MECHANISTIC ROOT WATER AND PESTICIDE UPTAKE MODELING: SIMULATION EXAMPLES AND APPROACHES FOR PARAMETERIZATION AND VALIDATION.

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INTRODUCTION

- Description of a mechanistic model for water and pesticide uptake by roots.
- Simulation results
- Parameterization and validation of simulation models
- Derivation of simplified models

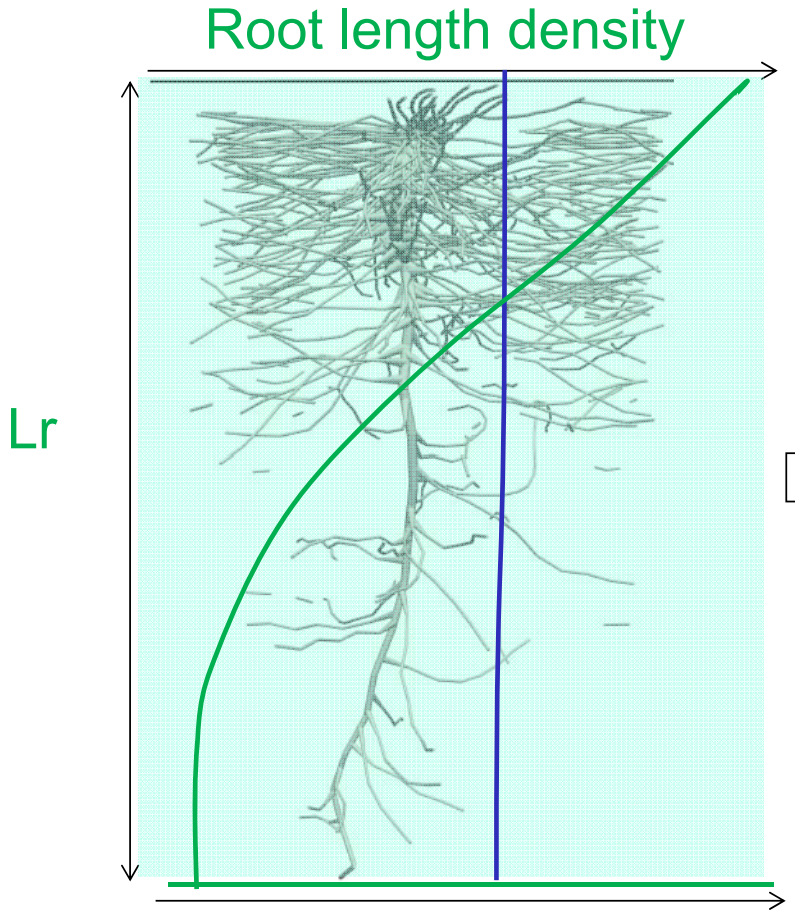
ROOT WATER UPTAKE AND SINK TERMS

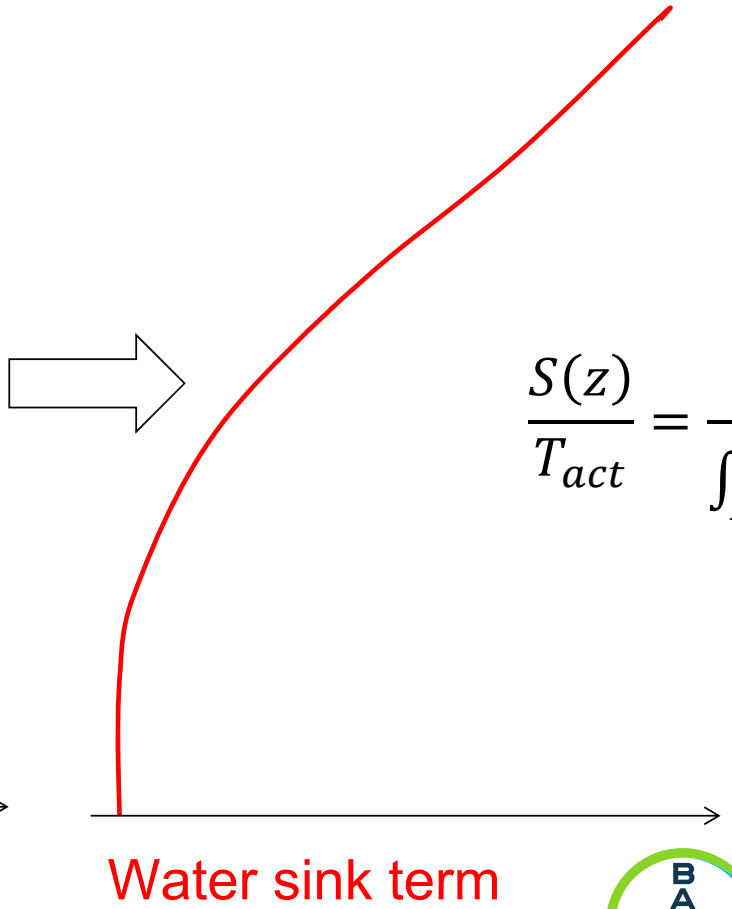
Basic equations

- Soil water balance: Leaching = Prec + Irr –T – E – ΔStorage
- Soil water balance $\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z}\left[K(\psi_s) \frac{\partial \psi_s}{\partial z} \right] - S_{water}(z,t)$
- Relation between transpiration and sink term $T_{act}(t) = \int_{L_r} S_{water}(z,t)dz$
- Relation between transpiration and soil water content/water potential:

$$T_{act} = T_{pot} f(\psi_s(z), T_{act})$$

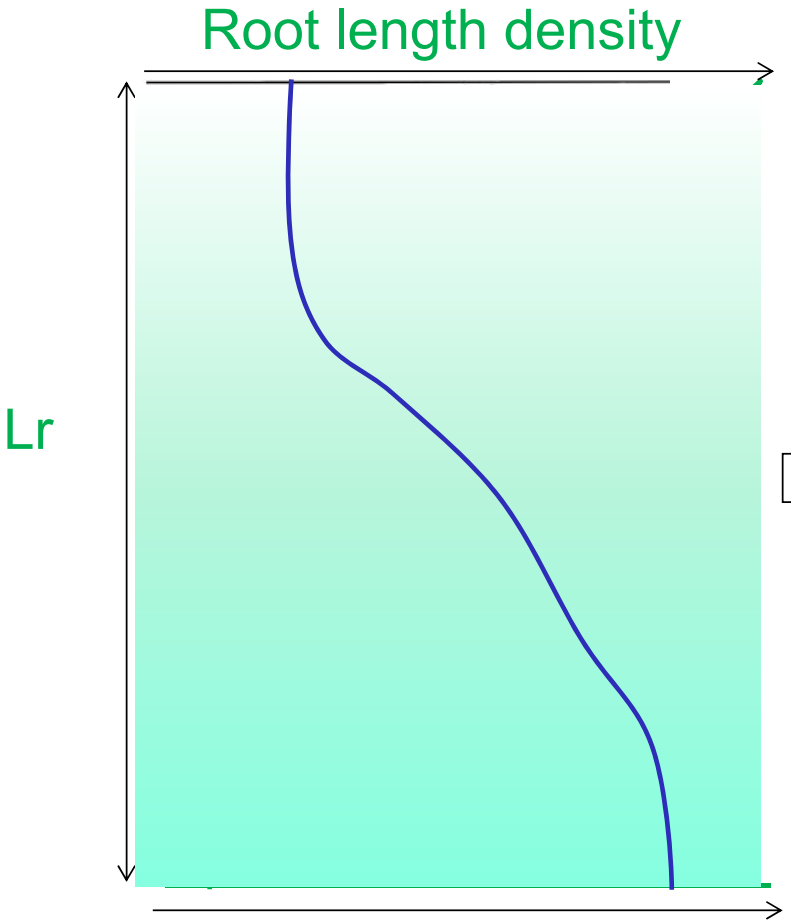
SINK TERM: UNIFORM WATER DISTRIBUTION

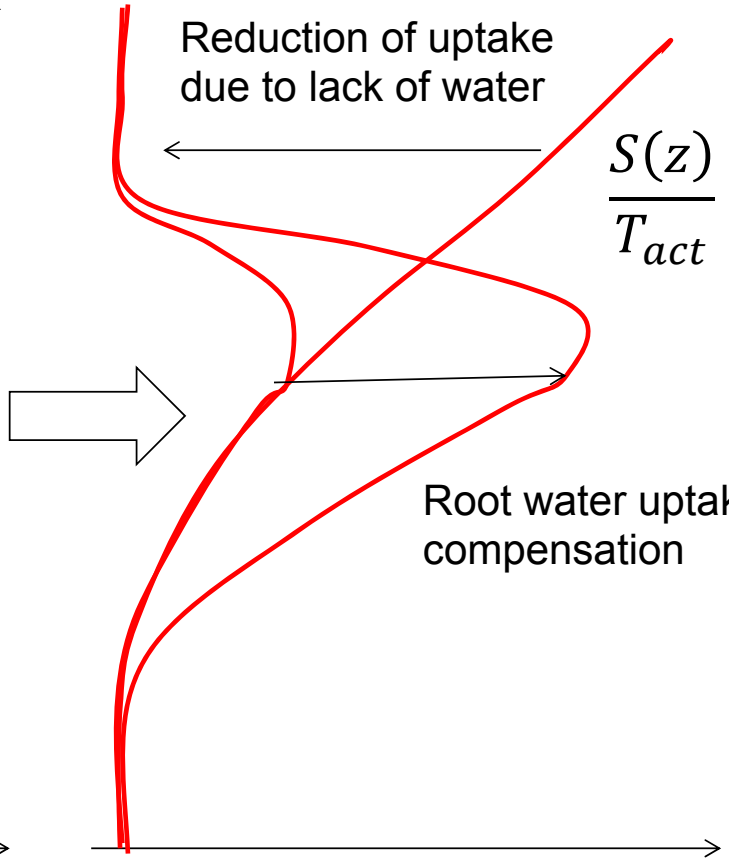




$$\frac{S(z)}{T_{act}} = \frac{rld(z)}{\int_{L_r} rld(z)dz}$$

SINK TERM: NON UNIFORM WATER DISTRIBUTION





$$\frac{S(z)}{T_{act}} = \frac{rld(z)}{\int_{L_r} rld(z)dz} f(\psi_s(z), T_{act})$$

PESTICIDE UPTAKE AND SINK TERMS

Basic equation

- Pesticide balance equation: $$(\theta + \rho_b K_d)\frac{\partial C}{\partial t} = -Jw\frac{\partial C}{\partial z} + \frac{\partial}{\partial z}\left(\theta D \frac{\partial C}{\partial z}\right) - \mu C - S_{pesticide}$$

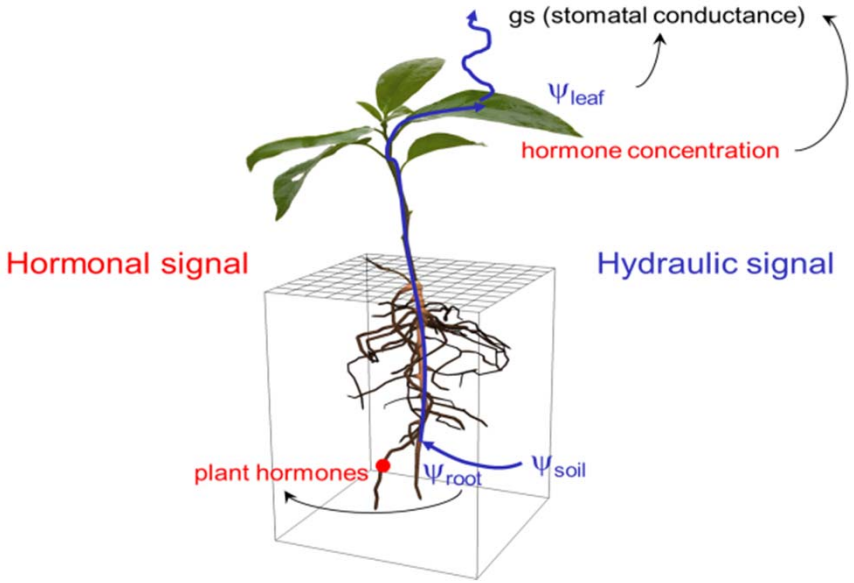
- Pesticide uptake by roots: $$S_{pesticide} = PUF\ C\ S_{water}$$

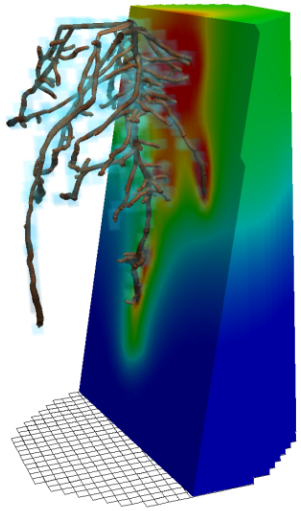
(PUF = Plant Uptake Factor)

- Total exclusion: PUF = 0
- Passive uptake with the water flow: PUF = 1

MECHANISTIC DESCRIPTION OF WATER UPTAKE

- Explicit representation of root architecture as a network of connected resistances.
- Simulation of flow and water potentials in this network
- Flow and potential in root segment network are coupled to the soil domain





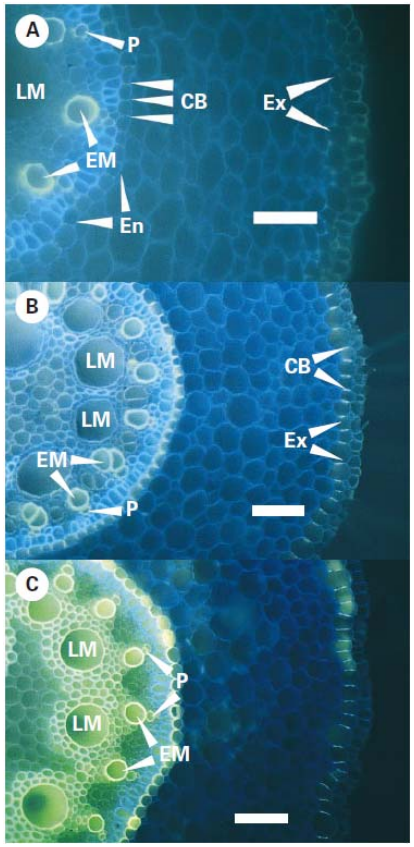
Input (parameters):

– Root architecture

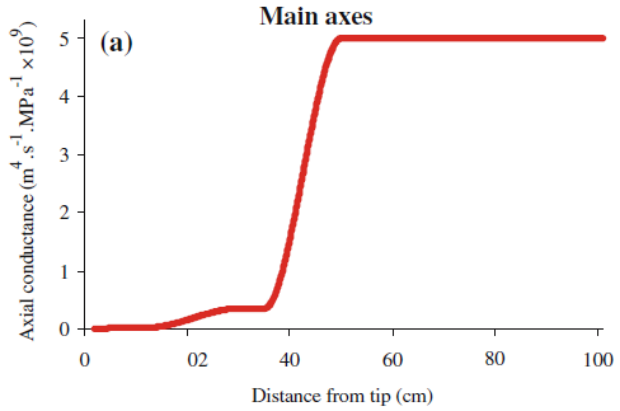
– Radial and axial root conductivity (as a function of root age and root order)

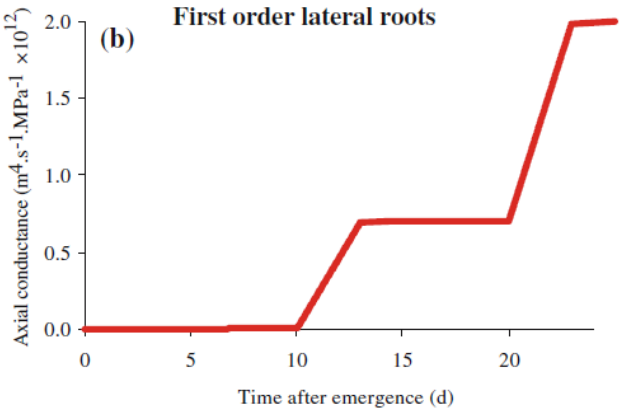
MECHANISTIC DESCRIPTION OF WATER UPTAKE

Root segment hydraulic properties



Steudle and Peterson, J Exp. Bot,1998





Pierret et al., Plant and Soil, 2006

MECHANISTIC DESCRIPTION OF WATER UPTAKE

Effect of root segment hydraulic properties on root water uptake from soil profile with uniform soil water potential

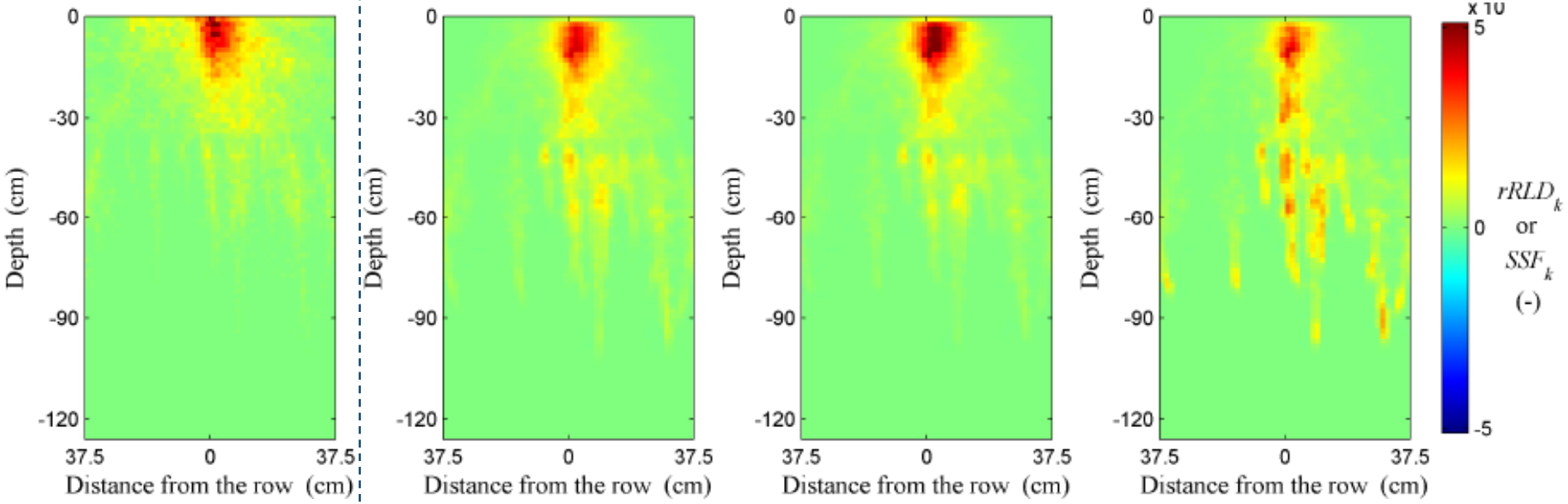
Root length density

Sink terms

Reference parameterization

Axial conductance of main root reduced by factor 10

Radial conductance of young roots increased by factor 10



Couvreur et al., 2012, HESS

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MECHANISTIC DESCRIPTION OF WATER UPTAKE

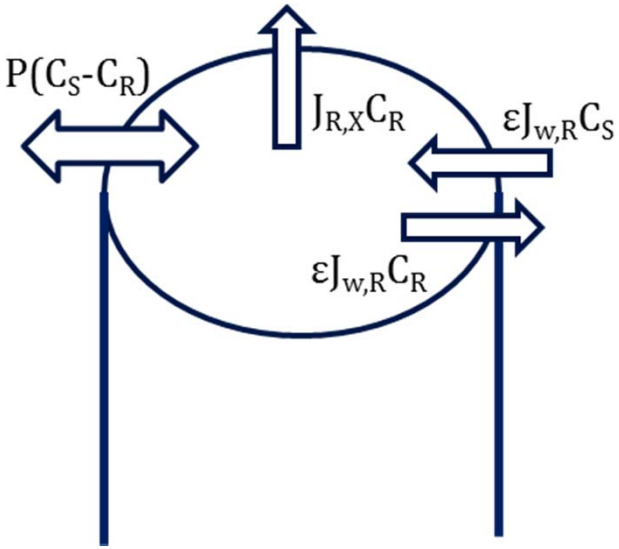
Simulation of root water uptake and water uptake compensation

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

- Hydraulic redistribution possible

Koebernick et al., 2015, Frontiers in Plant Sciences

MECHANISTIC DESCRIPTION OF PESTICIDE UPTAKE



Mechanism	Solute flux [M L^{-2} T^{-1}]	Example
Exclusion	$J_U = 0$	Salt
Passive – advection	$J_U = \varepsilon J_w C_S$	Nutrients, organic solutes (pesticides)
Passive – diffusion	$J_U = \frac{D}{\Delta x}(C_S - C_R)$	Organic solutes (pesticides)
Active uptake	$J_U = \frac{V_{max} C_S}{K_m + C_S}$	Nutrients, ions

Passive diffusive and advective (when water flux is from the root to the soil) uptake depend on root concentrations → concentrations in the root system must be simulated.

SIMULATION OF PESTICIDE UPTAKE

Small root system

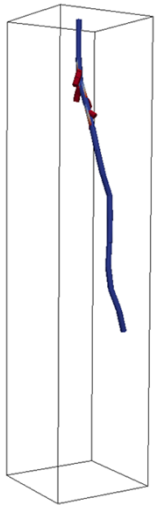
Soil:

- 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



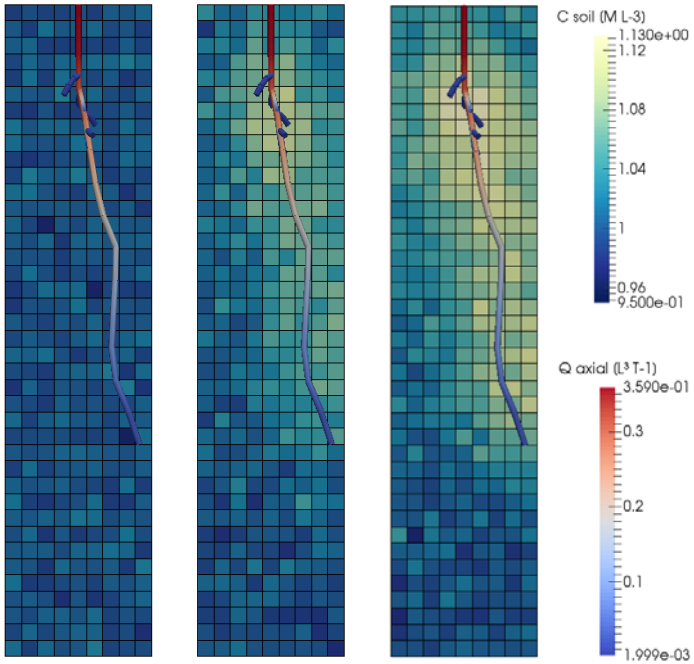
Uptake processes:

- diffusive and via membrane leakage

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

SIMULATION OF PESTICIDE UPTAKE

Small root system

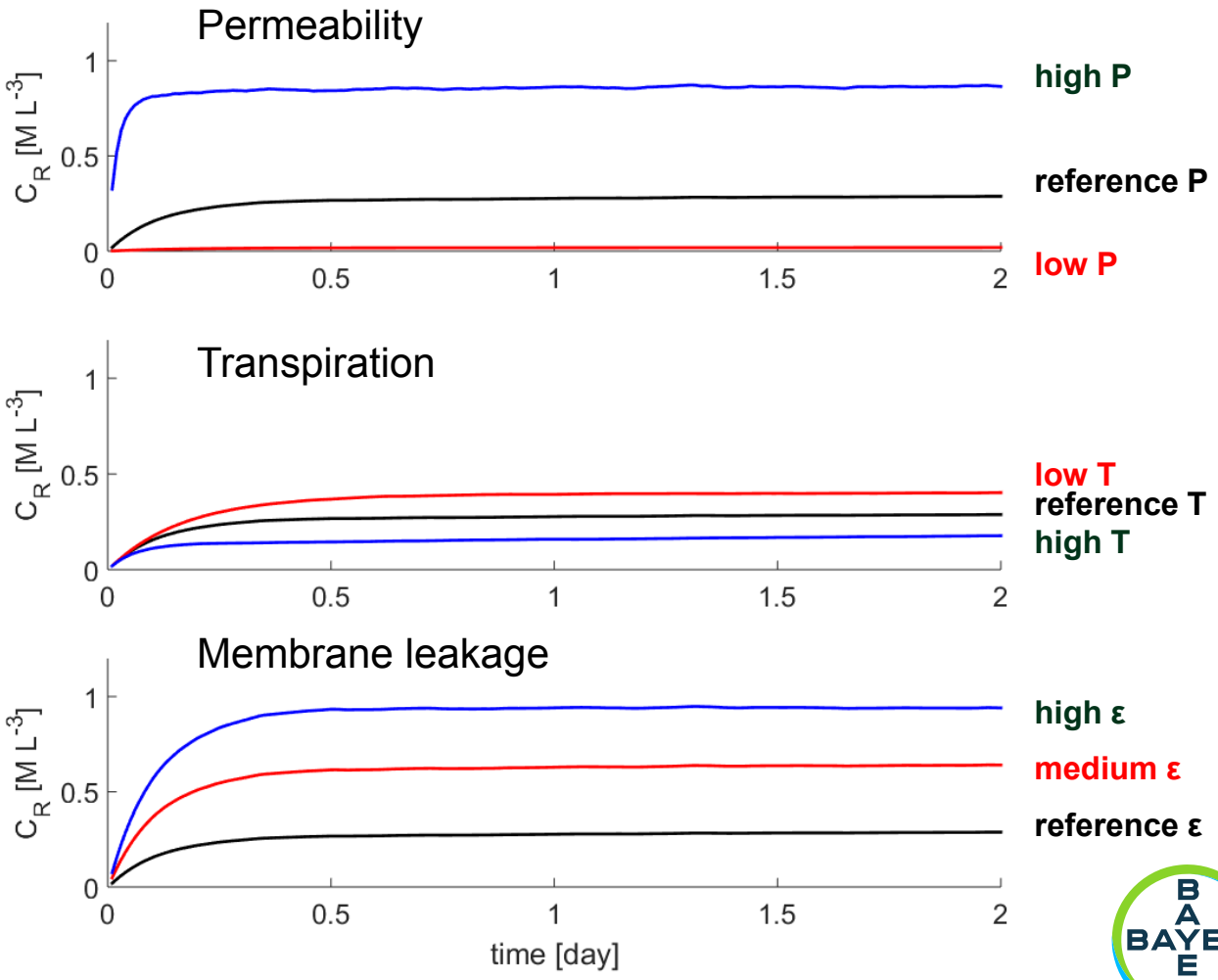


	P [cm day^{-1}]	ε [-]	T_{pot} [mm day^{-1}]
1	5.62e-2	0.0	0.71
2	"	"	0.04
3	"	"	1.71
4	"	0.5	0.71
5	"	1.0	"
6	2.69e-3	0.0	"
7	1.18	"	"

reference

SIMULATION OF PESTICIDE UPTAKE

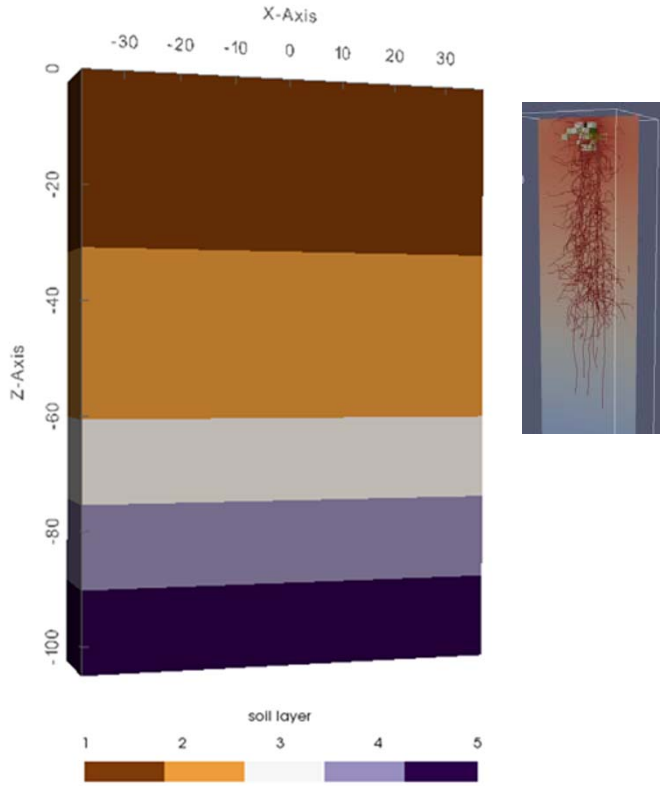
Small root system



SIMULATION OF PESTICIDE UPTAKE

Large root system

FOCUS groundwater scenario Hamburg with dummy compound B, maize crop



Root properties for solute uptake

Parameter	Unit	Value	
Lipophilicity *	$\log K_{OW}$ [-]	1.41	
Permeability **	P [cm/day]	13.44	> high P (1.18 cm/d in simulation 1)
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)**

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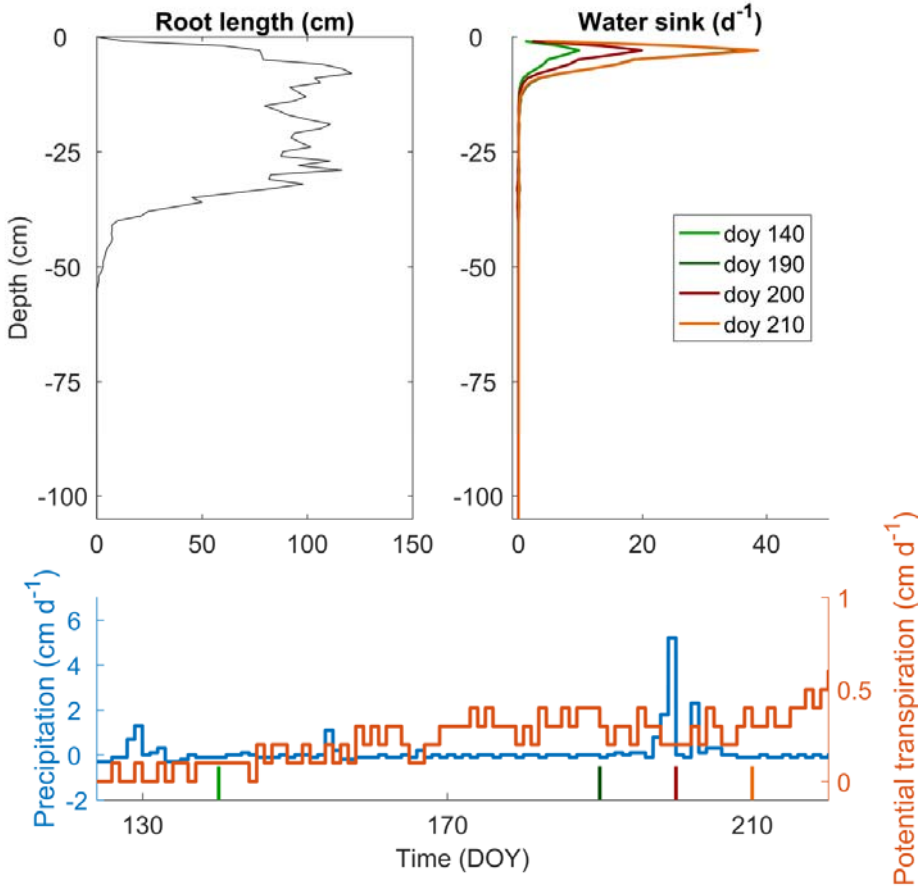
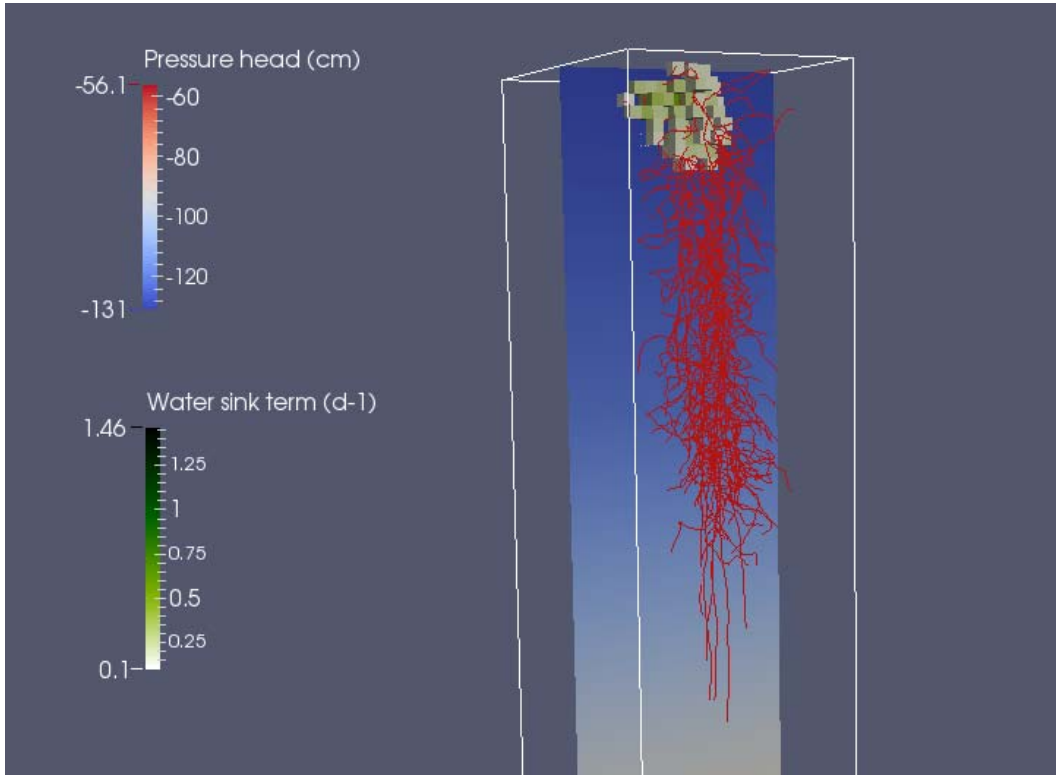
SIMULATION OF PESTICIDE UPTAKE

Large root system: water uptake





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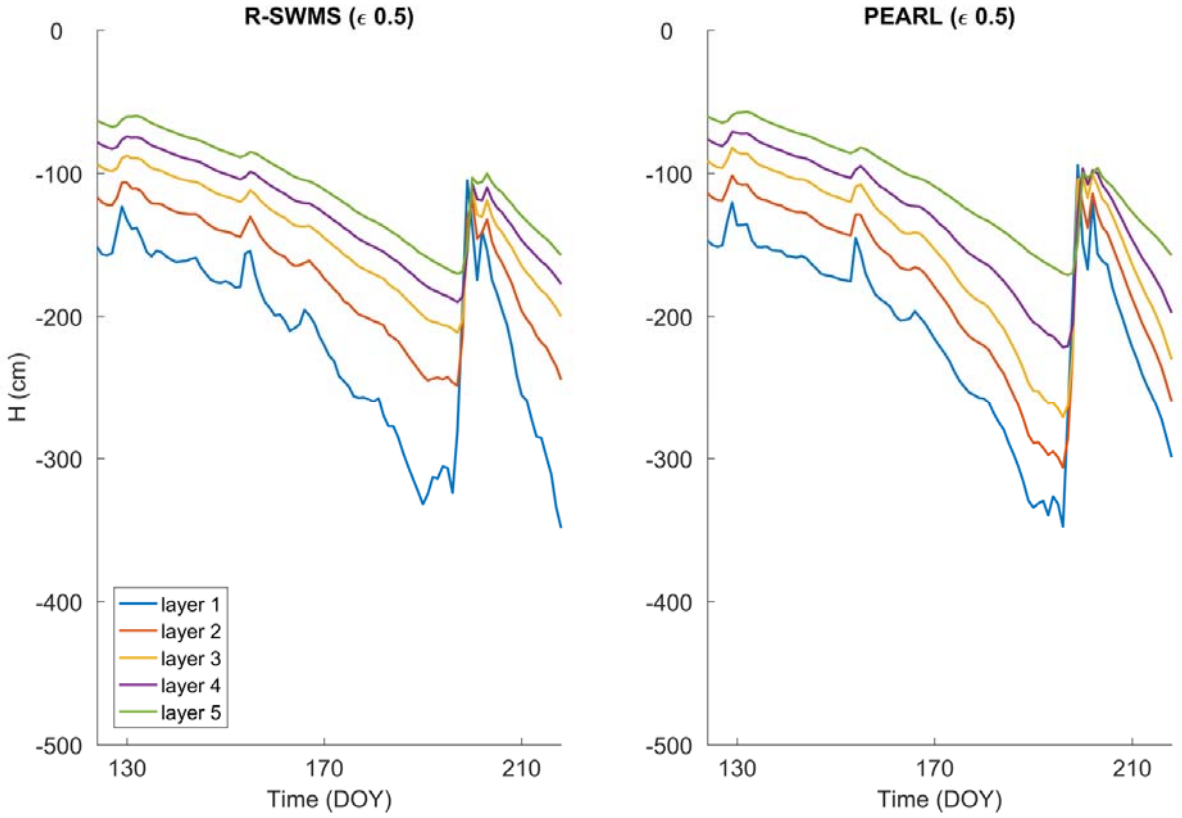
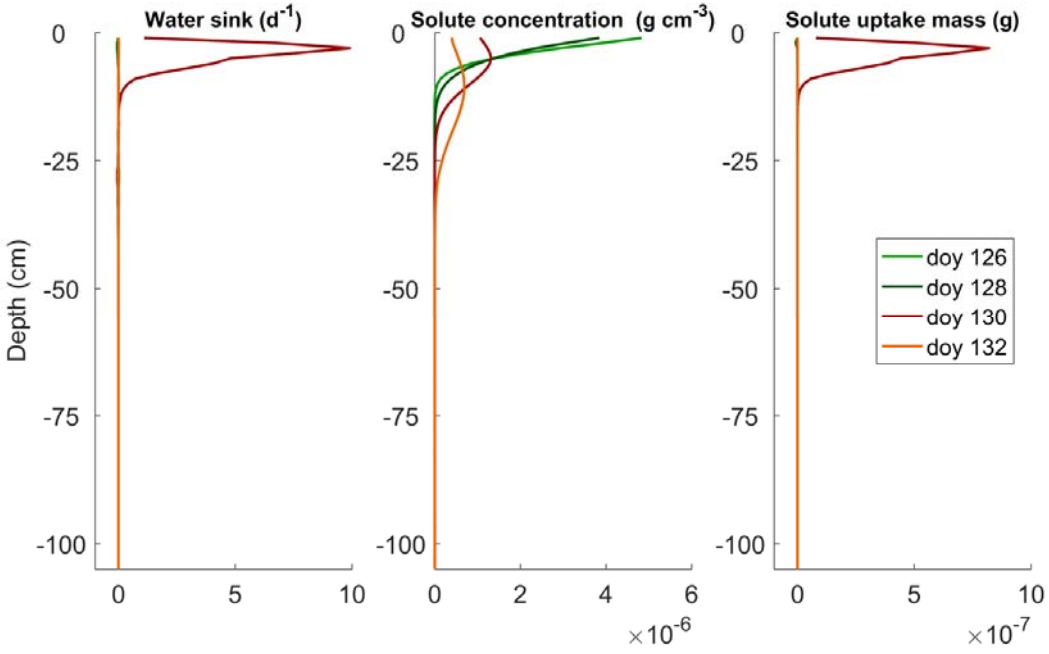
SIMULATION OF PESTICIDE UPTAKE

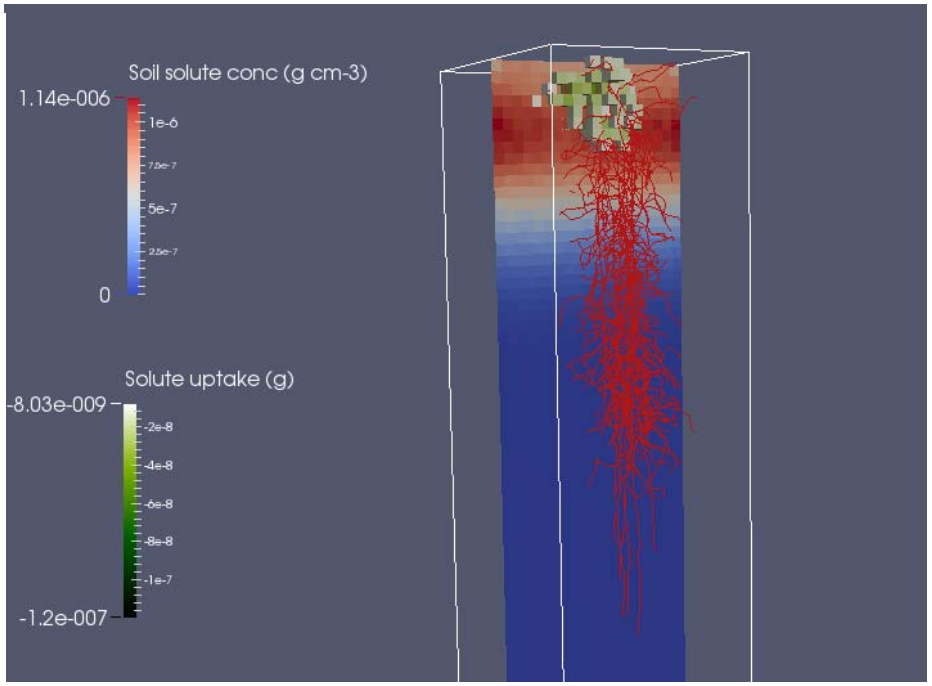
Large root system, water uptake, comparison with PEARL



SIMULATION OF PESTICIDE UPTAKE

Large root system, solute uptake

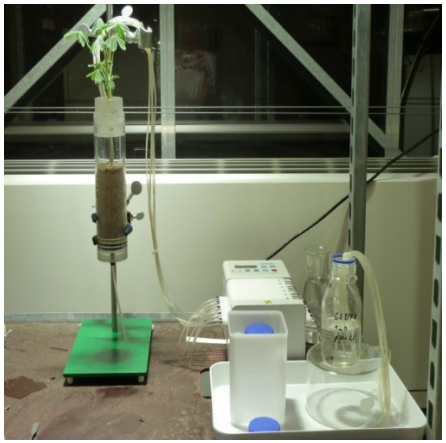




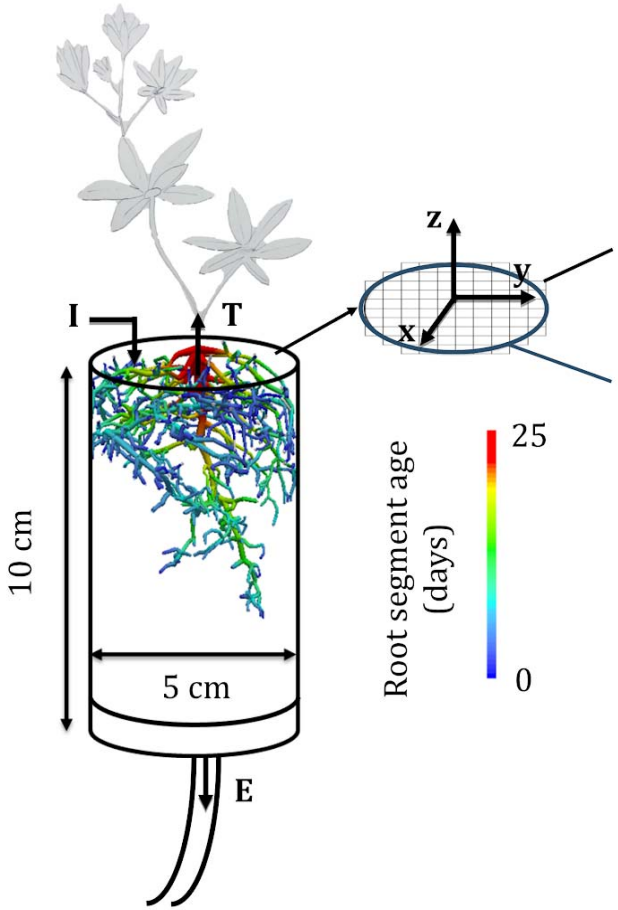
VALIDATION AND PARAMETERIZATION

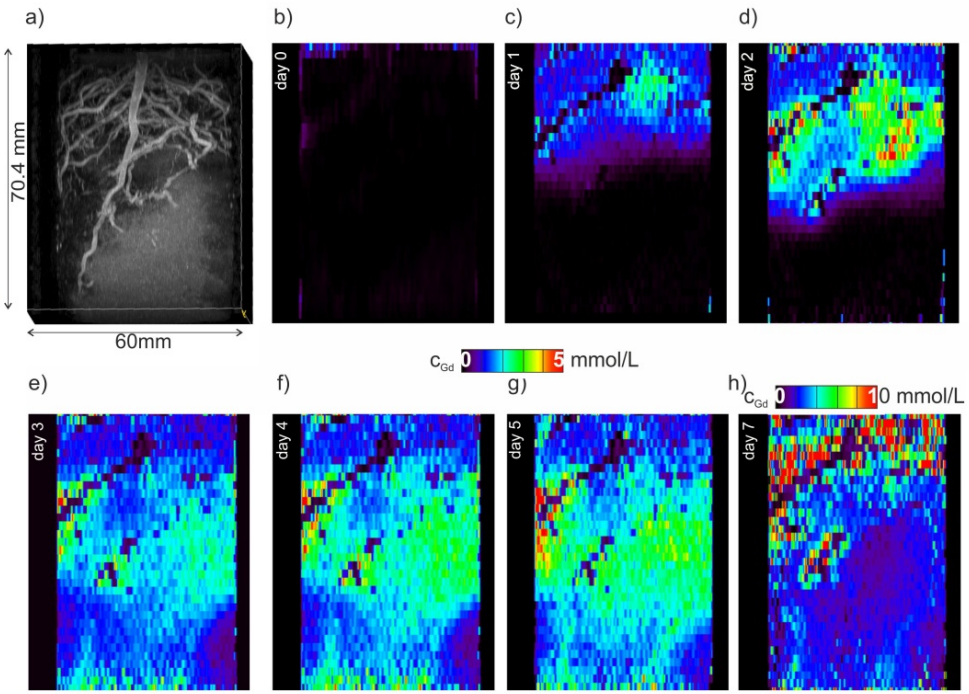
Small scale experiments (column scale) to validate model concept

MRI tracer experiments



Haber-Pohlmeier et al., 2017,
Water Resour. Res.





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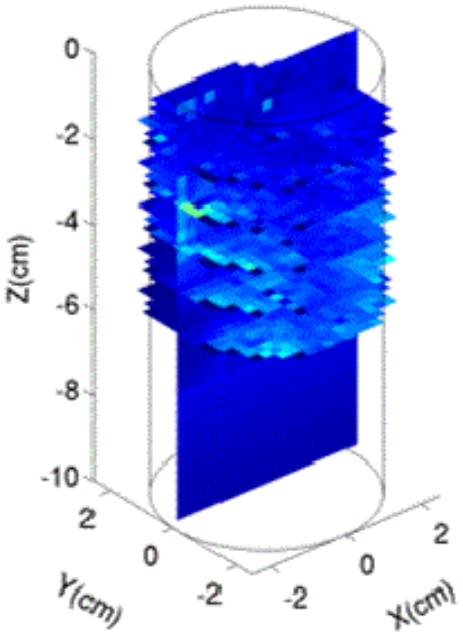
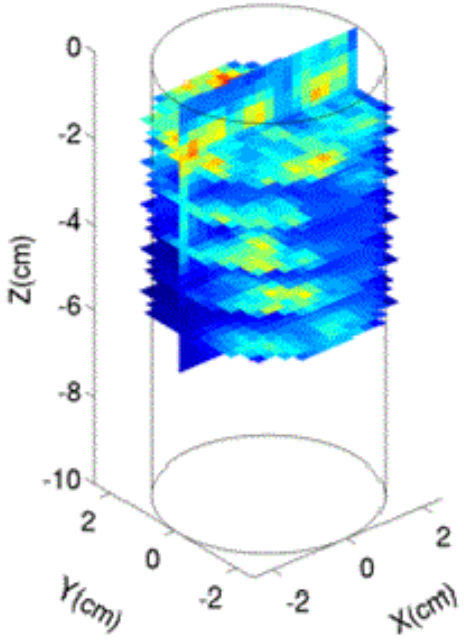
VALIDATION AND PARAMETERIZATION

Small scale experiments (column scale) to validate model concept

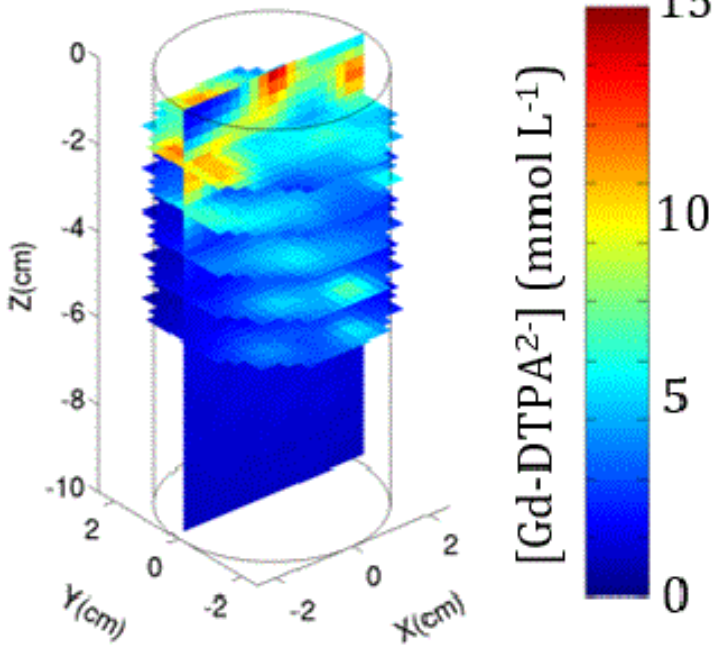
Gd concentration distribution at day 5 (initial condition for simulation)



MRI imaged Gd concentration at day 7



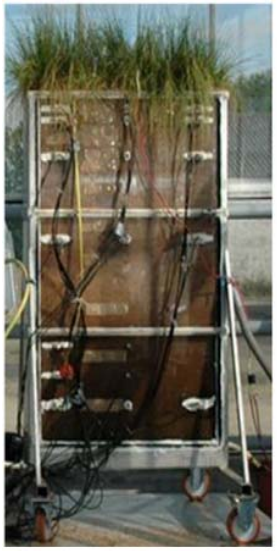
Simulated Gd concentration at day 7

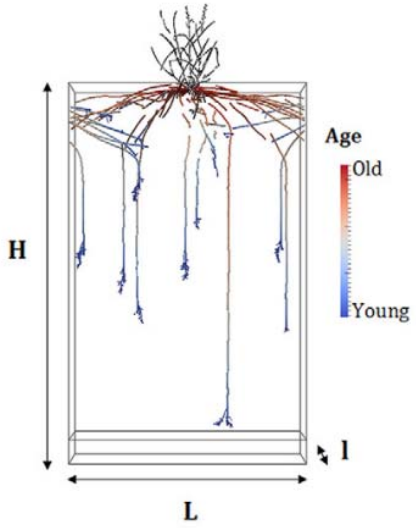


Koch et al., 2018, submitted

VALIDATION AND PARAMETERIZATION

Lysimeter scale experiments to validate hydraulic redistribution and hydraulic lift

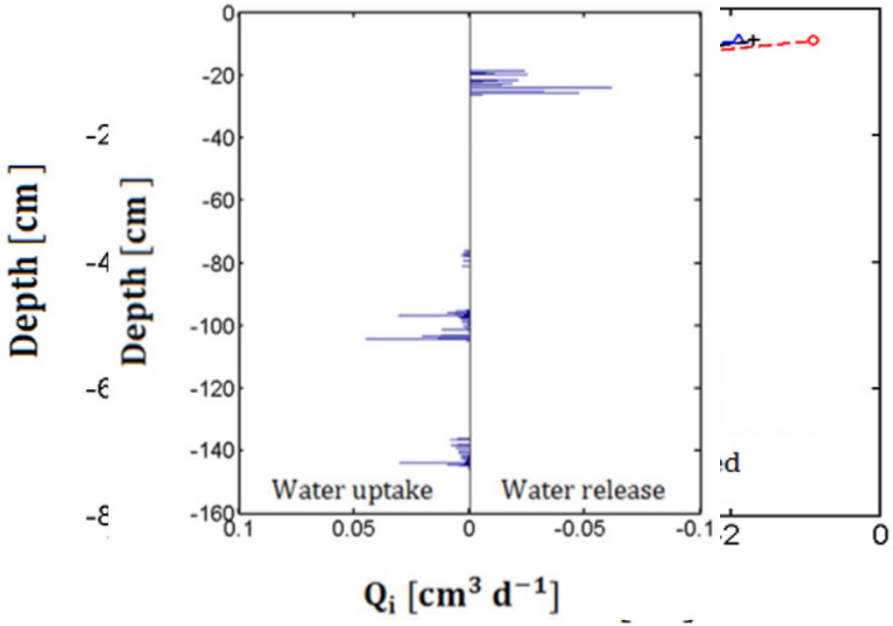




- Planted rhizotron monitoring of the water flow
- Measured root length densities and isotopic signatures of soil and plant collar
- Simultaneous measurements of soil water potential and content

- Experiment reproduced using RSWMS
- Root hydraulic properties were optimized to reproduce the isotopic profile
- Independent model validation using measured plant isotopic signatures

Meunier et al. 2017 VZJ



UPSCALING OF ROOT WATER UPTAKE MODEL

Based on the soil element instead of the root segment level

$$\mathrm{RWU}_k = K_{rs}(\bar{\psi}_s - \psi_{col})SSF_{\boldsymbol{k}} + K_{comp}\left(\psi_{s,k} - \bar{\psi}_s\right)SSF_k$$

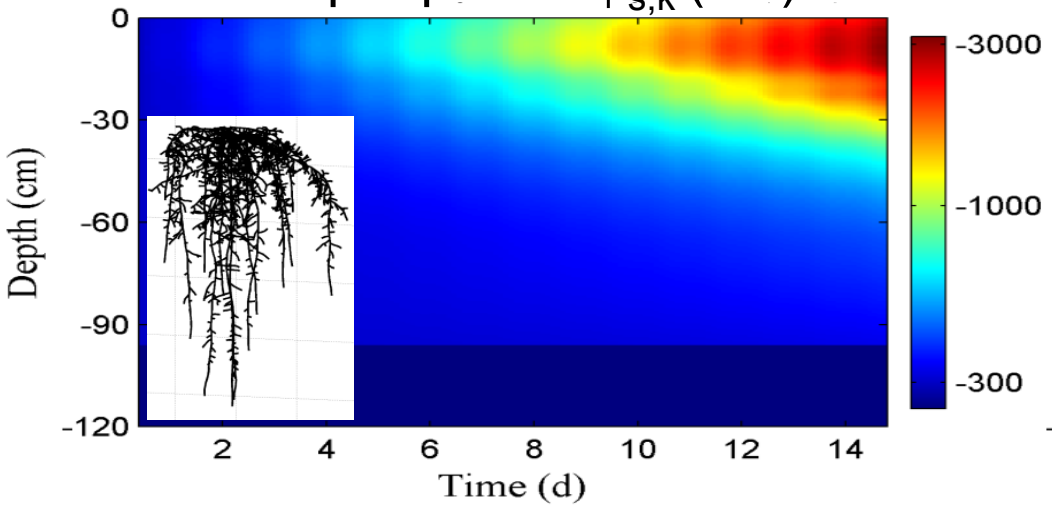
RWU_k (L T^{-1}): root water uptake in the k^{th} soil element
K_{rs} (T^{-1}): equivalent root system conductance
K_{comp} (T^{-1}): compensatory RWU conductance
SSF_k (-): standard sink fraction
ψ_{col} (L): total potential at the root collar
$\Psi_{s,k}$ (L): total potential in the k^{th} soil element

$$\bar{\psi}_s = \sum_{k=1}^{M} \psi_{s,k} SSF_k$$ equivalent soil water potential

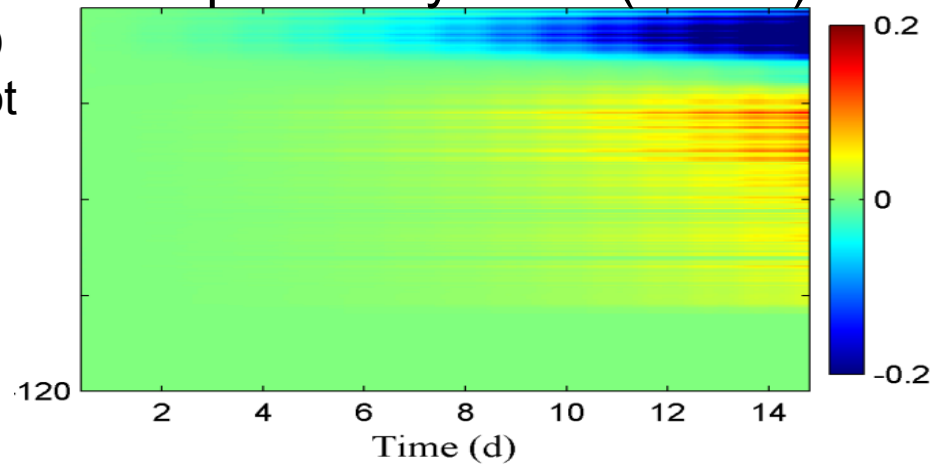
- **SSF**, K_{rs} and K_{comp} remain constant for static RSA
- For horizontally homogeneous root systems (wheat) → 1D sink term for RWU from knowledge of the 3D hydraulic root architecture
- Implemented in Hydrus1D, AgroC, CLM

Couvreur et al. 2012, HESS

1D depth profile $\psi_{s,k}$ (cm)



compensatory RWU (cm d^{-1})



SUMMARY AND CONCLUSIONS

- Using a mechanistic soil-root model, plant properties (root hydraulic properties and uptake properties) can be accounted for when describing water and pesticide uptake.
- The model can be parameterized using directly measurable properties of the root system.
- It can be validated.

- For water uptake, we have derived an upscaled version which could in principle be incorporated in regulatory models (but testing, parameterisation and validation is still required).
- For solute (pesticide) uptake, we need first further testing and analyses (work in progress).

THANK YOU