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# Integration of transport concepts for risk assessment of pesticide erosion



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## HIGHLIGHTS

# GRAPHICAL ABSTRACT

- Parsimonious risk assessment model of pesticide transfer by soil erosion is developed.
- Integration of pesticide transport variability in soil and overland flow erosion.
- Modular approach enables easy incorporation of more complex model software.



# article info abstract

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Environmental contamination by agrochemicals has been a large problem for decades. Pesticides are transported in runoff and remain attached to eroded soil particles, posing a risk to water and soil quality and human health. We have developed a parsimonious integrative model of pesticide displacement by runoff and erosion that explicitly accounts for water infiltration, erosion, runoff, and pesticide transport and degradation in soil. The conceptual framework was based on broadly accepted assumptions such as the convection-dispersion equation and lognormal distributions of soil properties associated with transport, sorption, degradation, and erosion. To illustrate the concept, a few assumptions are made with regard to runoff in relatively flat agricultural fields: dispersion is ignored and erosion is modelled by a functional relationship. A sensitivity analysis indicated that the total mass of pesticide associated with soil eroded by water scouring increased with slope, rain intensity, and water field capacity of the soil. The mass of transported pesticide decreased as the micro-topography of the soil surface became more distinct. The timing of pesticide spraying and rate of degradation before erosion negatively affected the total amount of transported pesticide. The mechanisms involved in pesticide displacement, such as runoff, infiltration, soil erosion, and pesticide transport and decay in the topsoil, were all explicitly accounted for, so the mathematical complexity of their description can be high, depending on the situation. © 2015 Elsevier B.V. All rights reserved.

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# 1. Introduction

Pesticides are widely used in agriculture, horticulture, and forestry, and pesticide pollution has become an important issue worldwide [\(Damalas, 2009; Enserink et al., 2013](#page--1-0)). The high risks and long-term effects of pesticides on ecosystems have been studied for various components of the environment ([Geissen et al., 2010; Ruiz-Suarez et al., 2014;](#page--1-0) [Thomsen et al., 2014\)](#page--1-0). Great efforts have been made to enhance pesticide monitoring and to reduce potential risks by adopting policies of pesticide use and its properties [\(EPA, 2003; Peeters et al., 2014](#page--1-0)) and by establishing a desired level of environmental quality ([Horst et al.,](#page--1-0) [2014; Rousseau et al., 2012; Valk et al., 2014](#page--1-0)).

Pesticides applied to fields are generally taken up by plants, adsorbed by soil particles, or volatilised into the atmosphere. Pesticides directly or indirectly enter soils with rainwater and/or from the root system [\(Köhne et al., 2009; Passeport et al., 2013](#page--1-0)) and become subject to soil physicochemical processes, such as infiltration, transport, sorption, decay, accumulation, and mineralisation by microbial activities [\(Beyer et al., 2014; Jarvis, 2007; Riah et al., 2014; Watanabe](#page--1-0) [and Takagi, 2000](#page--1-0)). Thus, the fate of pesticides in environmental systems is quite complex [\(Gassmann et al., 2014\)](#page--1-0). European Union (EU) legislation provides rules to prevent and cure the chemical pollution of water: the selection and regulation of substances of EU-wide concern (the priority substances) and the selection of substances by individual member states of national or local concern (pollutants specific to river basins) for control at the relevant level ([EC, 2012](#page--1-0)). As a general criterion, critical pesticide concentrations of 0.1  $\mu$ g l<sup>-1</sup> have been defined as admissible in drinking water in the EU. With increasing pesticide use, pesticide occurrence is high, and some pesticides have been banned for years [\(Zhong et al., 2014\)](#page--1-0). Many studies have been conducted on the dispersion of pesticides and their accumulation and translocation in water, soil, and plants, but identifying their source is difficult due to the qualification and quantification of hundreds of compounds with different physicochemical properties in different climatic conditions ([Parween et al., 2014; Steffens](#page--1-0) [et al., 2014](#page--1-0)).

Pesticide transport in soil has two important paths: vertical leaching and horizontal washing. Both are involved in water-soil interphase reactions associated with pesticide degradation and ad/desorption. To assess the risks of pesticide leaching, mathematical models have been proposed [\(Styczen et al., 2011](#page--1-0)), such as the one-dimensional MACRO [\(Jarvis et al., 1994\)](#page--1-0) and PRZM\_GW model ([Carsel et al., 1985](#page--1-0)). Other leaching models such as LEACHM ([Hutson et al., 1989](#page--1-0)), PLM ([Nicholls](#page--1-0) [et al., 2000](#page--1-0)), PEARL [\(Leistra et al., 2001](#page--1-0)), and GeoPEARL [\(Tiktak et al.,](#page--1-0) [2002\)](#page--1-0) have been developed either based on principles of chemical dispersion or drawing on advanced technology. Surface runoff is another important mechanism for pesticide transport, especially in highly erodible areas. Heavy rains can move pesticides both in the runoff water and attached to eroded soil particles [\(Majewski et al., 2014\)](#page--1-0). This displacement may adversely affect ponds, lakes, rivers, and aquatic ecosystems in general [\(Blann et al., 2009](#page--1-0)). Models have been developed to simulate pesticide transport with surface water, such as ARM [\(Donigian and](#page--1-0) [Davis, 1978](#page--1-0)), CREAMS [\(Knisel, 1980](#page--1-0)), ANSWERS ([Dillaha and Beasley,](#page--1-0) [1983\)](#page--1-0), AGNPS ([Young et al., 1986](#page--1-0)), RZWQM [\(Ahuja et al., 2000\)](#page--1-0), and PeLM ([Chen et al., 2004\)](#page--1-0). These models for assessing the risks of pesticides mainly focus on the dissolved portion, and the pesticides absorbed on particulate particles have rarely been characterised ([McGechan and](#page--1-0) [Lewis, 2002\)](#page--1-0).

In the present paper we quantify pesticide transport in soil, taking a first-order decay into account, by integrating models of runoff and erosion with variable rates of infiltration and sorption. The duration of pesticide decay before erosion and degradation rate was also included in the developed model. Basic model concepts and algorithms to verify pesticide transport associated with these processes are tested and discussed based on the performance of the selected reference output values.

## 2. Theory and governing equations

Pesticides applied to the soil surface that bypass the foliage are transported to deeper soil layers by infiltrating rainwater. Water ponding and surface runoff by Hortonian or Dunne overland flow can occur under certain circumstances, e.g. if rainfall exceeds the infiltration capacity of the soil or if the soil contains a low amount of stored water, which may induce soil erosion and pesticide displacement, either dissolved in runoff or entrained with the eroded soil. The quantity of pesticide actually moved to the surface water or depressions on the soil surface therefore depends on the amounts of runoff, erosion, and pesticide in the eroded soil. The latter in turn depends on the depth to which the pesticide has penetrated into the soil and how much of it has degraded.

# 2.1. Runoff and infiltration

Surface runoff occurs if the soil is saturated and its capacity to store infiltrating water has become depleted, but it occurs also if rain intensity exceeds the hydraulic conductivity of the soil. Surface runoff and overland flow are complex processes, and modelling can be highly demanding on the data and computational power ([Van der Ploeg et al., 2012\)](#page--1-0). Concerning runoff and erosion strongly depending on local micro- and mesotopogrophy but not only on "global" hillslope, we have chosen to parsimoniously model a relatively flat agricultural terrain. The runoff rate could thus be expressed as a functional relationship among precipitation rate, infiltration rate, and surface-soil roughness. Rearranging the terms of the equation presented by [Appels et al. \(2011\)](#page--1-0) yields:

$$
\frac{r(t)}{p(t)} = \left(1 - \frac{i(t)}{p(t)}\right) \cdot f\left[\frac{P - I}{DSC}\right] \tag{1}
$$

which can be rewritten as:

$$
r(t) = p(t) \left( 1 - \frac{i(t)}{p(t)} \right) \cdot f \left[ \frac{P - I}{DSC} \right] \tag{2}
$$

where t is the rainfall time (min),  $r(t)$  is the runoff rate (m min<sup>-1</sup>),  $p(t)$ is the precipitation rate (m min<sup>-1</sup>),  $i(t)$  is the infiltration rate  $(m min<sup>-1</sup>)$ , P is the cumulative precipitation  $(m<sup>3</sup>)$ , I is the cumulative infiltration ( $m<sup>3</sup>$ ), and DSC is the storage capacity of depressions ( $m<sup>3</sup>$ ), where the latter three may be expressed per  $m<sup>2</sup>$ . In these equations, precipitation (either as a cumulative value or as a rate) is a forcing function that is derived from observations or climatic data. Eq. (2) is based on the assumption of a fill-and-spill mechanism for surface depressions that overflow, with an instantaneous redistribution of runoff water in a unit area  $(m^2)$ . A more dynamic modelling of runoff has been described by [Yang and Chu \(2015\).](#page--1-0) Their method is computationally much more demanding, and produces similar results to those by [Appels et al.](#page--1-0)  $(2011)$ . Therefore, it was decided to use Eqs.  $(1)-(2)$ .

The function f[.] in Eq. (2) depends on the micro-, meso-, and macrotopographical features of the soil and is often sigmoid. The logistic function is a suitable and flexible function that captures experimental forms well:

$$
f[x] = \frac{1}{(1 + ae^{-bx})}
$$
\n<sup>(3)</sup>

where *a* and *b* are dimensionless parameters, and  $x = (P-I)/DSC$ .

The value of DSC is governed by the roughness of the soil surface, which in turn depends on the presence of soil aggregates (at small or local topographical scales), tillage meso-structure, and the (macroscopic or global) slope of the field. We corrected the DSC-value for slope based on our observations and those by R. Barneveld [Bioforsk, Aas, Norway, pers. comm., 2014] according to:

$$
DSC(S) = DSC(0) \cdot e^{\alpha S} \tag{4}
$$

where S is the slope of the terrain ( $\degree$ ), and  $\alpha$  is a coefficient ( $\degree$ <sup>-1</sup>).

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