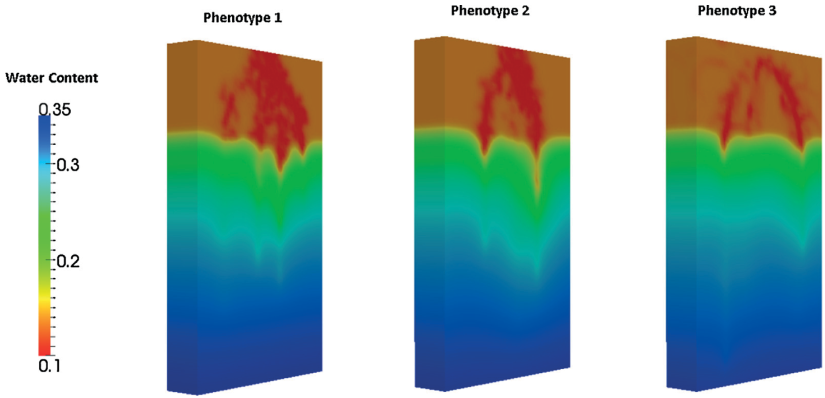
$$J_a = -K_a \left(\frac{\delta\psi_p}{\delta\zeta} - \rho g | \frac{\partial x_{root}}{\delta\zeta} |_z \right) \tag{13}$$

$$q_r = 2\pi r k_r \left(\psi_m \psi_p \right) \tag{14}$$

No-flux boundary conditions at the root tips and at the root collar a switch from Neumann to Dirichlet when stress occurs: $\begin{cases} J_a = T_{pot} & \text{if } \psi_{total} > \text{-1.5 MPa} \\ \psi_{total} = \text{-1.5 MPa} & \text{otherwise} \end{cases}$

ψ_p pressure potential in xylem, $\psi_t = \psi p + \rho g z$, ζ arc length along the root segment, $x_{root}(\zeta)$ corresponding position in Cartesian space, K_a axial hydraulic conductance, k_r radial conductivity

Output


Water Content
0.35
0.3
0.2
0.1
Phenotype 1
Phenotype 2
Phenotype 3

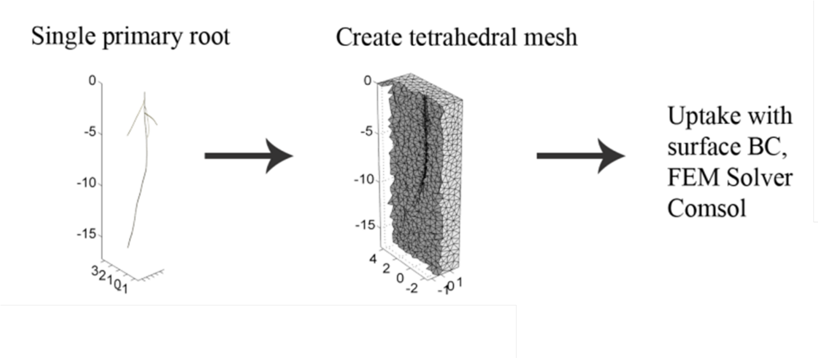
Non-equilibium in the rhizosphere

$$\frac{\partial \theta}{\partial t} = \nabla \cdot \left(K(\nabla h - 1) + (R-1)\frac{1}{\tau(\theta_M)}\left(h - h_{eq}(\theta_M)\right)\right) - S \qquad (15)$$

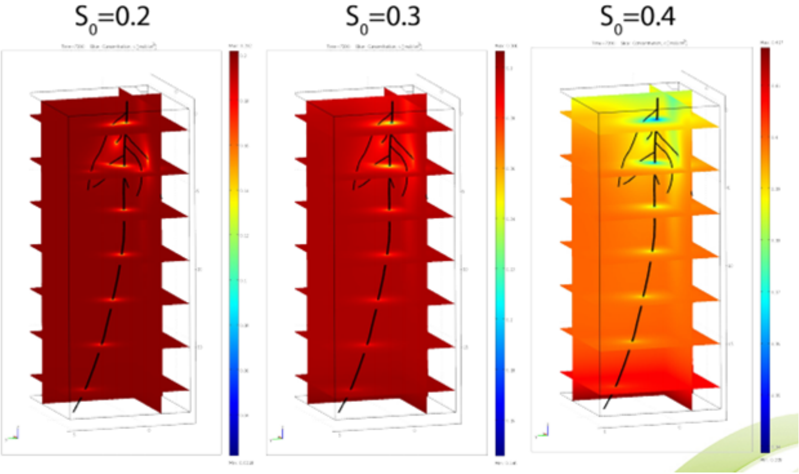
$$\frac{\partial \theta_M}{\partial t} = \frac{1}{\tau(\theta_M)}\left(h - h_{eq}(\theta_M)\right) \qquad (16)$$

R is the fraction of elementary soil volume influenced by mucilage, τ relaxation time, h_{eq} equilibrium pressure head in the rhizosphere, θ_m water content in the mucilage pore.

Water uptake by roots physically present in the domain



Sample results



Summary

- Our models can mostly be written in the general form $\mathbf{A}(\mathbf{U})\frac{\partial \mathbf{U}}{\partial \mathbf{t}} + \nabla \cdot \mathbf{F}(\mathbf{U}) + \mathbf{S}(\mathbf{U}) = \mathbf{0}$
- Solution-dependent sink term
- Sink term coupled to 1D geometry (root branching structure)
- Root systems are growing
- There can be small concentration gradients around the roots $\rightarrow$ upscaling approach or grid refinement