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Introducing the 2-DROPS model for two-dimensional simulation of crop roots and pesticide within the soil-root zone

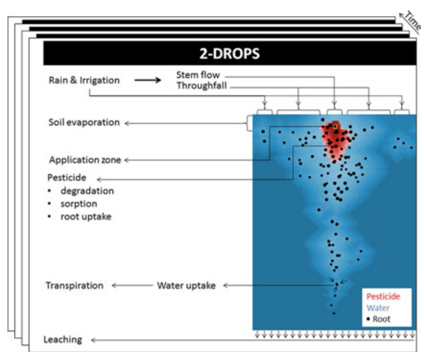
Annika Agatz *, Colin D. Brown

Environment Department, University of York, Heslington, York, United Kingdom

HIGHLIGHTS

- We lack predictive tools to guide development of pesticide placement technologies.
- A new 2-D model to predict water and pesticide movement in soils is developed.
- First predictive tool accounting for explicit and stochastic root development.
- Soil and pesticide properties drive the shape of the pesticide distribution zone.
- Developed model parameterised for maize but applicable to all crops.

GRAPHICAL ABSTRACT



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ABSTRACT

Mathematical models of pesticide fate and behaviour in soils have been developed over the last 30 years. Most models simulate fate of pesticides in a 1-dimensional system successfully, supporting a range of applications where the prediction target is either bulk residues in soil or receiving compartments outside of the soil zone. Nevertheless, it has been argued that the 1-dimensional approach is limiting the application of knowledge on pesticide fate under specific pesticide placement strategies, such as seed, furrow and band applications to control pests and weeds.

We report a new model (2-DROPS; 2-Dimensional ROots and Pesticide Simulation) parameterised for maize and we present simulations investigating the impact of pesticide properties (thiamethoxam, chlorpyrifos, clothianidin and tefluthrin), pesticide placement strategies (seed treatment, furrow, band and broadcast applications), and soil properties (two silty clay loam and two loam top soils with either silty clay loam, silt loam, sandy loam or unconsolidated bedrock in the lower horizons) on microscale pesticide distribution in the soil profile.

2-DROPS is to our knowledge the first model that simulates temporally- and spatially-explicit water and pesticide transport in the soil profile under the influence of explicit and stochastic development of root segments. This allows the model to describe microscale movement of pesticide in relation to root segments, and constitutes an important addition relative to existing models. The example runs demonstrate that the pesticide moves locally towards root segments due to water extraction for plant transpiration, that the water holding capacity of the top soil determines pesticide transport towards the soil surface in response to soil evaporation, and that the soil type influences the pesticide distribution zone in all directions. 2-DROPS offers more detailed information on microscale root and pesticide appearance compared to existing models and provides the possibility to investigate strategies targeting control of pests at the root/soil interface.

* Corresponding author.
E-mail addresses: annika.agatz@york.ac.uk (A. Agatz), colin.brown@york.ac.uk (C.D. Brown).

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1. Introduction

Mathematical models of pesticide fate and behaviour in soil have been developed over the last 30 years. Applications of these models include use as research tools, support for environmental safety assessments, and design of approaches to manage risks of pesticides (Addiscott and Wagenet, 1985; Köhne et al., 2009). In many cases, models simulate fate of pesticides in soil as a necessary step in quantifying transfer into non-target compartments including groundwater (Boesten, 1994; Brouwer, 1994, Tiktak et al. 2002), surface water (Carsel et al. 1985; Singh and Kanwar, 1995; Jarvis and Larsbo, 2012), crops (Fantke et al. 2013), and air (Bedos et al. 2009). In each instance, it has been sufficient to treat soil as a 1-dimensional system; this system varies in the vertical plane due to variation in boundary interfaces, soil properties, root distribution, pesticide inputs, water fluxes and so on, but variation in the horizontal plane is ignored. Some authors have coupled 1-dimensional models for leaching of pesticides through the soil unsaturated zone with 2- or 3-dimensional simulation of transport in groundwater where lateral transport is the norm (Hantush et al. 2000; Zhu et al. 2013).

Thus the 1-dimensional approach to modelling pesticide fate in soil has been successful in supporting a range of applications where the prediction target is either bulk residues in soil or receiving compartments outside of the soil zone. The 1-dimensional approach addresses the requirements for model parsimony, whereby model descriptions should be as simple as possible whilst fulfilling the prediction need. Nevertheless, it can be argued that the 1-D approach has been a limiting factor on the application of knowledge on pesticide fate. A range of strategies are available to target placement of pesticides into the soil profile, such as seed treatment, in-furrow applications and banding. These strategies afford more targeted placement to control pests and weeds whilst reducing overall inputs of pesticides into the system. However, innovation in this space has been limited because we lack predictive tools to guide development of placement technologies and to reward technologies by assessing the benefits for risks to the environment.

The literature includes a small number of 2-dimensional models for pesticide fate in soil. The TRANSMIT model (Hutson and Wagenet, 1995) is a multiregion model that comprises multiple iterations of the one-dimensional model LEACHP; transfer of water and chemical between regions allows application to 2-dimensional geometries and non-uniform surface boundary conditions such as drip irrigation or band applications of pesticides. The most frequently applied 2-dimensional model in recent years has been HYDRUS (Šimůnek et al. 2013). HYDRUS is a flexible software package applicable for simulating water, heat and solute movement in 1-, 2- and 3-dimensional porous media. Spatially-explicit solutions of the Richards' equation and convection-dispersion equation are supplemented by routines to describe sorption and degradation processes for reactive solutes such as pesticides and the simulation of nonequilibrium transport for two-region/dual porosity systems. HYDRUS-2D was used to evaluate preferential flow processes along a sloping transect at a field site in southern Sweden, demonstrating that a dual permeability description of preferential flow better matched transport of MCPA (2-methyl-4-chlorophenoxyacetic acid) to tile drains than simulations based on mobile/immobile regions or dual porosity (Gärdenäs et al. 2006). More recently, the model has been coupled with measurements of heterogeneity in soil properties across study sites to describe transport of pesticides through field soils (Suarez et al. 2013; Filipović et al. 2014, 2016). Simulation of root growth has been a constraint in HYDRUS with a simplified rooting pattern and definition via input parameters that did not consider the feedback between root growth and conditions in the soil. Recently, these feedbacks with soil water content or temperature have been added to HYDRUS-1D and partially implemented in HYDRUS-2D via an additional root growth module (Hartmann and Šimůnek, 2015). Finally, there has been a limited amount of work to describe fate of soil fumigants in two dimensions, for example following addition in drip irrigation and including the impacts of two dimensional cultivation beds and differentiated temperature fluctuations across the soil surface (Ha et al. 2009a,b; Luo et al. 2011).

Here we report a new model called 2-DROPS (2-Dimensional ROots and Pesticide Simulation) that describes the spatial and temporal distribution of crop roots and pesticides in the soil-root zone. The model captures spatial differentiation in inputs of precipitation and irrigation to soil (for example due to leaf cover and stem flow), and spatial differentiation in pesticide inputs (for example due to application as seed treatment). Root development is simulated as a spatially explicit and stochastic process within constraints that are specific to the crop, whilst transport of water (modelled according to the capacity approach) and chemical occurs in both vertical and horizontal planes according to hydraulic gradients arising from inputs of water at the surface, soil evaporation and extraction of soil water by the roots. Leaching out of the soil profile is again a spatially explicit process. Overland flow is ignored in the current version of the model but could readily be added as a future development.

2. Model description

2.1. Overview

The aim of this work was to derive a model to predict the temporally- and spatially-explicit transport of water and pesticide in the soil profile with particular focus on the influence of temporally- and spatially-explicit development of the plant root system. 2-DROPS simulates water transport and pesticide fate for a vertical soil profile of 76 ∗ 100 cm (x- and y-axes) and 1 cm depth (z-axis) with each patch/grid representing 1 cm^3. These dimensions were selected to represent the root zone of a single plant in a commercial maize field; the spatial dimensions could be modified to describe crops with different rooting systems. The model is implemented in NetLogo 5.0.5 (Wilensky 1999) and runs at a daily resolution from the beginning of a year (Julian day 1) until a day specified by the user. Irrigation can be implemented by the user, which then alters the above ground plant development and initiates an irrigation schedule that is dependent on climate and soil type. Whilst water can move in either direction horizontally and vertically, water leaching from the base of the soil profile is considered lost from the system. The soil can be divided into up to four horizons with differing soil characteristics. A schematic flow chart illustrating the order of processes incorporated in the model is presented in Fig. 1.

Inputs for 2-DROPS in addition to those described in the detailed model description (Section 2.2) and the Appendix A (Nomenclature) are the soil horizon boundaries, whether irrigation occurs, the planting and application day, and the application type and application rate.

2.2. Details

2.2.1. Evapotranspiration

The general formula to calculate the crop specific evapotranspiration $\mathbf{ET_a}$ from the reference evapotranspiration and two crop-specific coefficients is:

$$ET_a = K_o * K_c * ET_r$$

where $\mathbf{K_c}$ is the crop coefficient, $\mathbf{K_o}$ is the water stress coefficient and $\mathbf{ET_r}$ is the daily reference evapotranspiration (Allen et al. 1998). The latter can either be direct input data from a weather station or can be calculated using weather data and for example the FAO Penman-Monteith method.

The crop coefficient $\mathbf{K_c}$ for maize is given as a function of time after plant emergence $\mathbf{T_{spe}}$ using the duration of different plant growth stages and the corresponding crop coefficients given in the literature (Allen et al. 1998):

$$K_c = 0.3 \quad \text{for } T_{spe} < 30$$