FORSCHUNGSZENTRUM JÜLICH

BAYER Science For A Better Life

Coupled root water and solute uptake – a functional structural model

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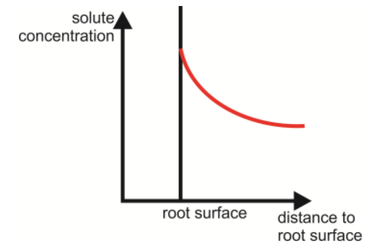
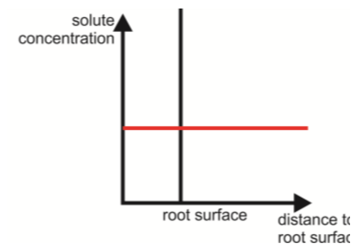
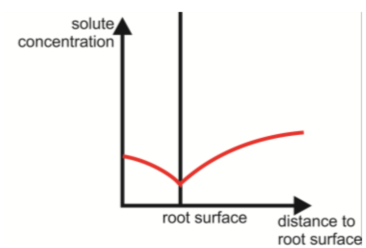
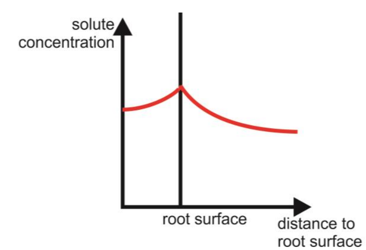
6 September, 2017

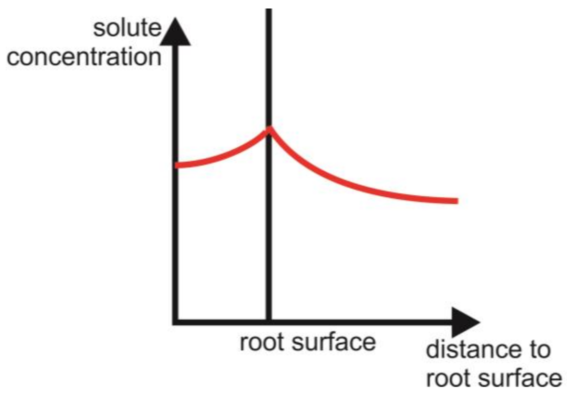
Motivation 1

Root solute uptake mechanisms:

Exclusion	$J_U = 0$	Salt	
Advective uptake (with transpiration stream)	$J_U = \varepsilon J_W C_S$	Nutrients Organic solutes	
Active uptake (Michaelis-Menten)	$J_U = (\frac{V_{max} C_S}{K_m + C_S})$	Nutrients Ions	
Diffusive uptake (gradient dependent)	$J_U = \frac{D}{\Delta x}(C_S - C_R)$	Organic solutes ➢ pesticides	

Motivation 1

Diffusive uptake



Challenge:
Simulate solute uptake of roots considering
- soil solute and root concentration
- with interaction and feedback between soil and root system.

Motivation 2

EU model for pesticide legislation

$$J_U = J_W * f * C_S \quad [M\ T^{-1}\ L^{-2}]$$

Uptake factor f:

$$TSCF = \frac{C_X}{C_S} \in [0,1][-] \quad \neq \quad PUF = \frac{C_{upt}}{C_s} \in [0,1][-]$$

- C_X: Solute concentration in plant shoot [M L^{-3}]
- C_S: Solute concentration in soil water [M L^{-3}]
- J_W: Root water flux [L T^{-1}]

- $C_{upt} = \frac{m_{upt}}{V_{upt}}$ [M L^{-3}]
- Experimentally determined with hydroponics
- Cumulative solute uptake

TSCF: Transpiration Stream Concentration Factor

PUF: Plant Uptake Factor

i.a. PEARL, Tiktak et al. 2015

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Is a constant factor sufficient to represent solute uptake processes?

- Solute characteristics
- Time dependency
- Root structure
- Application procedure
- Soil characteristics

Challenge: Gain an understanding of the dynamics and dependencies of root solute uptake and their representation by TSCF and PUF

Methods

Soil and root water flow and uptake

Soil

$$\frac{\partial\theta}{\partial t} = \nabla\cdot\left[\mathrm{K}(\theta)\,\nabla(h+z)\right] - S(x,y,z,t)$$

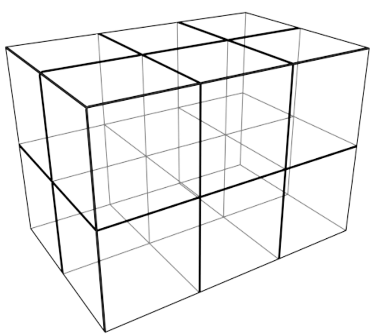
Richards 1931

Plant Root

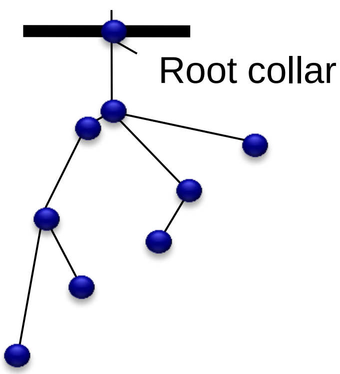
$$J_x = K_x^* A_x \frac{dH_x(z)}{dl}$$

$$J_R = K_R^* s_R\left[H_S(z) - H_X(z)\right]$$

Doussan et al. 2006



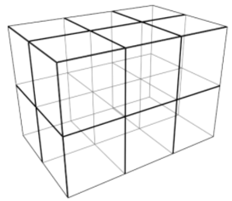
$$S = \frac{\sum_{i=1}^{n} J_{R,i}}{V_s}$$



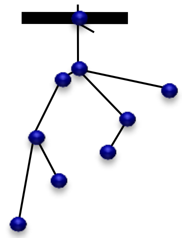
Javaux et al. 2008

Soil and root solute transport and uptake

Soil



Plant Root

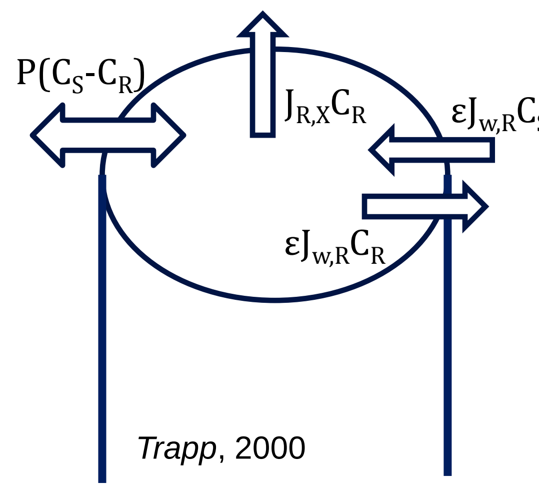


$$\frac{\partial(\theta_S + \rho_S K_{D,S})C_S}{\partial t} = \nabla \cdot (D\tau\theta_S \nabla C_S - \mathbf{J}_w C_S) - (\theta_S + \rho_S K_{D,S})k_S C_S + S_S$$

$$(\theta_R + \rho_R K_{D,R})\frac{\partial C_R}{\partial t} = \nabla \cdot (-\mathbf{J}_{w,R} C_R) - (\theta_R + \rho_R K_{D,R})k_R C_R + S_R$$

$$S_R = \frac{A_R}{V_R}\left(P(C_S - C_R) + \varepsilon J_{w,R} C_S\right)$$

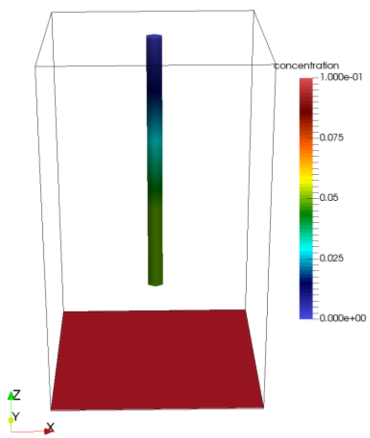
$$S_S = -\frac{\sum_{i=1}^{n} A_{R,i}\left(P(C_S - C_{R,i}) + \varepsilon J_{w,i} C_S\right)}{V_S}$$



Trapp, 2000

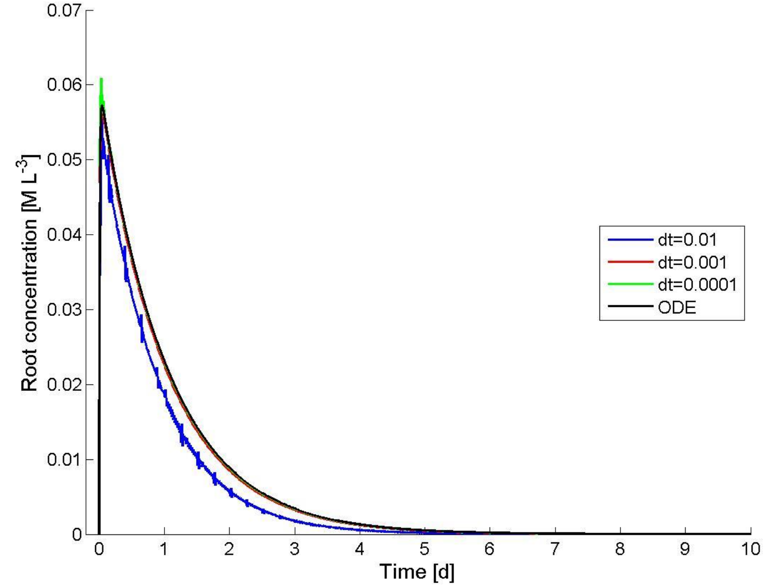
PARTRACE
Bechtold et al., 2011
Schröder et al., 2012

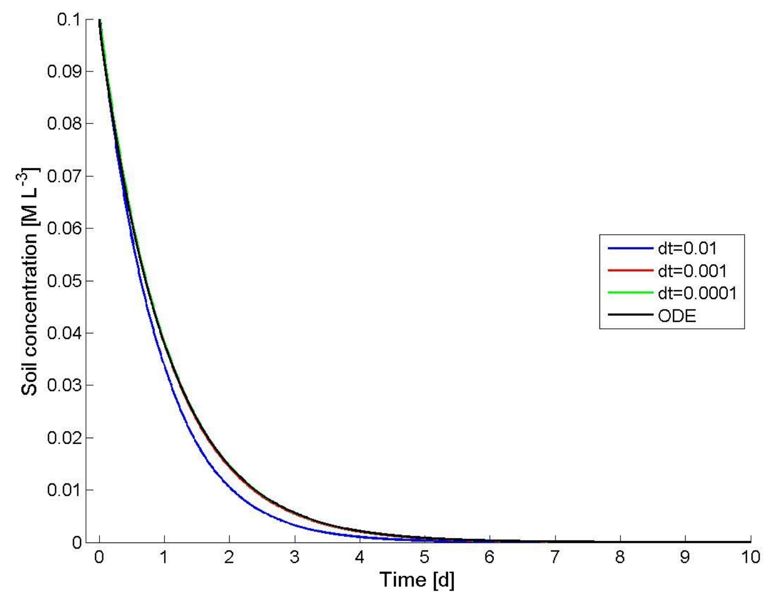
Benchmark scenario



Soil:
domain: 0.6 x 0.6 x 1 cm^3
$c_{S,ini}$ = 0.1 mg cm^{-3}
Prec = 0.067 cm^3 d^{-1}

Root:
l = 0.75 cm
P = 0.864 cm d^{-1}
T_{pot}= 0.067 cm^3 d^{-1}
$C_{R,ini}$= 0 mg d^{-1}





Sensitivity analysis

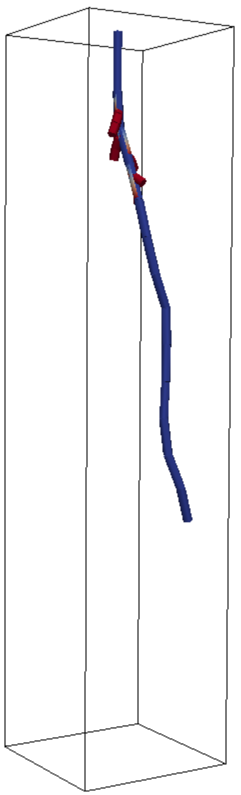
Soil:

- No flux boundaries
- No soil sorption
- $C_{S,ini}$ = 1 mg cm^{-3} at t=0
- domain: 2.25 * 2.25 * 10 cm³
  with Δx = Δy = Δz = 0.25 cm

Root:

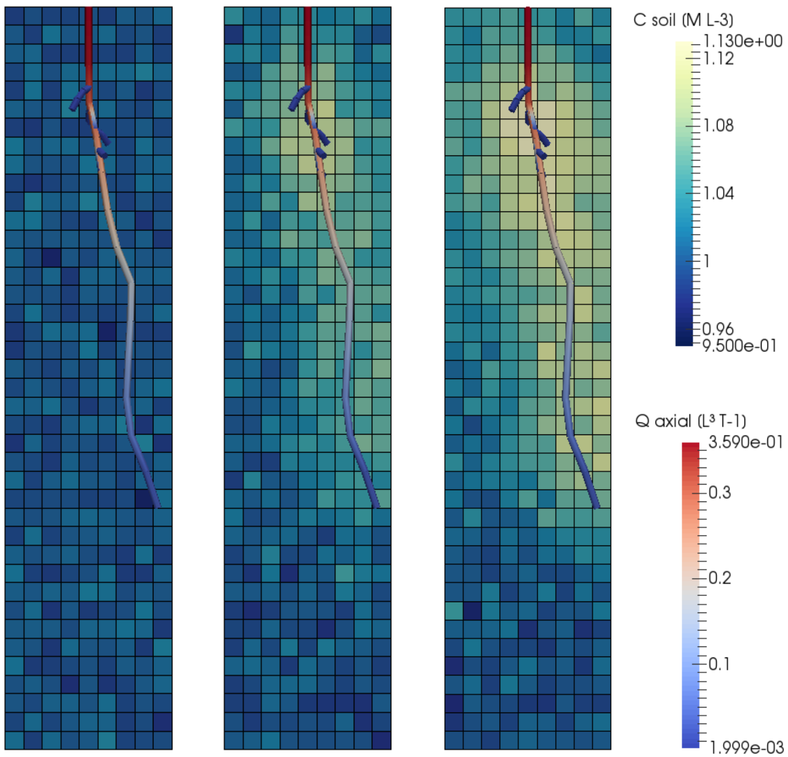
- Static root system (age 2 days)
- T_{pot} = 0.359 cm³ day^{-1}
- P = 5.62*10^{-2} cm day^{-1} (low permeability)
- No sorption in root system
- $C_{R,ini}$ = 0 mg cm^{-3} at t=0

- 2 days simulation time



Parametrization and results

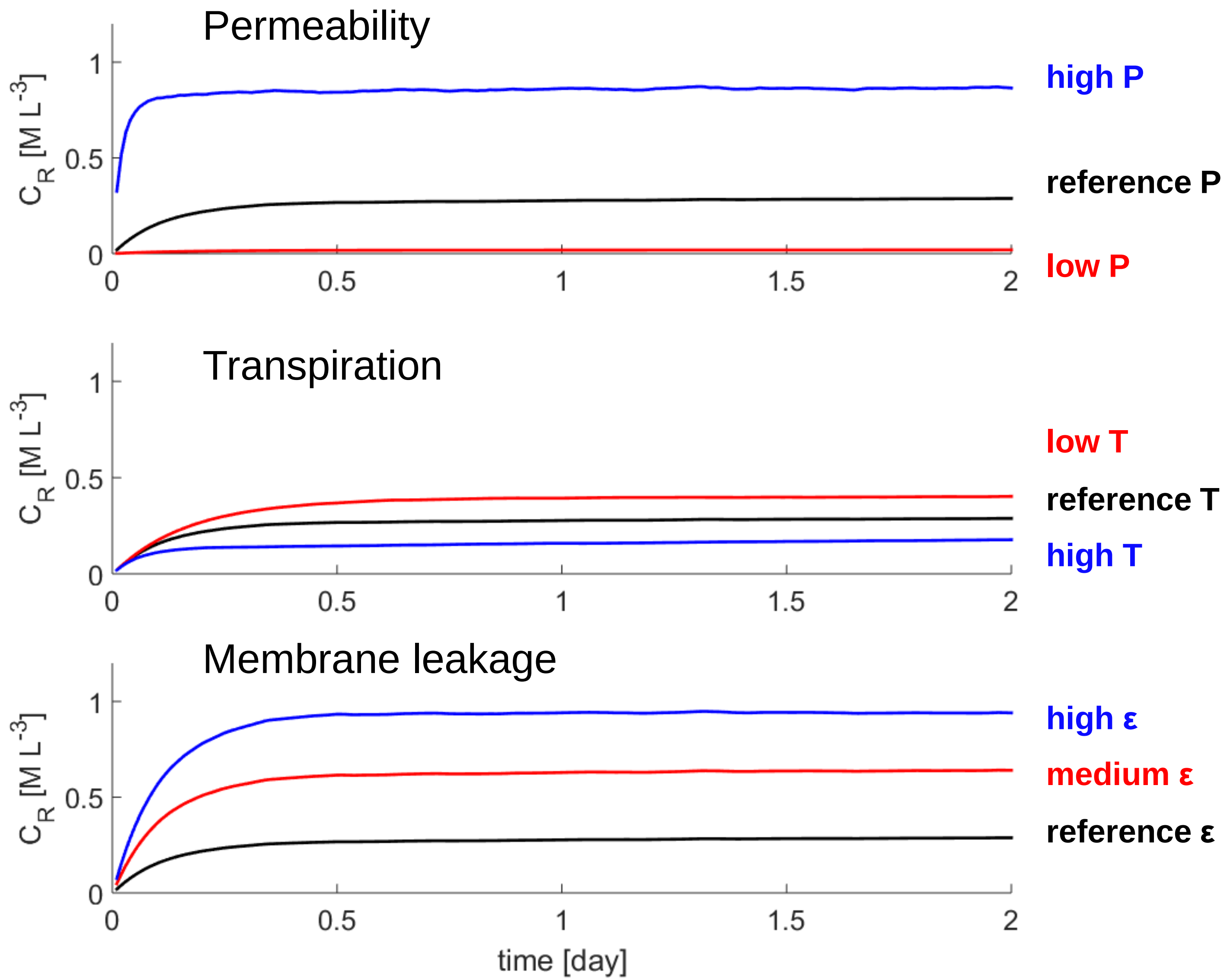
reference case



Day 0 Day 1 Day 2

	P [cm day^{-1}]	ε [-]	T_{pot} [cm³ day^{-1}]	
1	5.62e-2	0.0	0.359	reference
2	“	“	0.019	
3	“	“	0.868	
4	“	0.5	0.359	
5	“	1.0	“	
6	2.69e-3	0.0	“	
7	1.18	“	“	

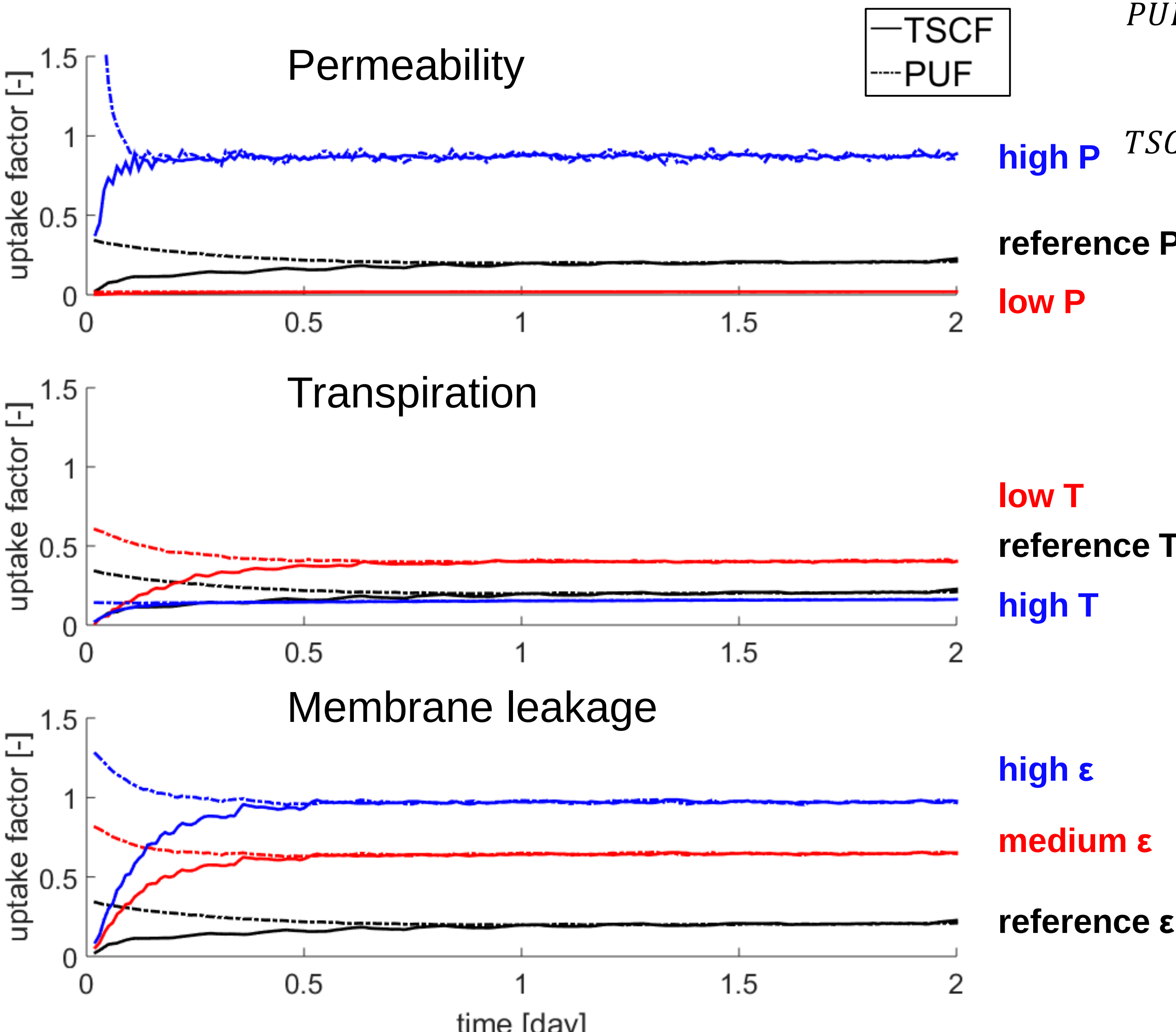
Results: root concentration



Results: uptake factors

$$PUF(t_i) = \frac{\sum_1^j m_{upt,i,j}/V_{upt,i}}{\overline{C_S}(t_i)}$$

$$TSCF(t_i) = \frac{\overline{C_X}(t_i)}{\overline{C_S}(t_i)}$$



Conclusion

- We implemented diffusive solute uptake as suggested by e.g. Trapp (2000) in a 3D multidimensional and dynamic root – soil model
- We are able to identify sensitive parameters (membrane permeability, transpiration, leakage factor) which influence the uptake and concentration of pesticides in root and soil
- We can relate the plant uptake factors to the transpiration rate and the root properties
- For the small system considered the uptake factors both reached a constant value
- Further studies with longer runtime, larger domains, more complex root systems, and more realistic boundary conditions will give a better indication how uptake factors vary in time and space or if a constant factor might be sufficient

Concentration gradients around the roots - 1D radially symmetric model

$$(\theta_R + \rho_R K_{D,R})\frac{\partial C_{R,f}}{\partial t} = \frac{A_R}{V_R}\left[P\left(C_{S,f} - C_{R,f}\right) + \varepsilon J_W C_{S,f}\right] - \frac{Q_x}{V_R} C_{R,f} - k_R \theta_R C_{R,f}$$

$$(\theta_S + \rho_S K_{D,S})\frac{\partial C_{S,f}}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r}\left(r D \tau \theta_S \frac{\partial C_{S,f}}{\partial r}\right) + \frac{r_0}{r} J_W \frac{\partial C_{S,f}}{\partial r} - k_S \theta_S C_{S,f}$$

boundary conditions

$$D\tau\theta_S \frac{\partial C_{S,f}}{\partial r} + J_W C_{S,f} = P\left(C_{S,f} - C_{R,f}\right) + \varepsilon J_W C_{S,f}$$

$$\frac{\partial C_{S,f}}{\partial_r} + \frac{r_0 J_W}{r D \tau \theta_S} C_{S,f} = 0$$

initial conditions at t=t_0

$$C_{R,f} = 0$$

$$C_{S,f} = C_{S,0,f}$$

Model setup

Soil:

- θ_S = 0.3 $cm^3\ cm^{-3}$
- D = 6.5E-6 $cm^2\ s^{-1}$
- $C_{S,0,f}$ = 1E-6 g cm^{-3}

Root flow:

- Q_X(low) = 1.27E-8 $cm^3 s^{-1}$
- Q_X(med) = 1.26E-7 $cm^3 s^{-1}$
- Q_X(high) = 5.67E-6 $cm^3 s^{-1}$

Solutes

- compound 1

  log K_{OW} = 0.8
  P_M = 1.64E-6 cm s^{-1} *[Lichtner and Cronshaw, 1986]*
  $K_{D,S}$ = 5.6E-2 $cm^3\ g^{-1}$
  $K_{D,R}$ = 5.03 $cm^3\ g^{-1}$ *[Trapp, 2000]*
- compound 2

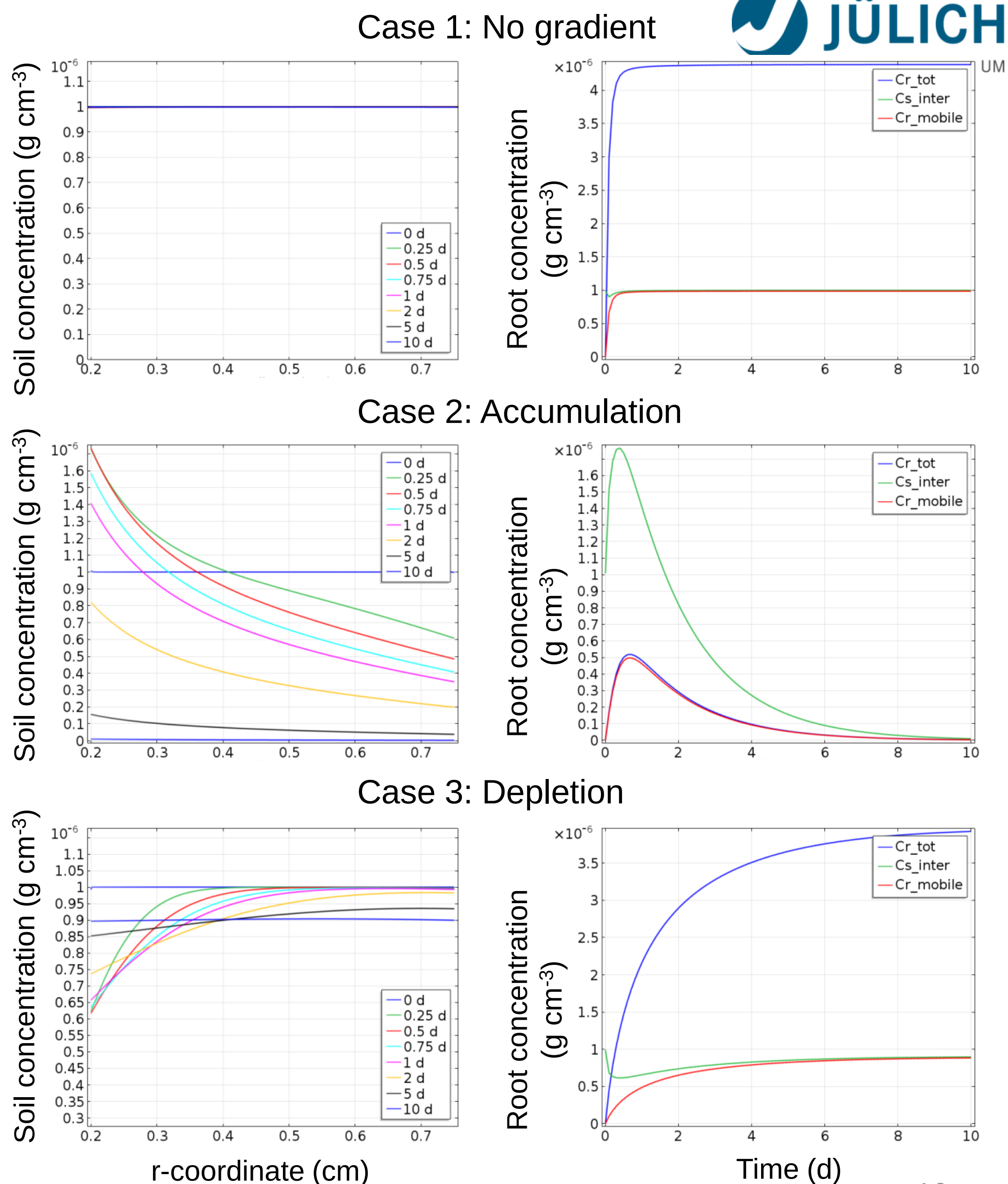
  log K_{OW} = 2.8
  P_M = 7.48E-6 cm s^{-1}
  $K_{D,S}$ = 2.33 $cm^3\ g^{-1}$
  $K_{D,R}$ = 174.73 $cm^3\ g^{-1}$

- Uptake by diffusion and advection: $\varepsilon = 0.05$
- BC root-soil interface: flux
- BC at r=r1: no flux
- 10 days of simulation

Results

Case	Compound	water uptake
1	2 (high $logK_{OW}$)	small
2	1 (low $logK_{OW}$)	high
3	2 (high $logK_{OW}$)	med

Case	Root solute uptake vs. soil solute transport	Solute sorption in roots
1	uptake ≈ transport	large
2	uptake < transport	small
3	uptake > transport	large



Conclusion

- Gradients develop within the first 0.5 cm
- This study can be used to estimate voxel discretization for numerical models
- Root-soil interface gradients cannot be neglected for all model parameterizations
- Different general types of gradients at the root-soil interface can be distinguished already by comparing the relevant model parameters.

Thank you!