Coupled root water and solute uptake – first applications of RoSI model to real-world scenarios

18 June 2018 / K. Hammel H.J. Guerra, A. Schnepf, J. Vanderborght, M. Javaux, K. Huber, C. Oberdörster, H. Vereecken

Introduction

Current model representations of root water and solute uptake often use simplified approaches (including regulatorily used models such as PEARL)

- spatially static root water uptake distribution
- no interaction between root and soil system
- lumped description of solute uptake (e.g. plant uptake factor PUF, transpiration stream concentration factor TSCF)

from the PEARL manual

$$R_{u,p} = R_{u,L}\, f_u\, c_L$$

with:

$R_{u,p}$ = volumetric mass rate of pesticide uptake, kg m^{-3} d^{-1}

$R_{u,L}$ = volumetric volume rate of water uptake, m^3 m^{-3} d^{-1}

f_u = transpiration stream concentration factor, -

Introduction

Yet advanced concepts are available which allow to describe the relevant processes more mechanistically

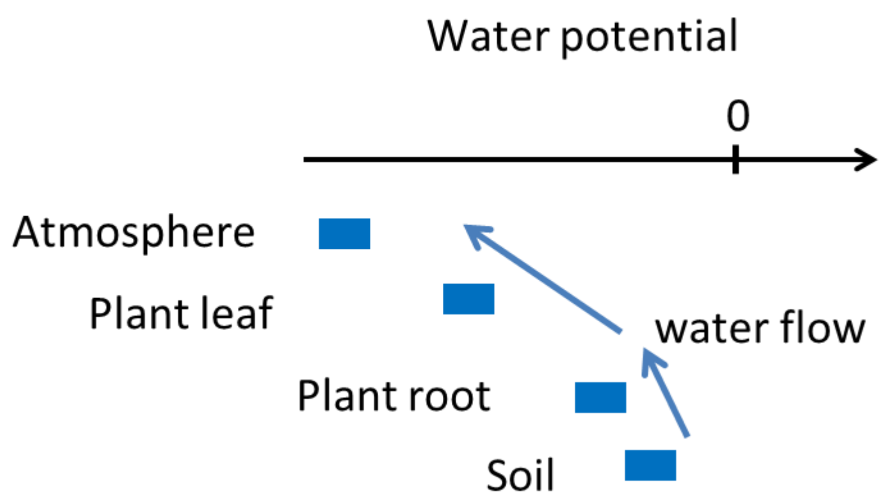
- roots as hydraulic system driven by water potential gradients
- interaction between root and soil system concerning growth and exchange of water and chemicals
- mechanistic description of root solute uptake
  - active uptake (Michaelis-Menten kinetic)
  - diffusive uptake via bio-membranes (solubility-diffusion theory, e.g. Trapp, 2004*)
  - advective uptake (membrane leakage)

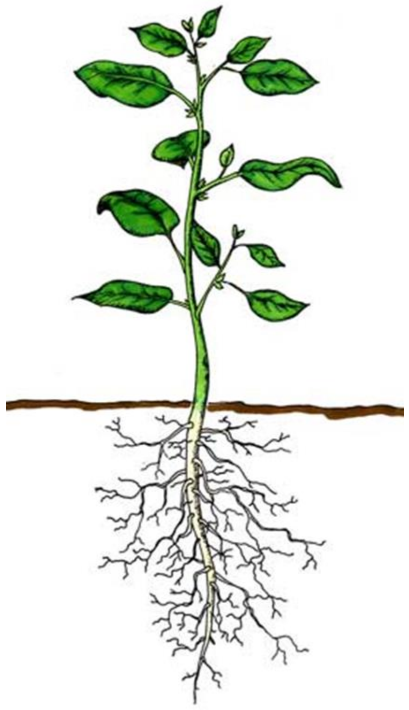
→ development of the RoSI** model based on the existing R-SWMS model at Forschungszentrum Jülich in collboration with Bayer AG

*Trapp, S. 2004. Plant Uptake and Transport Models for Neutral and Ionic Chemicals. Environ Sci & Pollut Res 11 (1) 33 – 39
**www.rosi.science

Root water uptake

Soil plant atmosphere continuum





Water transport through plants driven by water potential gradients and root hydraulic conductivities

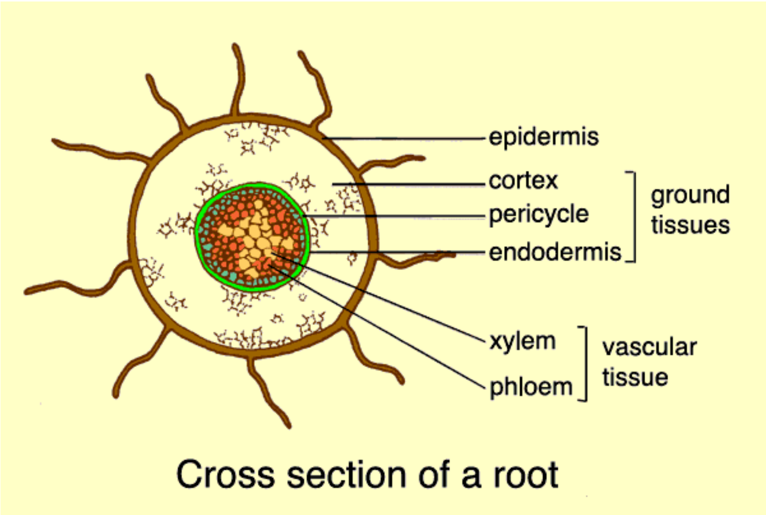
- „Automatic" adjustment of water uptake over the root system due to local soil water availability and local root hydraulic conductivity
- Hydraulic redistribution possible

Diffusive uptake

Membrane permeability P and solute uptake

$$P = K \cdot D / \Delta x$$

K partition coefficient membrane /water (usually approximated by Kow)
D diffusion coefficient across membrane
Δx membrane thickness
→ permeability is essentially a function of lipophilicity (and molar weight)

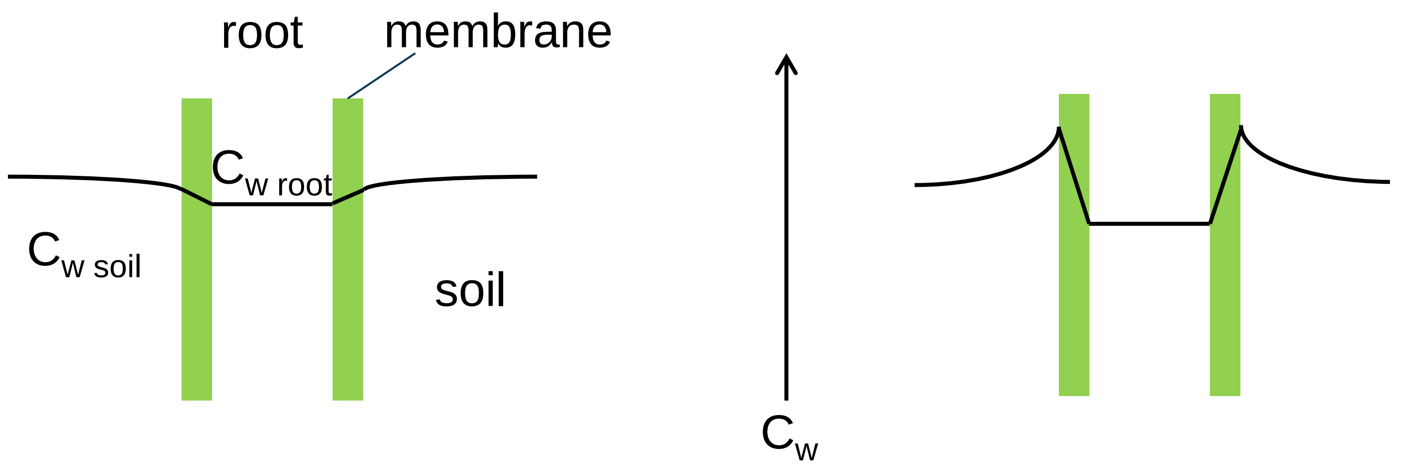


$$j_{up} = P \cdot (C_{w\ soil} - C_{w\ root})$$

C_w concentration in liquid phase
j_{up} solute flux across interface soil-root
→ solute flux can be in both directions
driven by concentration gradient

Diffusive uptake

High and low membrane permeability of chemical



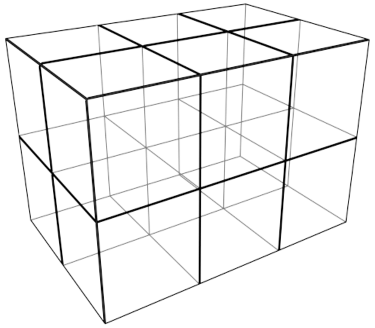
high permeability
- substance taken up as fast as water
- small gradients

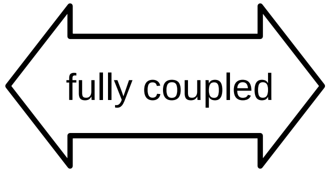
low permeability
- substance taken up slower than advective uptake
- larger gradients
- accumulation in rhizosphere

RoSI Model

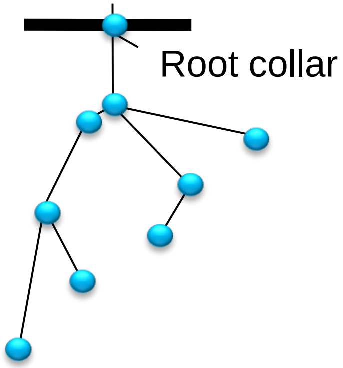
RoSI is a further development of the RSWMS software

Soil





Plant Root



Soil water flow and solute transport

- 3-D Richards equation and convection-dispersion
- Freundlich sorption and first order decay

Numerical implementation of solute transport

- particle tracking in both soil and root (to be able to handle steep gradients)
- coupling of both systems is complex and numerical implementation is a challenge

Representation of root by discrete segments

- different hydraulic conductivites axial/radial and young/old roots
- growth
- advective solute transport, adsorption, and first order decay

Simulations I

Exploration of effective parameters for plant uptake (PUF, TSCF) as used in 1-D regulatory models (e.g. PEARL)

$$j_{up} = j_w \cdot f \cdot C_{w\ soil}$$

Uptake factor f

$$TSCF = C_x / C_{w\ soil} \neq PUF = C_{upt} / C_{w\ soil}$$

- C_X solute concentration in plant shoot
- j_w root water uptake flux
- $C_{upt} = \frac{m_{upt}}{V_{upt}}$ ratio of cumulative mass to cumulative water volume uptake
- PUF plant uptake factor
- TSCF transpiration stream concentration factor

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

Simulations I

Parameterisation

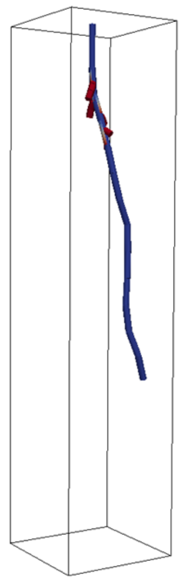
Soil:

- no flux boundaries
- no soil sorption
- $C_{w\ soil,\ ini} = 1\ mg\ cm^{-3}$ at $t = 0$
- domain: $2.25 * 2.25 * 10\ cm^3$
  with $\Delta x = \Delta y = \Delta z = 0.25\ cm$

Root:

- static root system (age 2 days)
- $T_{pot} = 0.71\ mm\ day^{-1}$
- $P = 5.62*10^{-2}\ cm\ day^{-1}$ (low permeability)
- no sorption in root system
- $C_{w\ root,\ ini} = 0\ mg\ cm^{-3}$ at $t = 0$

- 2 days simulation time



Uptake processes:

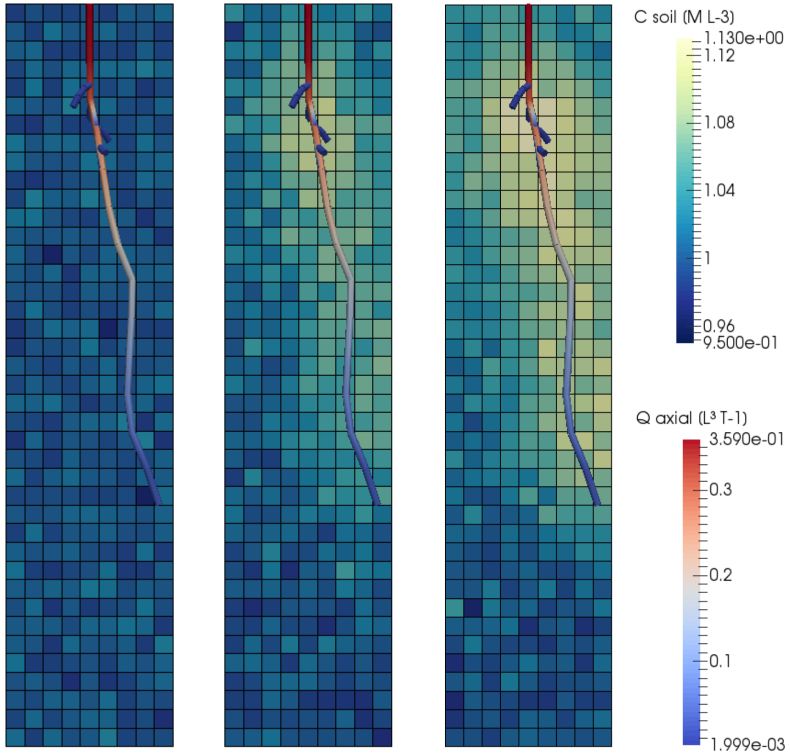
- diffusive and via membrane leakage with leakage factor ε

$$j_{up} = P \cdot (C_{w\ soil} - C_{w\ root}) + j_w \cdot \varepsilon \cdot C_{w\ soil}$$

Simulations I

Results for reference case and parameter combinations studied

reference case



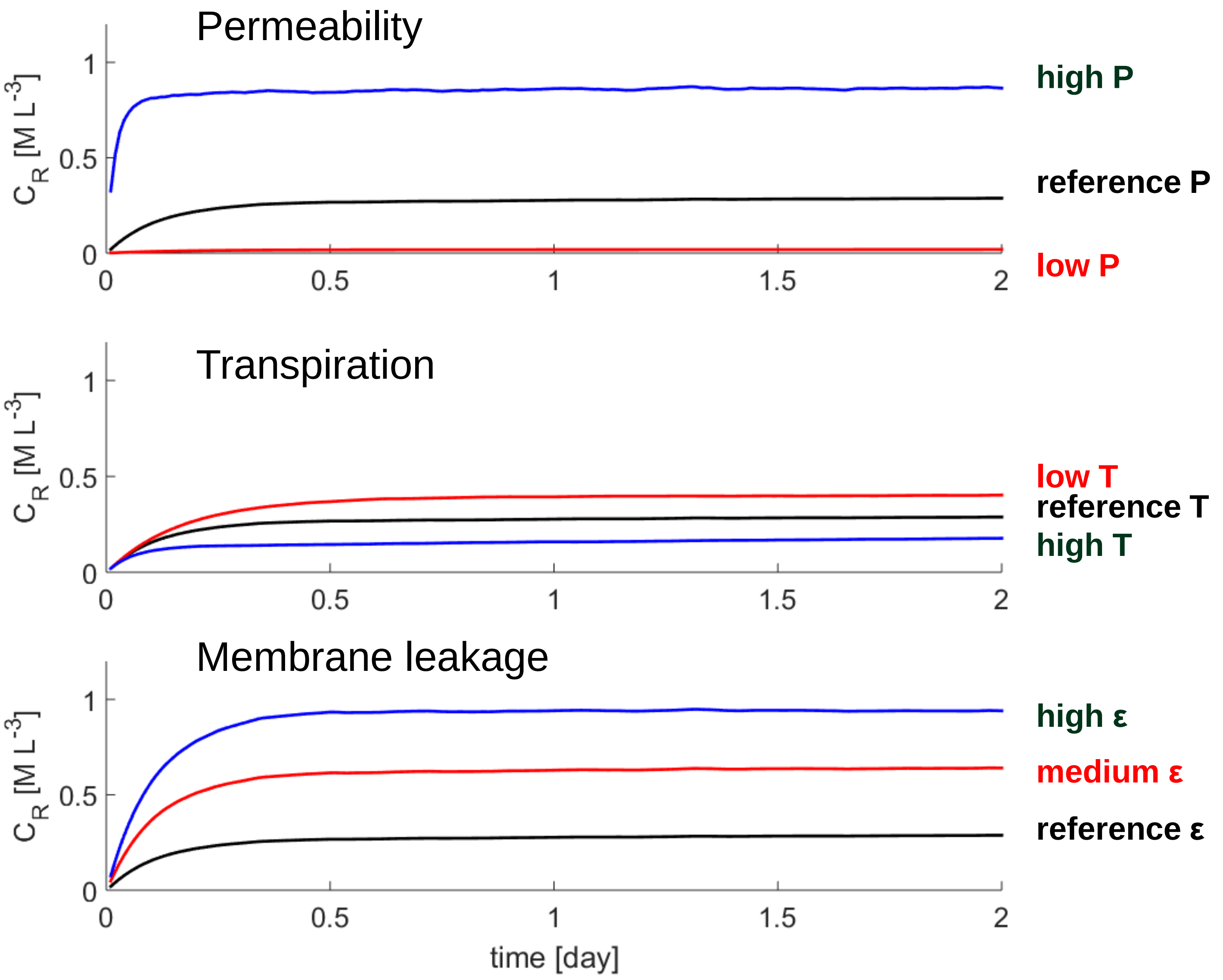
Day 0 Day 1 Day 2

	P [cm day^{-1}]	ε [-]	T_{pot} [mm day^{-1}]
1	5.62e-2	0.0	0.71
2	"	"	0.04
3	"	"	1.71
4	"	0.5	0.71
5	"	1.0	"
6	2.69e-3	0.0	"
7	1.18	"	"

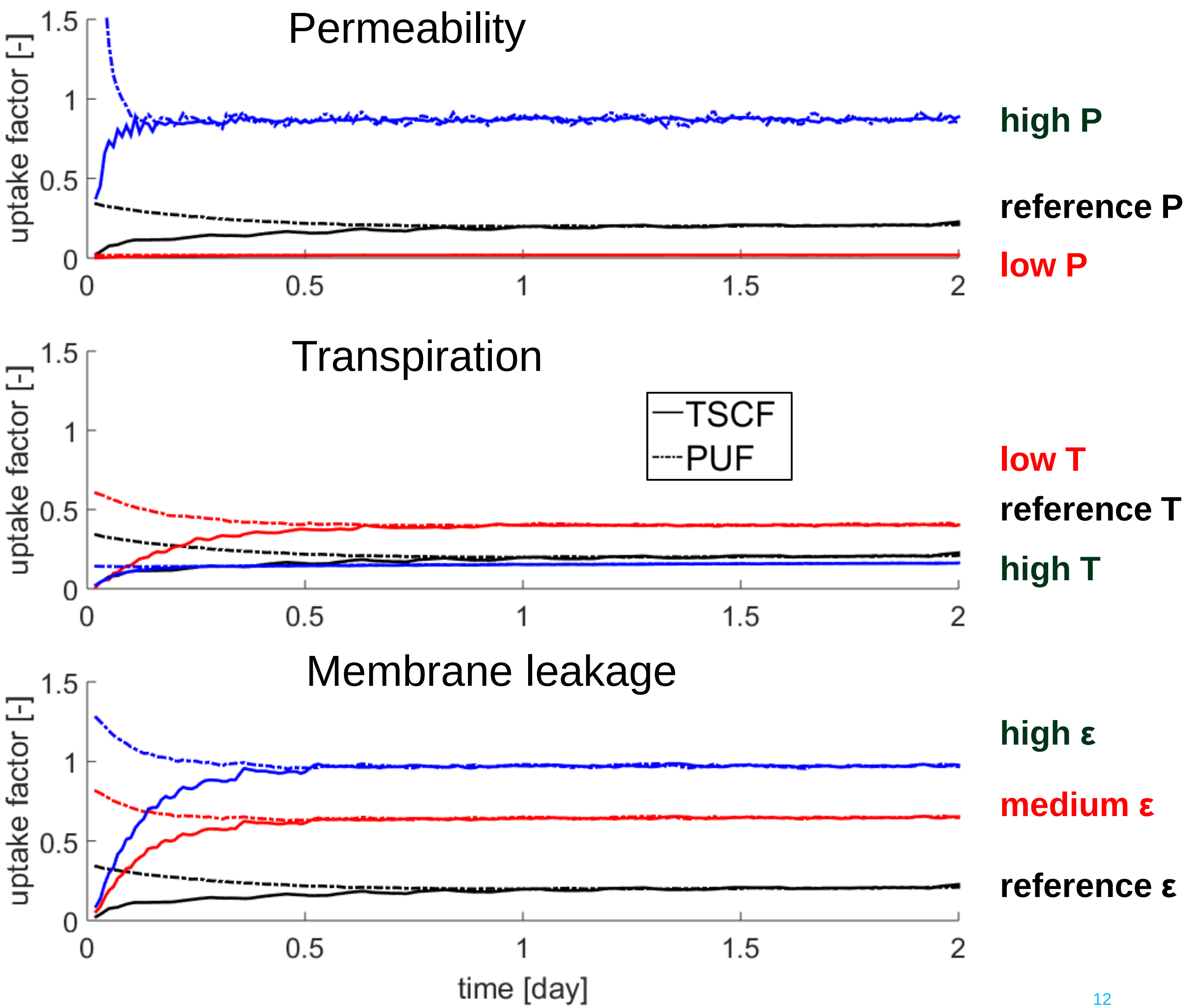
reference

Simulations I

Concentrations in root ($C_R = C_{w\ root}$)



Simulations I



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

$$TSCF(t_i) = \frac{C_X\,(t_i)}{\overline{C_{w\,soil}}(t_i)}$$

C_X taken at root collar

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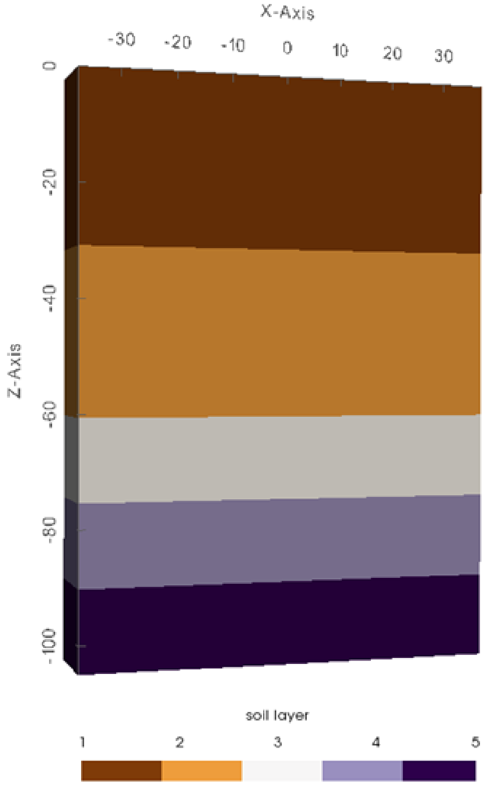
Simulations II

First simulations using the FOCUS groundwater scenario Hamburg with dummy compound B, maize crop



Depth	θ_s	θ_r	α	n	m	K_{sat}	λ	ρ_S	OC	K_D*
cm	$m^3\ m^{-3}$	$m^3\ m^{-3}$	m^{-1}	-	-	$*10^{-6}\ m\ s^{-1}$	-	$g\ cm^{-3}$	%	$cm^3\ g^{-1}$
Hamburg										
0-30	0.391	0.036	1.491	1.468	0.3188	23.33	0.5	1.5	1.5	1.545
30-60	0.370	0.030	1.255	1.565	0.3610	31.67	0.5	1.6	1.0	1.030
60-75	0.351	0.029	1.808	1.598	0.3742	28.33	0.5	1.56	0.2	0.206
75-90	0.310	0.015	2.812	1.606	0.3773	28.33	0.5	1.62	0	0.0
90-105	0.310	0.015	2.812	1.606	0.3773	28.33	0.5	1.6	0	0.0

	Planting	Emergence	Senescence	Harvest	Root depth
	dd/mm (doy)	dd/mm (doy)	dd/mm (doy)	dd/mm (doy)	m
Hamburg	20/04 (110)	05/05 (125)	21/08 (234)	20/09 (264)	1.0

Root properties for solute uptake

Parameter	Unit	Value
Lipophilicity *	$\log K_{OW}$ [-]	1.41
Permeability **	P [cm/day]	13.44
Lipid content **	L [$M\ M_R^{-1}$]	0.02
Water content **	θ_R [$cm^3\ cm^{-3}$]	0.942
Advective uptake fraction **	ε [-]	0.05
Root sorption coefficient **	$K_{D,R}$ [$cm\ g^{-1}$]	0.298

***Seth *et al.* (1999), **Trapp (2000)**

> high P (1.18 cm/d in simulation 1)

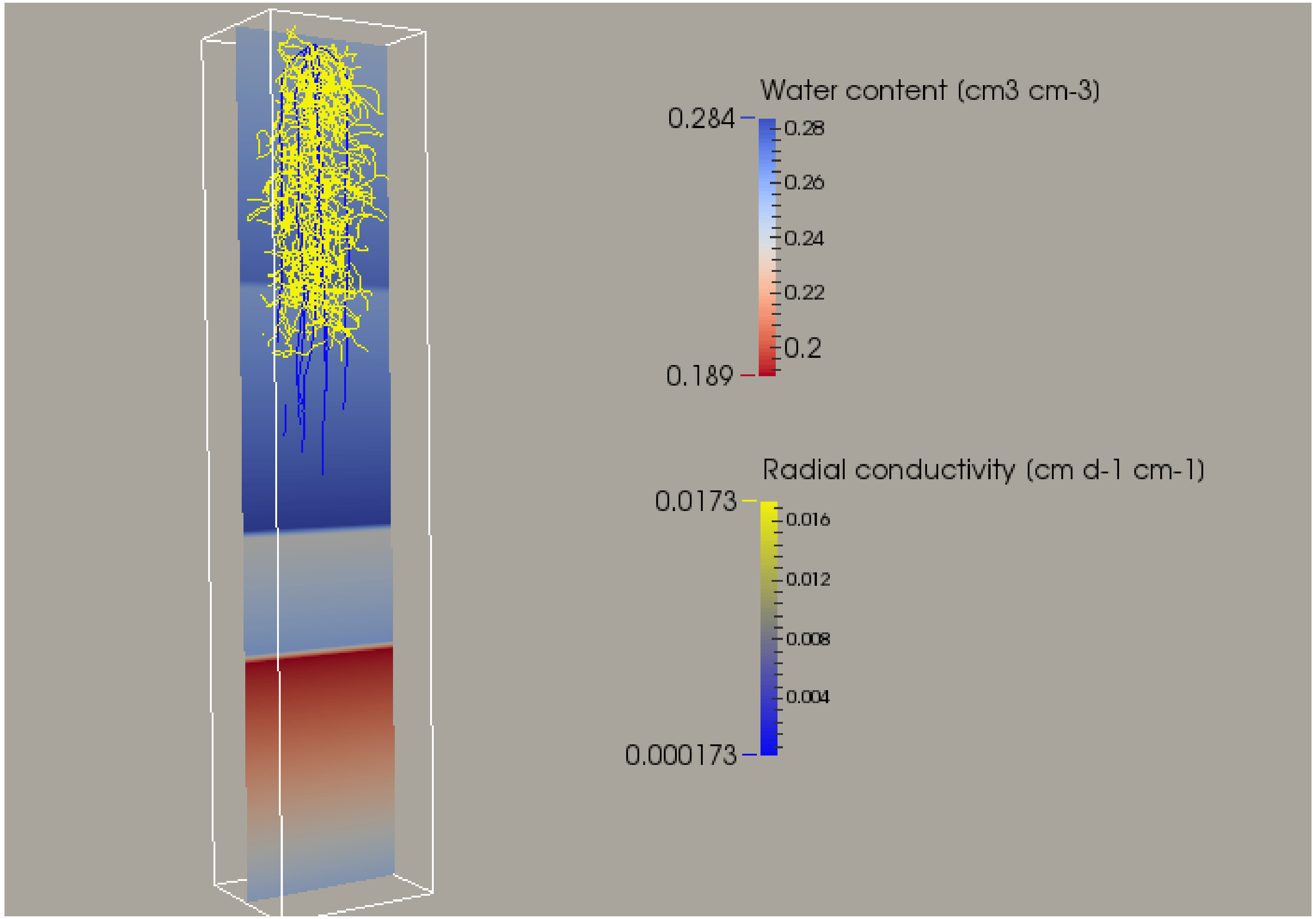
Simulations II

Root hydraulic properties

Maize root system			
Radial conductivity ($cm\ d^{-1}\ cm^{-1}$)	Age 0 - 10 days	Age 10-16 days	Age >16 days
1st order roots	0.00181	0.00181-0.000173	0.000173
2nd order roots	0.181	0.181 - 0.0173	0.0173
3rd order roots	0.181	0.181 - 0.0173	0.0173
Axial conductivity ($cm^4\ d^{-1}\ cm^{-1}$)	Age 0 - 10 days	Age 10 - 16 days	Age >16 days
1st order roots	0.0432	0.0432	0.0432
2nd order roots	0.0432	0.0432	0.0432
3rd order roots	0.0432	0.0432	0.0432

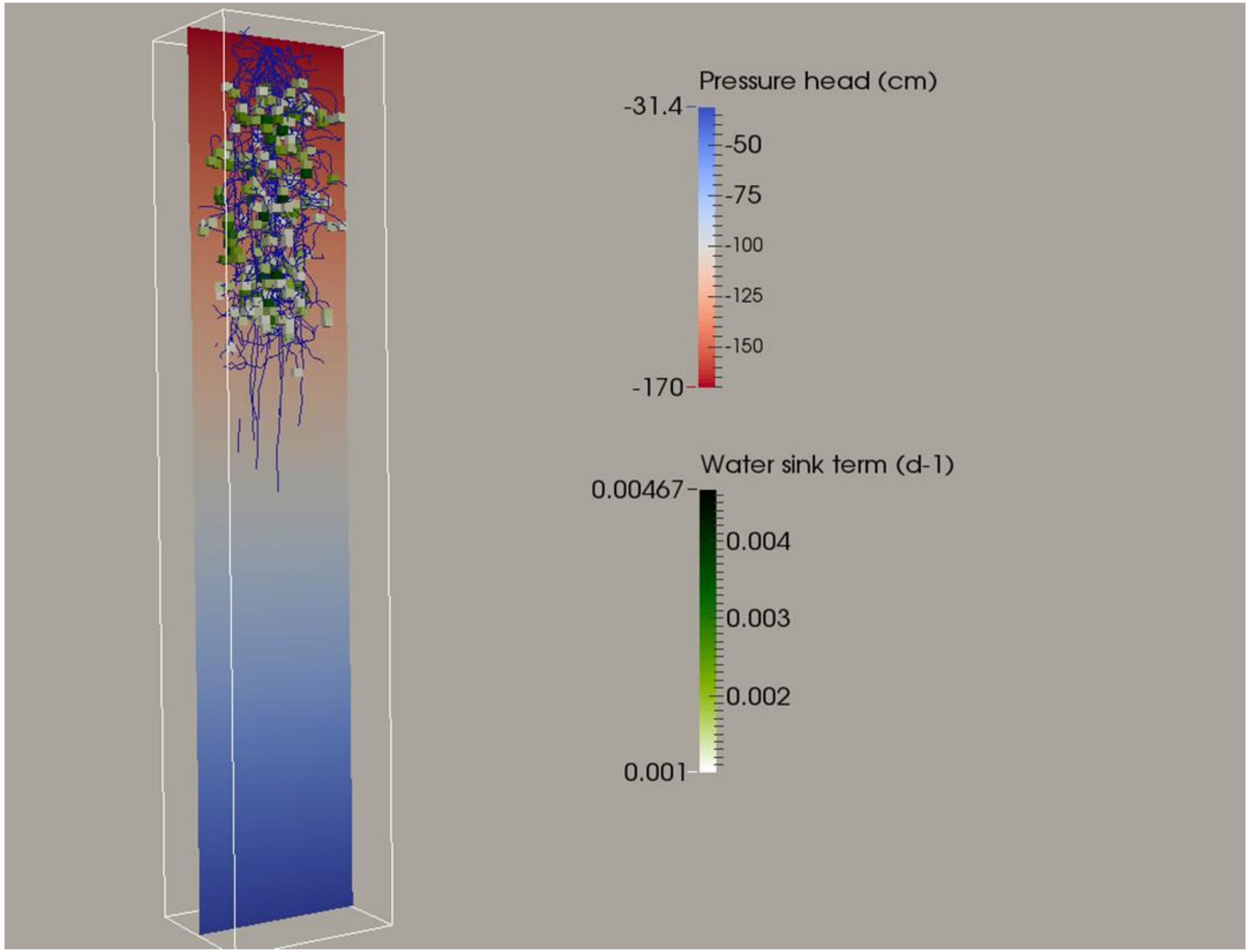
Simulations II

Results for water content and radial conductivity



Simulations II

Results for pressure head and water uptake



Simulations II

Results on solute transport

.... currently under evaluation

Summary and Conclusion

- We implemented diffusive solute uptake as suggested by e.g. Trapp (2000) in a 3D multidimensional and dynamic root – soil model
- It could be shown that for a small, quasi-static system comparable to the situation in a hydroponic test system both uptake factors, PUF and TSCF reached a constant value after relatively short time
- The values of PUF and TSCF obtained were found to depend on membrane permeability and transpiration (and leakage factor)

Summary and Conclusion

- First simulations of a real-world scenario (FOCUS gw Hamburg) revealed a good reproduction of the soil hydraulic conditions and illustrated the ability of RoSI to model the spatially variable root water uptake of a realistic root system with root age/order dependent properties
- Next steps will be thorough evaluation and analysis of solute transport especially considering effective uptake factors and their behaviour
- ... and further applications over longer time-periods and with different compound properties, crops, and environmental scenarios

Thank you!

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