Simulation of atrazine and metolachlor transport in andisol using HYDRUS-1D model

HYDRUS-1D モデルを用いた黒ボク土壌中のアトラジンとメトラクロールの挙動シミュレーションについて

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1. Introduction

Inappropriate use and management of pesticides may affect the aquatic as well as terrestrial environments. Thus, the prediction and assessment of the pesticide fate and transport in soil is required to minimize the adverse impacts on the environment. Atrazine and metolachlor are the commonly used pesticides to control broadleaf weeds for the protection of corn, tea, sugarcane, etc (Celestino Ladu J.L. et al, 2011). HYDRUS-1D model was used to investigate the transport of these herbicides in andisol soil (Šimůnek J. et al, 2013). The objective of this work was to simulate and assess the atrazine and metolachlor concentrations in the soil column.

2. Material and method

Soil samples were collected at an experimental field of Tokyo University of Agriculture and Technology from the surface to 5 cm of depth. The soil samples were air-dried and ground to pass through a 2-mm sieve before visible roots and organic residues were removed. The soil samples were packed to a soil column at the dry bulk density of 0.498 g.cm^{-3} and were saturated. After 24 hours, the atrazine and metolachlor were mixed to the soil surface with 0.33x10^{3} mg.L^{-1} for atrazine and 0.32x10^{3} mg.L^{-1} for metolachlor. Water was applied at 0.2 cm.minute^{-1} to the soil surface for 210 minutes. The soil physical characteristics and the conditions of numerical experiments for running HYDRUS-1D model are described in Table 1. To simulate pesticide transport with HYDRUS-1D, we first experimentally obtained adsorption

Table 1. The soil characteristics and pesticides parameters values for HYDRUS-1D model simulation.

Parameters	Soil column	
Residual soil water content (cm^{3}.cm^{-3})	0.1	
Saturated soil water content (cm^{3}.cm^{-3})	0.37	
Saturated hydraulic conductivity (cm.minute^{-1})	0.49	
	Atrazine	**Metolachlor**
Molecular diffusion coefficient (cm^{2}.minute^{-1})	334.73 x10^{-6}	305.76 x10^{-6}
Adsorption isotherm coefficient (cm^{3}.mg^{-1})	0.0045	0.003
First-order rate constants (minute^{-1})	2.013x10^{-5}	1.944x10^{-5}

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isotherm coefficients and first-order rate constants for both pesticides. The study compared the HYDRUS-1D model output with the experimental data to assess the accuracy of the simulation.

3. Results and discussion

Fig 2 shows the simulated breakthrough curves (BTCs) of the two pesticides with the experimental conditions using the single porosity model considering equilibrium. At middle of the soil column, the soil water concentrations increased to maximum values of 2.21 and 2.3 mg.L^{-1} at 35 and 32 minutes and decreased to 0.6 and 0.58 mg.L^{-1} at the final time for atrazine and metolachlor, respectively. At other nodes, the concentration has the same trend with different in time of peak and amount of concentration.

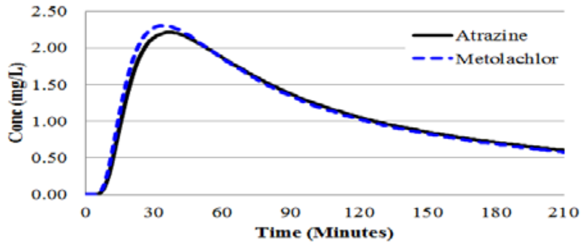

Fig 2. The soil water concentrations of atrazine (line) and metolachlor (dot) at the middle of the soil column.

The study compared observed data with the simulated concentrations at 35cm depth (Fig 3). In general, the HYDRUS-1D simulated the observed herbicide concentrations with high accuracy up to the maximum concentrations for both atrazine and metolachlor. The maximum observed concentrations in the soil water at outlet of the soil column were about 1.19 and 1.28 mg.L^{-1}, respectively. After the maximum concentrations, simulated values have started to deviate from observed values for both herbicides. The RMSE values between the simulated results and the observed data were about 0.25 for atrazine and 0.26 for metolachlor. On the other hand, the comparison of sorbed concentrations showed difference shapes at final time. The shapes of simulated values are inverted with observed data. The simulated sorbed concentration values were higher than observed data from 4.4 to 5.2 times. Therefore, it seems more calibration effort for input parameters such as equilibrium partitioning coefficient and dispersivity may be required for more accurate simulation.

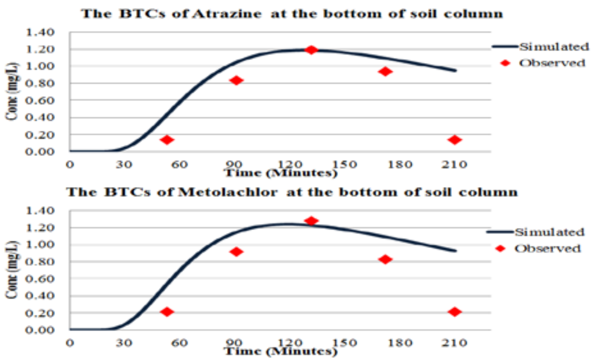

Fig 3 . The comparison of observed and simulated BTCs for these herbicides.

4. Conclusions

This study simulated the transport of atrazine and metolachlor in the soil column using the HYDRUS-1D. For the simulation, dispersivity and equilibrium partitioning coefficient which might have effect on the simulation results had been adjusted by manual calibration. Finally, the tendency of pesticide movement was similar for the soil water concentrations of simulated values and observed data. However, farther calibrations of transport parameters are required for improving the simulation of experimental data for concentration in the soil column.

References: Celestino Ladu J.L., Zhang .D.R,(2011). Modeling atrazine transport in soil columns with HYDRUS-1D. Journal of Water Science and Engineering, Vol.4No.3, 258-269; Šimůnek J., Šejna M., Saito H., Sakai M., and van Genuchten M. Th.,(2013). The HYDRUS-1D Software user manual version 4.16, 115-132.