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Simulating Dissolved Chemical Transport from Saturated Soil to Overland Flow by Interfacial Diffusion and Raindrop Dispersion

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Abstract

Interfacial diffusion and raindrop dispersion both affect solute and pollutant transfer from soil to overland flow. In this study, we propose a modified model to describe the transfer of dissolved chemicals from saturated soil to overland flow. The model was based on the concept of a diffusion-like model by taking into account the impact of raindrop dispersion. The model was solved analytically under non-infiltration conditions. Experimental data were collected for model parameters estimation and model validation. Results showed the interfacial diffusion by concentration gradient contributed about 80% of the chemical transfer from soil to runoff water, while raindrop dispersion contributed about 15%. The model predicted well for both the chemical concentration in runoff water and in soil profile.

Introduction

➢Solute transfer at the soil surface/overland flow interface is an important process that controls pollutant transport in runoff water. Mathematical models are often used to represent this process.

➢ The existing models that describe the transfer of chemicals at the interface can be divided into three categories.

(1) Mixing layer models

They have been used for decades due to their simplicity of fewer parameters. But the depth of the mixing zone in the models cannot be easily quantified. The theory becomes more complex if infiltration and non-steady state runoff processes are included.

(2) Diffusion-like models

They are physically based and expandable by combining with other models to solve more practical issues. However, the current diffusion-like models do not consider the effect of raindrop detachment on solute transfer.

(3) Mixing layer-raindrop dispersion models

Raindrop impact is combined with the mixing layer theory in the models. Chemical transfer at the interface is assumed to be completely controlled by raindrop dispersion while the mass transfer induced by concentration gradient is not considered.

Objective

Since the current models all have their deficiencies, the objectives of this research are to:

(1) Develop an improved model to describe the transfer of dissolved chemicals at the soil surface and overland flow interface. The model accounts for both interfacial diffusion and raindrop ejection;
(2) Inversely estimate the model parameters by using the analytical solutions of the model and the experimental data of chemical concentration change in runoff water and at soil surface; and
(3) Evaluate the modified model using the chemical concentration change with time along the soil profile.

Model Description

➢ Diffusion-like Model

● Soil solution

$$\frac{\partial}{\partial t}[RC_s] = -\frac{\partial}{\partial z}[D\frac{\partial C_s}{\partial z}] + \frac{\partial}{\partial z}(uC_s)$$

Upper Boundary Condition

$$\left(uC_s - D\frac{\partial C_s}{\partial z}\right) = -K_L[C_s(0,t) - C_r]$$

● Overland flow

$$\frac{\partial(hC_r)}{\partial t} + \frac{\partial(qC_r)}{\partial x} = K_L[C_s - C_r] - IC_r$$

The mass transfer coefficient, K_L (LT^{-1}), is the rate of chemical transfer at the interface induced by concentration gradient. It can be calculated approximately based on channel flow parameters.

$$K_L = \frac{\rho g D_w}{\mu} f R_a^{1/3} J^{1/2}$$

It is a function of water density ρ, water viscosity μ, soil surface roughness f, hydraulic gradient J, and hydraulic radius Ra.

In the diffusion-like model, impact of raindrop ejection is neglected.

➢ Mixing Layer-Raindrop Dispersion Model

● Overland flow

$$\frac{\partial(hC_r)}{\partial t} + \frac{\partial(qC_r)}{\partial x} = E_r\left(C_m - \lambda C_r\right) - IC_r$$

● Mixing layer

$$\frac{\partial\left(\theta\varepsilon C_m\right)}{\partial t} = -D\frac{\partial C_s}{\partial z} + E_r(\lambda C_r - C_m) + I\left(C_r - C_m\right)$$

Er (LT^{-1}) is the rate that soil-water is ejected into the runoff:

$$E_r = \frac{mP}{\rho_s}\theta_s$$

Er is related to soil detachability m, rainfall intensity P, and soil dry bulk density ρ_s.

➢ Modified model

- K_L: mass transfer rate by concentration gradient
- E_r: mass transfer rate by rainfall dispersion

Since both coefficients describe the rate of dissolved chemical transfer at the interface, we define a new coefficient as interfacial transfer coefficient, let

$$T_L = K_L + E_r$$

Here, T_L represents the rate of mass transfer from soil surface to overland flow induced both by raindrop dispersion and by interfacial diffusion of dissolved chemicals. T_L is affected by rainfall, slope and roughness of soil surface, and hydraulic properties of soil.

The modified model with new coefficient is:

● Soil solution

$$\frac{\partial}{\partial t}[RC_s] = -\frac{\partial}{\partial z}[D\frac{\partial C_s}{\partial z}] + \frac{\partial}{\partial z}(uC_s)$$

Upper Boundary Condition

$$\left(uC_s - D\frac{\partial C_s}{\partial z}\right) = -T_L[C_s(0,t) - C_r]$$

● Overland flow

$$\frac{\partial(hC_r)}{\partial t} + \frac{\partial\left(qC_r\right)}{\partial x} = T_L\left(C_s - C_r\right) - IC_r$$

Results

➢ Model Parameter Optimization

The least square method was employed to optimize the model parameters using the average Br^{-1} concentrations measured from runoff water and in the top soil segment during a period of 36 min.

(1) The diffusion coefficient from model optimization was 7.2 times greater than the calculated value by the Millington & Quirk equation (1961).

The impacts of rainfall on the solute diffusion process at the soil surface may be attributed to the following two physical processes:

- Soil particles may be loosened by the raindrop splash so that there is less resistance for the solution diffusion;
- Fine particles are removed preferentially in the runoff water resulting in a layer of coarse particles near the surface so that it is easier for solute to diffuse out of the soil.

(2) The model predicted value of interfacial transfer coefficient is:

$$T_L = 3.16\times10^{-3}\ \text{cm s}^{-1}$$

The calculated values of parameters by above equations are:

$$K_L = 2.48\times10^{-3}\ \text{cm s}^{-1}$$

$$E_r = 4.5\times10^{-4}\ \text{cm s}^{-1}$$

- The sum of the calculated K_L and E_r is 2.93×10-3, which is very close to the model optimized T_L;
- About 80% of chemical transfer from soil into overland flow was induced by diffusion while near 15% was from raindrop dispersion;
- The result indicates that the modified model predicted the experimental data well, and it shows that both diffusion and rainfall dispersion are important in solute transfer at the interface.

➢ Experimental Measurement vs. Model Prediction

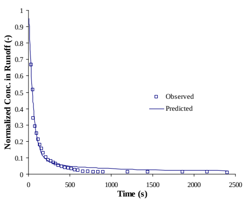

Fig. 1. Experimental and model predicted Br^{-1} concentration change with time in the runoff water. The observed points are average values of all treatments.

The chemical concentration in runoff decreased rapidly in the first 5 min. After that, it was reduced to less than 0.1C$_0$. The model prediction agreed well with the experimental data (R^2 = 0.9875) and the relationship is significant at a a level of 0.05 by Wilcoxon Rank Sum (WRS) test with P = 0.164.

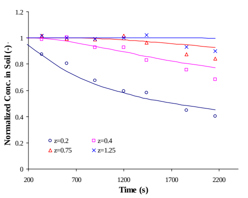

Fig. 2. Experimental and model predicted soil solution Br^{-1} concentration change with time at 0.2, 0.4, 0.75, and 1.25-cm depths. Symbols are observed data; lines are model predictions.

- The Br^{-1} concentrations below the 1.5-cm layer were nearly unchanged at 1.0C$_0$ and were not shown in the figure.
- Model prediction and experimental data were not significantly different by WRS test (P = 0.329, 0.310, 0.398, and 0.512 for the four depths, respectively).

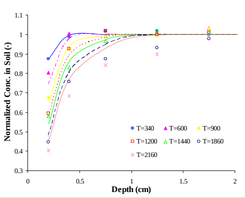

Fig. 3. Experimental and model predicted Br^{-1} concentration dynamics of the soil solution in the soil column. Symbols are data points; the lines are predicted data by model.

The predicted average soil Br^{-1} concentration agreed well with the experimental observations. The regression coefficients, R^2 for the top four layers were 0.9637, 0.9505, 0.9013 and 0.8916, respectively while WRS tests did not indicate any significant difference at P level of 0.05. Nevertheless, the model overestimated the soil Br^{-1} concentration for longer time predictions, and the errors increased with soil depth and time. Thus the model prediction is more suitable for the upper soil layers during a relatively short-time period.

Conclusions

(1) The predicted diffusion coefficient by model optimization was 7.2 times that of the calculated value;

(2) The modified model predicted the experimental data well. The mass transfer by concentration gradient at interface contributes about 80% to the total amount transfer from soil to overland flow, while rainfall dispersion contributes about 15%;

(3) For chemical concentration dynamics in the soil, the model can predict the short-term change occurred in the upper soil profile better than the long-term change in the lower profile.