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Model prediction uncertainty of bromide and pesticides transport in laboratory column

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Knowledge of transport parameters of reactive solutes such as pesticides is a prerequisite for reliable predictions of their fate and transport in soil porous systems. Water flow and transport of bromide tracer and five pesticides (atrazine, imazaquin, sulfometuron methyl, S-metolachlor, and imidacloprid) through an undisturbed soil column of tropical Oxisol were analyzed using a one-dimensional numerical model. Laboratory column leaching experiment with three flow interruptions was conducted. The applied numerical model is based on Richards' equation for solving water flow and the advection–dispersion equation for solving solute transport. A global optimization method was used to evaluate the model's sensitivity to transport parameters and the uncertainty of model predictions. Within the Monte Carlo modeling framework, multiple forward simulations searching through the parametric space, were executed to describe the observed breakthrough curves. All pesticides were found to be relatively mobile. Experimental data indicated significant non-conservative behavior of bromide tracer. All pesticides, with the exception of imidacloprid, were found less persistent. Three of the five pesticides (atrazine, sulfometuron methyl, and S-metolachlor) were better described by the linear kinetic sorption model, while the breakthrough curves of imazaquin and imidacloprid were more appropriately approximated using nonlinear instantaneous sorption. Sensitivity analysis suggested that the model is most sensitive to sorption distribution coefficient. The prediction limits contained most of the measured points of the experimental breakthrough curves, indicating adequate model concept and model structure for the description of transport processes in the soil column under study.