Hydrus 2D applied to modelling transport of agrochemicals in drip irrigation scenarios



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Overview

HYDRUS (2/3D) is an higher tier alternative to regulatory models that are commonly accepted for estimating fate and transport of agrochemicals in groundwater. One of the advantages of HYDRUS is the flexibility in creating scenarios to model agrochemical fate in specific agronomic situations. User defined scenarios can be created in 1, 2 or 3D for a particular type of irrigation/chemigation method (e.g. drip, in-furrow), product application technique (chemigation/spray/granular) with appropriate site-specific soil and weather files. To investigate transport of agrochemicals applied via drip irrigation, scenarios in HYDRUS 2D were designed for 1m width x 1m depth domains. Theoretical root zone (RZ) 30cm x 30cm were placed in the domain to track porewater concentrations (PWCs) in rootzone for a hypothetical pesticide. Sensitivity analysis of input parameters (degradation rates, sorption, irrigation amount) was tested to assess their impact on PWCs in RZ (for single year simulations). For this work, product RZ PWCs of 0.5-3 ppm is assumed for product efficacy. Results show that HYDRUS 2D can also predict concentrations in a similar range to that of regulatory models and have the potential to be a useful tool to understand pesticides fate under actual agronomic use conditions, especially for drip irrigation, where current regulatory models are less effective in simulating such situations.

Objective

Material/Methods/Inputs

- To identify input parameters; soil degradation (DT50), sorption (KOC) and agronomic parameters (irrigation amount) impacting RZ PWCs in drip irrigation scenarios - To compare and show similarity in predicted porewater concentrations from PEARL 4.4.4 and Hydrus 2D

Multiple factors influence rootzone (RZ) PWCs. Rootzone is the zone where core root mass lies and most of nutrients/pesticides are taken up by plants. Fig 1 shows the hypothetical RZ in the simulated HYDRUS domain. Agronomic parameters such as amount and frequency of irrigation for a fruiting crop was obtained through consultation with FAO and internal field development team at DuPont. For simplicity, the emitter was assumed to be placed at/near the surface directly above the RZ. Input parameters for PEARL 4.4.4 and HYDRUS 2D were derived based upon these consultations together with environmental fate inputs for FOCUS test substance A.

Note: For sensitivity analysis, product RZ PWCs of 0.5-3ppm is assumed for product efficacy)



Fig 1. Illustration of a drip irrigation with a subsurface emitter (figure not to scale) and predicted concentrations at rootzone at Day X after application of product

Results

| PARAMETER | UNIT | DUMMY A |
|-------------------|-------------|-------------------|
| Mol. Mass | g/mol | 300 |
| Vapour Pressure | Pa | 1.0 E-7 |
| Sol water | Mg/L | 900 |
| DT50 | D | 60 (range 20-100) |
| Kom | L/kg | 60 (range 50-200) |
| 1/n | L/kg | 0.9 |
| Crop | (-) | Fallow |
| Application rate | Kg/ha | 1 |
| Irrigation timing | Daily | |
| | (variable) | |
| Soil type | Sandy (95%) | - |

Table 1. Input parameters (FOCUS test substance A from HYDRUS 2D was used). All other default modeling parameters from PEARL 4.4.4 were used (as appropriate).



Fig 2. Simple sensitivity analysis with RZ PWCs over time vs variation in KOC(left) and variation DT50 (right)

Impact of irrigation amounts for optimum average PWCs in RZ

Theoretical irrigation amounts varying between 0.25° - 0.75° (0.64-1.91 cm) every 2 days were applied in the drip system to assess impact of irrigation on pesticide RZ PWCs. For a simplistic case, results show that for ideal PWCs, irrigation amounts should be between 0.25° to < 0.75° (0.64-1.91 cm) every two days but not higher than the latter as the product might be 1) diluted and 2) mobilized away from the RZ.



Fig 3. RZ PWCs variation with irrigation amount

Hydrus vs Pearl 4.4.4

'No crop' modeling was conducted in both HYDRUS 2D and PEARL 4.4.4 using equivalent environmental fate and default modelina parameters for drip irrigation scenario. Surface applications in both models were assumed and RZ PWCs modelled. Observation nodes were placed in HYDRUS 2D (identified by crosses below). Concentrations (over time) at each observation node were compared with PECs from PEARL 4.4.4 and plotted against each other.



Fig 4 (top). 2D illustration of a drip irrigation observation nodes placed at different depths (figure not to scale)

Fig 5 (right). RZ PWCs vs depth from Hydrus vs FOCUS PEARL 4.4.4. at day 1 to day 50

Concentration (ppm) 0.1 0.2 Pearl Hydrus Ê 0.3 0.4 Depth DAY 1 0.6 0.7 3 0.1 0.2 0.3 Ξ 0.4 Depth 0.5 **DAY 35** 0.5 1.5 Ê_{0.2} Depth Depth 0.6 DAY 50

Summary/Conclusions

- With 2D/3D possibilities, HYDRUS offers a robust option for not only predicting concentrations in soil/gw but also optimizing irrigation needs in agronomic settings
 RZ PWCs were impacted differently by DT50 and KOC values for Substance A. DT50 was a less sensitive parameter as the RZ PWCs did not vary significantly with varying DT50 (20-100d). Sorption is a more sensitive parameter that influenced RZ PWC as the concentrations decreased significantly with KOC (50 200 L/Kg)
 Irrigation between 0.25" to <0.75" (0.64-1.91 cm) every 2 days was optimum to produce RZ PWCs in the range of 0.5 3 ppm. Irrigation >0.75"(1.91 cm)/2 days (overwatering) may lead to greater dilution and mobilization of product from the root zone thereby decreasing RZ PWCs
- Concentrations in PEARL 4.4.4 were comparable in HYDRUS 2D. It is possible to create equivalent scenarios in HYDRUS 2D by taking agronomic/env inputs from PEARL 4.4.4. A setup combining regulatory models such as PEARL 4.4.4 with HYDRUS 2/3D could help understand answers in modeling and risk assessment where 1D regulatory models (like PEARL 4.4.4) cannot provide as complete context surrounding patterns of exposure within the soil domain