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Development and application of a catchment scale pesticide fate and transport model for use in drinking water risk assessment

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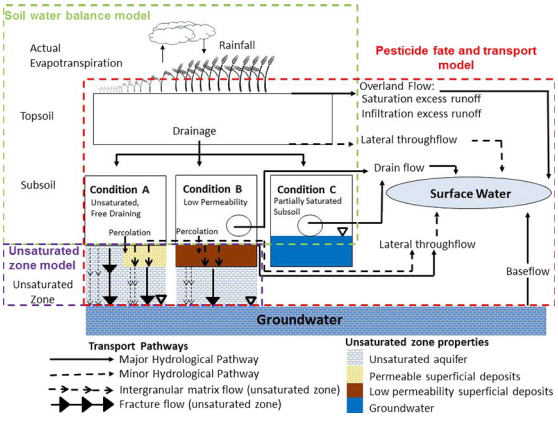
HIGHLIGHTS

- A new parameter-efficient catchment-scale pesticide exposure model is presented.
- Soil-type-specific boundary conditions determine active hydrological pathways.
- Applied and evaluated at the small sub-catchment and large catchment scales.
- Predicted exposure can inform water company risk assessments.

GRAPHICAL ABSTRACT



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ABSTRACT

This paper describes the development and application of IMPT (Integrated Model for Pesticide Transport), a parameter-efficient tool for predicting diffuse-source pesticide concentrations in surface waters used for drinking water supply. The model was applied to a small UK headwater catchment with high frequency (8 h) pesticide monitoring data and to five larger catchments (479–1653 km^2) with sampling approximately every 14 days. Model performance was good for predictions of both flow (Nash Sutcliffe Efficiency generally >0.59 and PBIAS <10%) and pesticide concentrations, although low sampling frequency in the larger catchments is likely to mask the true episodic nature of exposure. The computational efficiency of the model, along with the fact that most of its parameters can be derived from existing national soil property data mean that it can be used to rapidly predict pesticide exposure in multiple surface water resources to support operational and strategic risk assessments.

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1. Introduction

Pesticides are widely used in modern conventional agriculture and contribute to increased yield and quality. However, a small fraction of some active ingredients can be transported, via a range of different pathways, to ground and surface waters. If the receiving water body is used for drinking water supply, then these substances may periodically present compliance risks for water companies if the treatment technologies in place are unable to reduce concentrations to the limits required by the prevailing legislation. In the European Union (EU), individual pesticides must not have concentrations >0.1 μg L^{-1} in drinking water supplies (post treatment) and the total concentration of all pesticides must be <0.5 μg L^{-1} (Drinking Water Directive - DWD; EC, 1998). In order to anticipate the levels of exposure which will be experienced at different drinking water abstraction points under current or future land use and meteorological scenarios, water companies are increasingly employing numerical models (Bloodworth et al., 2015). These models can help to assess DWD compliance risks and guide timing of sampling and the choice of analytical methods used on samples collected at water intakes. They can also be used to explore the potential of different catchment management interventions for mitigating pesticide exposure (e.g. changing crop rotations, switching active ingredients, using different dose rates), as required by Article 7 of the Water Framework Directive (WFD; EC, 2000).

There are a number of pesticide fate models that describe pesticide transfers from soil to surface and ground waters that could be used at the catchment scale (understood in this context to be over 100 ha or 1 km^2; Köhne et al., 2009). These range from simple screening models such as the Groundwater Ubiquity Score (GUS) developed by Gustafson (1985), the soil fugacity model (SoilFug) of Di Guardo et al. (1994) and the Pesticide Risk Management Profiling Tool (PRoMPT: Whelan et al., 2007), all based largely on pesticide properties, through to detailed field-scale one dimensional models, such as MACRO (a model of water flow and solute transport in macroporous soil: Larsbo and Jarvis, 2003; Larsbo et al., 2005), Pesticide Emission Assessment at Regional and Local scales (PEARL: Tiktak et al., 2000), PEsticide Leaching Model (PELMO: Klein, 1991) and the Pesticide Root Zone Model (PRZM: Mullins et al., 1993). Many simpler models (e.g. GUS) are not dynamic (i.e. they are not able to make predictions in time) and often lack good description of spatial variations in leaching due to varying soil characteristics, weather, topography and land use. The latter one-dimensional models are all employed as risk screening tools using standardised scenarios in the pesticide registration process in the EU (e.g. FOCUS, 2000, 2001) but can also be up-scaled to catchment and regional scales (e.g. GeoPEARL: Tiktak et al., 2003 and MACRO-SE: Steffens et al., 2015). Although such up-scaling can be successful, detailed models typically have high data requirements and incur long run times to solve the partial differential equations describing one-dimensional transport of water and solutes by numerical methods. This is exacerbated when applied to large heterogeneous catchments which require simulations to be performed for various (independent or connected) units representing different soil type and land use combinations and topographic locations. They are, therefore, often unsuitable for catchment-scale applications where evaluations may be required for many different pesticides (possibly all feasible combinations of active ingredients currently on the market) and for many different combinations of weather, soil types and land uses.

The aim of the model described here is to predict pesticide transport from agricultural land to surface waters in order to inform and support water company risk assessments in multiple catchments over a range of scales. This application requires a model that contains a sufficient description of process complexity to yield realistic concentrations in a wide range of catchment types (i.e. it should be process-based rather than empirically-based) using readily available input data (e.g. on soil properties and meteorological data). However, it also needs to be computationally efficient so that it can be run for a wide range of pesticides, crops, soils and weather combinations over large heterogeneous areas. This problem of finding an optimal combination between fidelity to real process operation and simplicity (to reduce run times) is a perennial problem in environmental modelling and has recently been attempted for pesticides by, inter alia, Gassmann et al. (2013) and Steffens et al. (2015). In the case of ZIN-AgriTra, the model described by Gassmann et al. (2013), a fully distributed approach was taken with soil water and pesticide dynamics represented at 10 min time steps in 10 m grid cells across a 1.95 km^2 catchment in Switzerland. The explicit representation of material transfers within and between many grid cells in this catchment resulted in long run times which would be problematical for exposure assessments for several pesticides in larger catchments. In contrast, the one dimensional MACRO model is used in MACRO-SE model (Steffens et al., 2015) to calculate leaching to 2 m depth for a set of independent soil and crop combinations, which are then integrated at the catchment scale via weighted averaging. This approach is more efficient than running computations for all grid cells in a catchment (although it lacks the ability to account for landscape connectivity) but still requires a number of computationally intensive one-dimensional runs to be performed. Furthermore, whilst MACRO is based on a realistic and mechanistic representation of water and material transfers in one dimension, accurate catchment scale up of such models is not always straightforward and may require additional calibration (e.g. Beven, 1989).

This paper presents the development of IMPT (Integrated Model for Pesticide Transport), a conceptual, parameter efficient model for predicting pesticide fate and transport at the catchment outlet. It is intended to fill the gap between one dimensional aspatial leaching models such as the ones used in FOCUS and fully distributed catchment scale models which have yet to be employed widely for operational environmental management. The model was initially applied to a small (0.15 km^2) sub-catchment for which detailed data on flows and pesticide concentrations were available in order to demonstrate its ability to predict concentrations at the 'edge of field' scale and to underpin confidence in process representation. The model was then applied to five larger catchments (479–1653 km^2) to assess its performance under a range of different soil, land use, pesticide use and climatic conditions.

2. Model description

The underlying philosophy of the model is to represent soil-to-water transport in a simple, but physically realistic, way. This necessitates the implementation of a good hydrological model as catchment hydrological response plays a critical role in determining how solutes, including agriculturally-applied pesticides, are transported from land to water (Holvoet et al., 2005).

2.1. Soil water balance

The model is "semi-distributed" and performs calculations for homogenous soil type and land use combinations (sometimes referred to as Hydrological Response Units). A soil water balance model is used to predict the hydrological (and pesticide) transport pathways. For each soil type, the soil is divided into two discrete stores: the top soil and the subsoil. A separate moisture balance (e.g. Ward and Robinson, 1999) is calculated for each store i.e.

$$\frac{dS_{TOP}}{dt} = P - f_{TOP}.ET_a - q_{OLF} - q_{DRAIN} - q_{LAT\_top} \quad (1)$$

$$\frac{dS_{SUB}}{dt} = q_{DRAIN} - f_{SUB}.ET_a - q_{GW} - q_{LAT\_sub} \quad (2)$$

where $_{TOP}$ and $_{SUB}$ refer to the topsoil and subsoil stores, respectively, S is the storage in each layer (mm), t is time (days), P is the precipitation, ET_a is the actual evapotranspiration, f_{TOP} and f_{SUB} are the fractions of