Multidimensional reactive transport modelling of imidacloprid and clothianidin after seed treatment

Science For A Better Life

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Aim of Study

- Investigate the applicability of HYDRUS 2D for detailed investigations of transport processes at the vicinity of treated seeds.
- Gain insights in the behavior of active ingredients when applied as seed treatment.

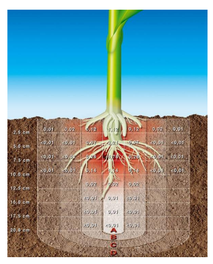
Introduction

- Seeds are usually treated with Plant Protection Products (PPPs) before plantation to reduce their undesired potential environmental exposures through drift or run-off/erosion and to increase their efficacy by providing higher concentrations at vicinity of the plant roots.
- A Lab soil column experiment was performed [1] with corn seeds treated with imidacloprid (IMD) and clothianidin (CTD). The soil moisture and mass distribution of IMD and CTD were measured at end of the experiment.
- In order to better understand the release and translocation processes of PPPs in soil around the treated seed at the presence of root plant uptake, the experiment were modelled with HYDRUS 2D software [2].

Material and Methods

Experimental Set Up:

- One seed inserted at a depth of 6 cm in the center of the column
- Column size: diameter 44 cm; Height 40 cm
- Moisture at 40% of maximum water holding capacity (MWHC) equivalent to 14% volumetric water content.
- Weekly irrigation and weighting
- Experiment duration: 30 days



Soil Sampling Equipment:

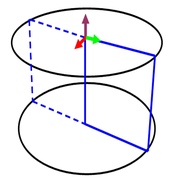
Tabelle 1: Physicochemical properties of Monheim soil

Parameter	Value	Unit
pH	6.9	-
Organic matter	2.36	%
Sand	63.5	%
Silt	26.3	%
Clay	10.2	%

Tabelle 2: Compound properties

Parameter	Value	Unit
Imidacloprid (IMD)		
DT_{50}	103	day
K_d	2000	m^3/kg
Freundlich exponent	0.85	-
Calibrated release rate ($\mathbf{k}_r$)	0.192	1/day
Initial mass	1×10^{-6}	kg /seed
Clothianidin (CTD)		
DT_{50}	153	day
K_d	2900	m^3/kg
Freundlich exponent	0.83	-
Calibrated release rate ($\mathbf{k}_r$)	0.085	1/day
Initial mass	0.474×10^{-6}	kg /seed

Model Set Up:



- Domain geometry
- 2D-Axisymmetrical vertical flow (Plane: XZ)
- Richards‘ equation for single phase flow with van Genuchten-Mualem model for parameterization of water retention and hydraulic conductivity functions.
- Soil hydraulic parameters were estimated by Rosetta pedotransfer function.
- Static root water uptake distribution, stress function for root water uptake according to Feddes.
- Space discretization: Galerkin finite element method (FEM).
- Time discretization: implicit scheme with automatic time stepping.
- Freundlich adsorption isotherm.
- Release of PPP from treated seed and biodegradation were modelle as first order decay process.

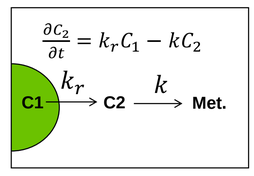


Tabelle 3: Model setup parameters

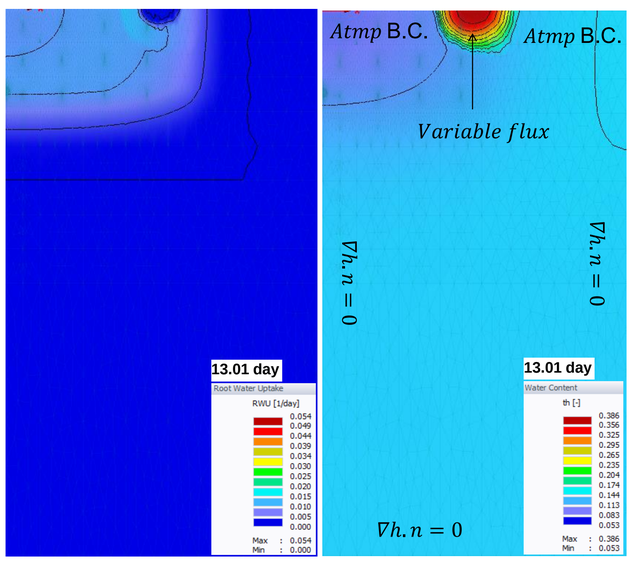
Parameter	Value	Unit
Column width (x axis)	0.22	m
Column height (y axis)	0.40	m
Bulk density	1300	kg/m^3
Longitudinal dispersion length	0.01	m
Transverse dispersion length	0.001	m
Molecular diffusion coefficient	0.43×10^{-4}	m^2/day
Corn seed radius	0.003	m

Tabelle 5: Calibrated parameters

Irrigation flux
Size of infiltration area
Root water uptake distribution
Compound release rates

Results

- **2D profiles (XZ plane) of (from left to right) root water uptake, soil water content , CTD concentration and spatial root water uptake distribution.**



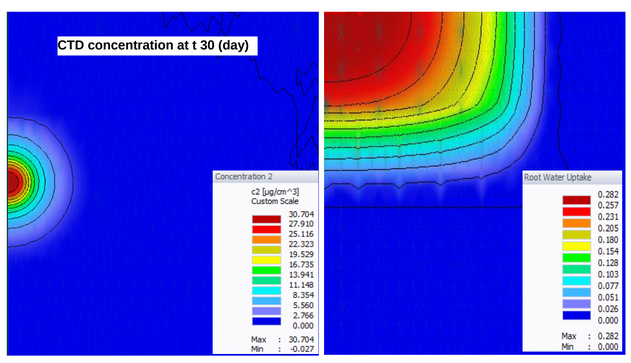
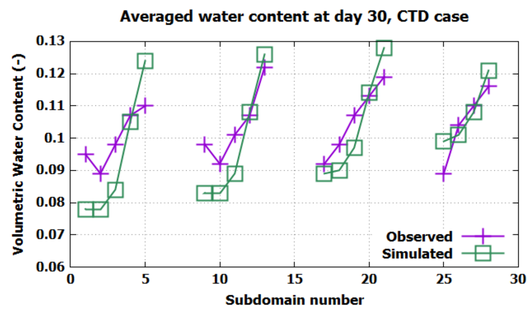
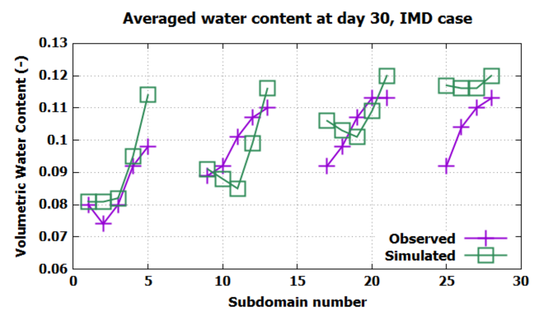
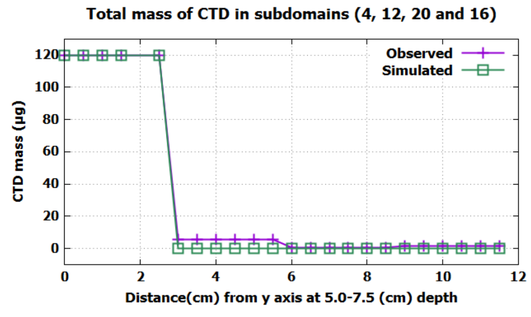


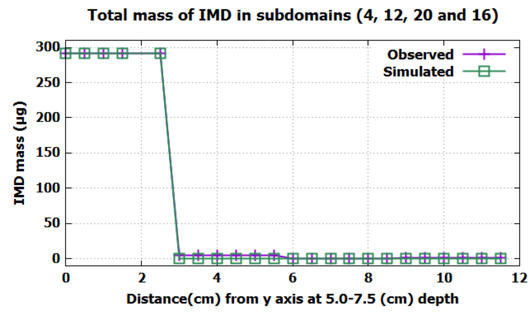
Tabelle 4: Numbering of subdomain intervals (row[x], column[z] (cm))

0.0	2.5	5.5	8.5	11.5
2.5	2	10	18	9
5.0	3	11	19	15
7.5	4	12	20	16
10.0	5	13	7	17
12.5	6	14	8	









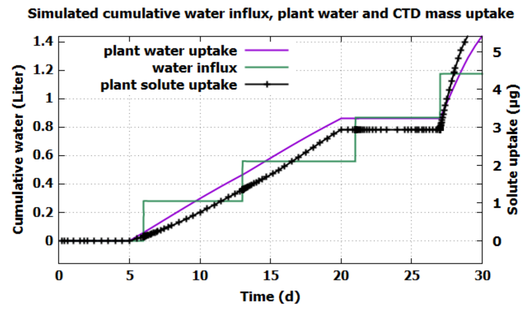


Tabelle 6: Total mass(μg) distribution of CTD in subdomains.

(cm)	2.5	5.5	8.5	11.5	2.5	5.5	8.5	11.5
	measured				simulated			
2.5	2.15	4.35	3.85	2.95	0.00	0.00	0.00	0.00
5.0	38.3	2.85	0.35	1.25	11.0	0.01	0.00	0.00
7.5	120	5.45	0.50	1.70	120	0.20	0.00	0.00
10.0	27.45	1.45	0.00	0.00	2.93	0.01	0.00	0.00
12.5	0.25	0.30	8.45	0.00	0.00	0.00	0.00	0.00

Conclusions

- **The simulation results of water content and mass distribution of IMD and CTD in soil agreed well with the measured data.**
- **The solute transport in soil under the experimental condition is dominated by diffusion.**
- **The simulations indicated that the implementations of plant uptake and the release rate had a substantial influence on the water and mass distribution of the compounds in the soil.**
- **Thus the direct determination of root distribution and release rates is likely to improve the simulations as is expected for the use of a dynamic root growth model.**

References

[1] Mittelstaedt, W. (2008) Verhalten und Verteilungsmuster von Imidacloprid, Clothianidin und Thiamethoxam in einem sandigen Lehm (Bi-Boden, Monheim) verschiedener Feuchtestufen nach Saatgutbeizung von Mais, Bayer AG Internal Report, ICG-4 00108, 2008.02.18.

[2] Šimunek, J., van Genuchten, M.Th., and Šejna, M. (2016) Recent developments and applications of the HYDRUS computer software packages, Vadose Zone Journal, 15(7), pp. 25, doi: 10.2136/vzj 2016.04.0033.