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SENSITIVITY ANALYSIS OF THE PESTICIDE LEACHING MODEL PEARL FOR THREE BRAZILIAN SCENARIOS

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ABSTRACT: Sensitivity analysis of mathematical models has the aim to identify the relationship between model inputs and outputs. For an accurate use of pesticide leaching models it is necessary to assess the sensitivity of input parameters. The aim of this work was to carry out sensitivity analysis of the pesticide leaching model PEARL for contrasting soil types using data of Rio Dourados watershed in Mato Grosso do Sul State, Brazil. Sensitivity analysis was done by carrying out many simulations with different input parameters and calculating their influence on the output values. The approach used was the so called one-at-a-time sensitivity analysis, which consists in varying independently input parameters one at a time and keeping all others constant with the standard scenario values. Sensitivity analysis was automated using SENSAN tool that was linked to the PEARL model. Results have shown that only soil characteristics influenced the simulated flux of water resulting in none variation of this variable for scenarios with different pesticides. All input parameters that showed the greatest sensitivity with regard to leached pesticide are related to soil and pesticide properties. Sensitivity of all input parameters was scenario-dependent, confirming the importance of using more than one standard scenario for sensitivity analysis of pesticide leaching models.
KEYWORDS: calibration, inverse modeling, PEST

INTRODUCTION: Pesticides used in the agriculture can pose contamination risks to groundwater and surface water resources. Risk assessment for each pesticide is necessary. However, this assessment at field scale for all combinations of pesticides, soil and climate conditions is time- and money consuming (BOESTEN, 2000). To overcome this limitation, mathematical models have been created to simulate pesticide leaching considering the diversity of climate conditions, soils and pesticides. Thus, the use of pesticide leaching models for risk assessment can result in economy of time and financial resources. One of these pesticide leaching models is the PEARL model (LEISTRA et al., 2002; TIKTAK et al., 2002), which has been used for pesticide risk assessment within the European Union. Sensitivity analysis of mathematical models has the aim to identify the relationship between model inputs and outputs (DUBUS et al., 2003). One important use of sensitivity analysis is to identify which are the most important parameters in a model. On the other way, sensitivity analysis can identify the least relevant parameters and suggest model refinement or simplification (WOLT et al., 2002). Moreover, sensitivity analysis can help in the selection of parameters for model calibration and probabilistic modeling. DUBUS et al. (2003) states that for an accurate use of pesticide leaching models it is necessary to assess the sensitivity of input parameters. Results of sensitivity analysis have shown to be scenario dependent. Thus, there is a need to carry out sensitivity analysis for different scenarios. Studies that show the sensitivity analysis of pesticide leaching models under Brazilian scenarios are scarce. The aim of this work was to carry out sensitivity analysis of the PEARL model for contrasting soil types using data of Rio Dourados watershed in Mato Grosso do Sul State, Brazil.

METHODOLOGY: The pesticide leaching model used for sensitivity analysis was PEARL version 3.3.3 (LEISTRA et al., 2002; TIKTAK et al., 2002). PEARL uses the SWAP model (VAN DAM et al., 1997) to describe the soil water flow using Richards's equation and considering a one-dimensional, vertical and transient flow. Soil temperature is simulated using the combination of Fourier's law and the conservation equation for heat in soil. The relationship between soil water content and its pressure head is described by the Van Genuchten model and the hydraulic conductivity by the Mualem model (VAN GENUCHTEN, 1980). In PEARL, the mass conservation equation of pesticide in soil is given by:

$$\frac{\partial C^*}{\partial t} = \frac{\partial}{\partial z}\left(q \cdot C_L - D_L \frac{\partial C_L}{\partial z} - D_G \frac{\partial C_G}{\partial z}\right) - R_T - R_U \quad (1)$$

where C^* is the total mass concentration of pesticide in soil (g cm^{-3}), t is time (day), z is depth (cm), q is the volume flux of water in soil (cm day^{-1}), C_L is the mass concentration of pesticide in the liquid phase (g cm^{-3}), D_L is the hydrodynamic dispersion coefficient (cm^2 day^{-1}), D_G is the gas diffusion coefficient (cm^2 day^{-1}), C_G is the mass concentration of pesticide in the gas phase (g cm^{-3}), R_T is the transformation rate of pesticides in soil (g cm^{-3} day^{-1}) and R_U is the pesticide uptake by plants (g cm^{-3} day^{-1}). Pesticide sorption is described with the Freundlich isotherm. The transformation rate of pesticides in soil is described by a first-order equation. Input data for PEARL were obtained in the literature and in-situ measurements. Meteorological data were obtained from a time-series of 27 years from 01 January 1980 until 31 December 2006 at the meteorological station at Embrapa Western Region Agriculture, in Dourados, MS. Sensitivity analysis was done by carrying out many simulations with different input parameters and calculating their influence on the output values. The approach used was the so called one-at-a-time sensitivity analysis (DUBUS et al., 2003). It consists in varying independently input parameters one at a time and keeping all others constant with the standard scenario values. Thus, it is possible to assess the sensitivity of each input parameter by observing the influence on model outputs. Sensitivity analysis was automated using SENSAN tool which is part of the inverse modeling PEST package (DOHERTY, 2000). This tool is linked to PEARL model using input and output files. SENSAN uses a template file to create PEARL input files. Thereafter, SENSAN runs simulations to obtain output files and carry out sensitivity analysis. SENSAN interferes in PEARL using its input and output files only and thus it is fully model independent. Variation in the output values was always calculated in relation to a pre-established standard scenario. Six different standard scenarios were used as a result of three soil types (0-100 cm depth) and two pesticides combination. The following three contrasting soil types from Dourados river watershed were used: a very clayey typical dystroferric Red Latossol (LVdf), a distrofic Red Latossol (LVd) and a distrofic Red Argisol (PV). The average values of clay content for 0-100 cm depth were 680 g kg^{-1} for LVdf, 230 g kg^{-1} for LVd, and 90 g kg^{-1} for PV. The range values of organic matter content for 0-100 cm depth were between 33.4 g kg^{-1} and 11.3 g kg^{-1} for LVdf, between 17.5 g kg^{-1} and 11 g kg^{-1} for LVd, and between 7.5 g kg^{-1} and 4.7 g kg^{-1} for PV. The range values of saturated soil hydraulic conductivities for 0-100 cm depth were between 1.21 and 7.34 m day^{-1} for LVdf, between 0.49 and 3.73 m day^{-1} for LVd, and between 0.8 and 6.98 m day^{-1} for PV. Two pesticides with contrasting field behavior were selected. The values of K_{OM} were 10 L Kg^{-1} for pesticide 1 and 120 L kg^{-1} for pesticide 2 and the half-life values were 20 days for pesticide 1 and 80 days for pesticide 2. The output variables in PEARL used for calculation of sensitivity analysis were cumulative volume flux of water percolated at 1 m depth (m) and cumulative areic mass of leached pesticide at 1m depth (kg ha^{-1}). Sensitivity of each input parameter for an individual scenario was assessed using the ratio of variation (ROV) given by the relationship between output and input variation. For each simulation, ROV was calculated based on five different input values. The sensitivity of the input value was represented by the maximum absolute ratio of variation (MAROV) given by (DUBUS et al., 2003):

$$MAROV = max\left|\frac{O - O_{ss}}{I - I_{ss}} * \frac{I_{ss}}{O_{ss}}\right| \quad (2)$$

where O is value of the output variable, O_{SS} is the value of the output variable for the standard scenario, I is the value of the input parameter and I_{SS} is the value of the input parameter for the standard scenario. The larger the MAROV value, the more influence a parameter has on model output. If MAROV equals 10, the disturbance of model input will be propagated through the model and amplified to result in a maximum variation of the output by 10 times more.

RESULTS AND DISCUSSION: Simulated cumulative volume flux of water percolated at 1 m depth for all six standard scenarios was in the range between 19,010 and 27,110 mm for the 27-year period. The total cumulative precipitation in this period was 39,410 mm. The simulated cumulative fluxes of water percolated at 1 m depth represented 48%, 54%, and 69% of the total precipitation for LVdf, LVd, and PV, respectively. As expected, only soil characteristics influenced the simulated cumulative flux of water resulting in none variation of this variable for scenarios with different pesticides. The simulated cumulative areic mass of leached pesticide at 1m depth for all six standard scenarios was in the range between 0.09 and 6.47 kg ha^{-1}. These amounts correspond to 0.09 and 6.47% of the applied amount (i.e. 100 kg ha^{-1}) and are in the range of the expected amount leached in the field of about 5% (CARTER, 2000). It means that standard scenarios used for sensitivity analysis can mimic a real situation in the field. The greatest pesticide leaching was on PV soil. Both soil and pesticide characteristics influenced the variable cumulative areic mass of leached pesticide at 1 m depth. Results from sensitivity analysis with regard to cumulative areic mass of leached pesticide show that the most sensitivity input parameters (i.e. MAROV >10) were: reference temperature in which half-life was measured (TR), pesticide half-life (HL), organic matter content (OM), organic matter/water distribution coefficient (KOM), Freundlich exponent (FE) and dry soil bulk density (DENS) (Figure 1).

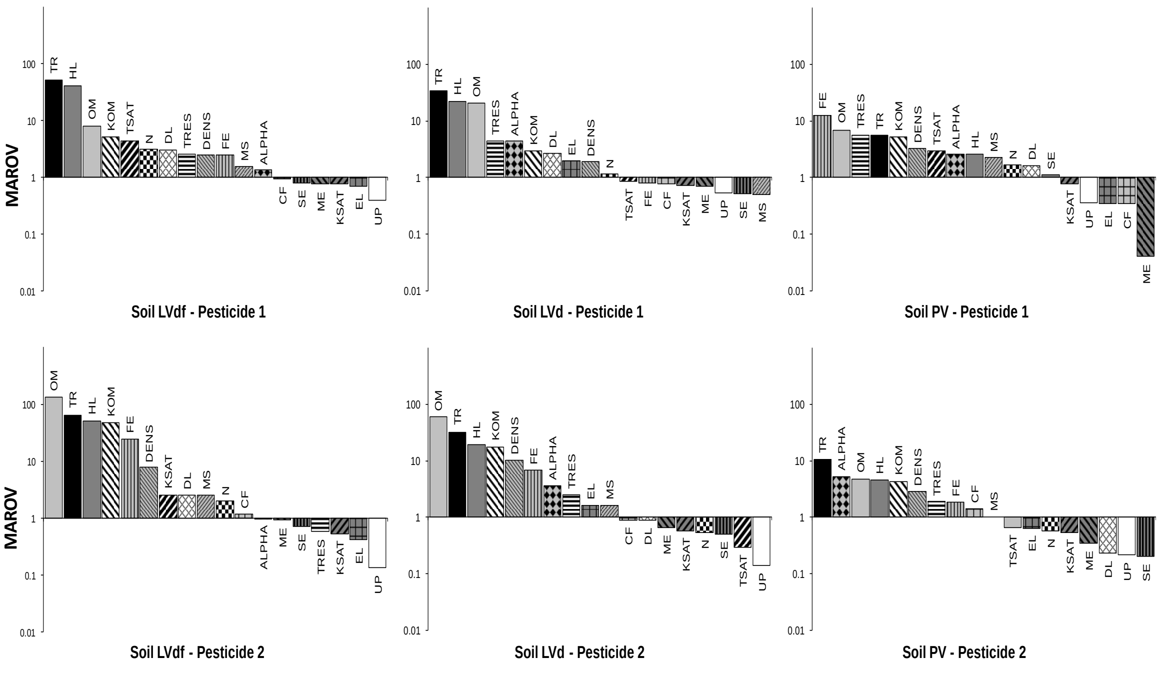

FIGURE 1. MAROV values for all six scenarios. TR = Reference temperature of half life, HL = half-life, OM = organic matter content, KOM = organic matter/water distribution coefficient, TSAT = saturated water content, N = Van Genuchten parameter, DL = dispersion length, TRES = residual water content, DENS = soil bulk density, FE = Freundlich sorption exponent, MS = molar enthalpy of sorption, ALPHA = Van Genuchten parameter, CF = crop factor, SE = parameter in soil evaporation reduction equation, ME = molar activation energy, KSAT = saturated hydraulic conductivity, EL = exponent for the effect of soil moisture content on degradation, UP = coefficient for uptake by plant.

All input parameters that showed the greatest sensitivity are related to soil and pesticide properties. Input parameters related to soil water flow and crop properties (e.g. residual water content – THETARES and crop factor – CF) did show low sensitivity with regard to cumulative areic mass of leached pesticide (Figure 1). Sensitivity of PEARL input parameters was scenario-dependent. Scenarios with LVdf soil type did show the greatest MAROV values followed by LVd and PV soil types, respectively. This confirms the importance of using more than one standard scenario for sensitivity analysis. Important to mention that the magnitude of the sensitivities was scenario-dependent and was smallest for scenarios where the greatest losses were predicted (i.e. PV soil type) and greatest for the scenario where the smallest losses were predicted (i.e. LVdf and LV soil types) (Figure 1).

CONCLUSION: Sensitivity analysis of the PEARL model was scenario-dependent under Brazilian conditions. Thus, it is important to know input parameters sensitivity based on the scenarios the model will be used before any application for pesticide risk assessment in Brazil.

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