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# Evaluation of two pesticide leaching models in an irrigated field cropped with corn

Dorothea D. Giannouli, Vassilis Z. Antonopoulos*

*School of Agriculture, Aristotle University of Thessaloniki, 54124 Thessaloniki, Greece*

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ABSTRACT

Pesticide leaching models is an easy and cost effective method used in the prediction of surface and groundwater pollution. In this paper, the ability of two pesticide leaching models, MACRO and PEARL, to describe soil water dynamics and atrazine's transport through the soil profile was examined. The data used for the comparison was obtained from an experiment in an irrigated corn field in the plain of the Ardas River, in north-eastern Greece. Both models were parameterized using pedotransfer functions, field and laboratory data. The uncalibrated simulation showed several discrepancies, therefore the retention curve and the sorption parameters were calibrated according to the trial and error method. The comparison of both models indicated that soil water flow was described similarly. The simulated results of atrazine's concentration were evaluated and compared to the measured concentrations at specific depths, using statistical criteria. Atrazine transport was simulated in a satisfactory manner as confirmed by model efficiency (*EF*) values, that are very close to unit. Coefficient of residual mass (*CRM*) values for both models are positive, indicating that both models underestimate the measured data. MACRO estimated higher accumulated actual evapotranspiration values, and less percolated water from soil profile than PEARL, and as a result, change in water content was higher in the latter. PEARL also predicted that half the amount of the applied mass was decayed two days earlier than the day estimated by MACRO. Generally, MACRO simulated the fate of atrazine in soil better than PEARL.



## 1. Introduction

Agriculture is one of the main sources of groundwater contamination, because of the extended use of pesticides and other agrochemicals. Several monitoring studies mention the presence of agrochemicals in surface and groundwater (Cooper, 1996; Reemtsma et al., 2013). Several studies confirm the presence of numerous pesticides in groundwater (Hallberg, 1989; Papastergiou and Papadopoulou-Mourkidou, 2001; Gonçalves et al., 2007). Apart from biotic, the extensive use of pesticides influences also the abiotic processes in soil (Zeng et al., 2012; Fenner et al., 2013). The European Union, in order to protect groundwater from pollution, promotes several directives such as the Water Framework Directive (2000/60/EC), the Groundwater Directive (2006/118/EC) and the recent Directive 2013/39/EU, regarding priority substances in the field of water policy. Besides, according to the Directive 98/83/EC, it is important that agrochemicals that reach groundwater do not exceed a concentration of 0.1 μg/L.

In Greece, water pollution is caused mostly by the plant protection products used in corn, rice and cotton crops. According to Albanis et al. (1998), the maximum concentration of DEA and metolachlor detected in river water samples reached a value of 0.53 and 0.56 μg/L, respectively. Atrazine has been detected in significant concentrations (1.51 μg/L) in the groundwater of corn-growing areas of Northern Greece (Papastergiou and Papadopoulou-Mourkidou, 2001). High concentration levels of atrazine were also detected at the depth of 35 cm (1166 μg/L, Vryzas et al., 2012). In a recent study (Kalogridi et al., 2014), several pesticides and especially triazines, were detected in the surface waters and sediments of Lakes Kerkini, Doirani and Volvi, in Northern Greece.

An efficient and low cost method for a preliminary assessment of groundwater vulnerability is the use of mathematical models. Various models like GLEAMS (Knisel and Davis, 2000), PRZM 3.21 (Carsel et al., 1998) and PEARL (Leistra et al., 2001) have been developed for the description of soil water movement and pesticide leaching. These models can simulate not only water flow and pesticides fate, but also most of the processes that compose the water

* Corresponding author.
*E-mail address:* vasanton@agro.auth.gr (V.Z. Antonopoulos).

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and mass balance. Vanclooster et al. (2000) presented an assessment of twelve models simulating water movement and pesticide transport in soil, with the purpose of describing the problems encountered in using these models, and to introduce a Good Modelling Practice. In recent years though, there has been a strong tendency to incorporate soil water movement through macropores, commonly known as preferential flow, into leaching models. For this reason, many models that account for preferential flow, such as HYDRUS (Šimůnek et al., 2005), RZWQM (Ahuja et al., 2000a,b) CRACK-NP (Armstrong et al., 2000b) and MACRO (Larsbo and Jarvis, 2003) have been developed. Despite the advantages a mathematical model can provide, when it comes to a comparison between two or more models, certain discrepancies may be observed. Armstrong et al. (2000a) and Persicani (1996) mention the variability in models' prediction.

Although many studies concerning pesticide leaching in soil columns or lysimeters can be found in literature, only a few are based on data derived from field scale experiments (Flury et al., 1995; Flury, 1996; Vanclooster et al., 2000). The lack of measured values, especially at field scale, led to the use of stochastic parameters (Köhne et al., 2009). Among the limited number of comprehensive field-scale tests of pesticide transport models is the work of Suarez et al. (2013), who studied the transport of simazine in a vineyard using the HYDRUS 2D model. Other works with measured field data include the validation of the PEARL model using data from two sites in the Netherlands and Sweden (Bouraoui, 2007), the testing of the MACRO model in a cracked clay soil in the Netherlands by Scorza et al. (2007), and the impact of different irrigation practises on herbicide leaching by Fait et al. (2010).

Recognizing the lack of site-specific data, this paper tries to contribute to the testing and the validation of two of the most commonly used in Europe models in the prediction of pesticide leaching. MACRO and PEARL models were used to simulate soil water dynamics and a solute's fate in a clayey soil, using the field data from an irrigated field cropped with corn in north-eastern Greece, under the climate and growing conditions of a Mediterranean area.

## 2. Method

### 2.1. Description of the MACRO and PEARL models

MACRO 5.2 (Larsbo and Jarvis, 2003) and PEARL 4.4.4 (Leistra et al., 2001) are two representative pesticide leaching models, and were chosen in this study because of their credibility and ease of use (Jarvis, 1995; Boesten and van der Linden, 2001; Scorza and Boesten, 2005; Scorza et al., 2007; Köhne et al., 2009; Fait et al., 2010). FOCUS team (Boesten et al., 2000) through realistic worst-case scenarios, evaluated MACRO and PEARL models as a first-tier assessment of a pesticide leaching to groundwater. Since a full description of MACRO and PEARL is given elsewhere (Larsbo and Jarvis, 2003; Tiktak et al., 2000), only a brief summary of the models will be presented here.

Both MACRO and PEARL are one-dimensional models which describe water flux, heat, and solute transport in soil matrix. Moreover, both account for a complete water balance including water flow, canopy interception and root water uptake, seepage to drains and groundwater. PEARL is linked with the SWAP model (Van Dam et al., 1997), whose soil hydrology is described by Richard's equation. MACRO is a dual permeability model which simulates preferential flow of water and solutes by dividing the soil matrix into the micropore and macropore domain, each one described by specific characteristics such as degree of saturation, conductivity and flux. Therefore, soil water flow in micropores is also described by Richards equation, and a kinematic wave equation is used in the macropore domain.

A convection–dispersion equation is used to describe the solute's transport, and in the macropore domain, MACRO uses only the convection equation. In both models, instantaneous equilibrium or kinetic sorption is described by either a linear or a Freundlich equation, and degradation by first order kinetics, depending on soil water content, temperature and depth. The degradation process in MACRO occurs in both domains. PEARL can also account for a pesticide's volatilization from soil or the plant's canopy, while MACRO does not account for this process.

Crop growth in both models is described by a simple model where both the leaf area index (LAI) and the rooting depth are a function of the development stage of the crop. In MACRO, LAI and root depth follow a logistic curve, when in PEARL both are linear. Potential evapotranspiration is calculated using the equation of Penman–Monteith (Allen et al., 1998) or can be pre-calculated and provided by the user, and can be partitioned into actual evaporation and transpiration through reduction functions. Finally, both models assume that runoff happens when infiltration capacity is exceeded. All these processes are also summarized in Table 1.

Several studies are included in literature where PEARL and MACRO models were used to describe the water flow and the pesticide transport in soil (Scorza and Boesten, 2005; Scorza et al., 2007; Leistra and Boesten, 2010; Stenemo et al., 2007). In some cases, MACRO did not considered for preferential flow, and was used only for the one-domain approach (Antonopoulos et al., 2013). Because of the importance of the flow through the soil macropores, Tiktak et al. (2012a,b) presented two studies where PEARL, through macropore modules, could account for preferential flow (or a two-domain approach). This version of PEARL though, is unavailable to general public due to further testings.

## 3. Field and computational data

### 3.1. Site description and data sets

The data used was derived from a 0.4 experimental field site in the Ardas River plain (41°37′ N, 26°21′E) in north-eastern Greece and was presented elsewhere in detail (Fragkoulis, 2003; Vryzas et al., 2007; Antonopoulos et al., 2011). Ardas River plain is one of the most important areas nationwide for corn production, and is characterized by warm summers and wet and cold winters, where

**Table 1**
Description of the MACRO and PEARL processes.

| | MACRO | PEARL |
|---|---|---|
| Water flow | Micropores: Richard's equation<br>Macropores: Kinematic wave | Richard's equation |
| Solute transport | Micropores: Convection dispersion equation<br>Macropores: convection (gravity flow) | Convection dispersion equation |
| Sorption | Linear or Freundlich<br>Instantaneous equilibrium and kinetic sorption for micro- and macropores | Linear or Freundlich, Instantaneous and non equilibrium |
| Degradation | First-order kinetics, separate rate coefficients for both solid and liquid phase of micro- and macropores | First-order kinetics |
| Water uptake | Empirical sink terms | A function of transpiration |
| Volatilization | No | Soil and canopy |
| Initial condition | Soil water content and temperature | Groundwater level |
| $ET_p$ | Penman–Monteith or input | Penman–Monteith, Makkink, or input |
| $ET_a$ | Reduction functions | Reduction functions |
| Crop growth | LAI as a Logistic function | LAI as a Linear function |