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

Xiaonan Shi\textsuperscript{a,b}, Weiping Chen\textsuperscript{a}, Laosheng Wu\textsuperscript{a}, Tingwu Lei\textsuperscript{b}

\textsuperscript{a}Department of Environmental Sciences, University of California, Riverside; \textsuperscript{b}College of Hydraulic and Civil Engineering, China Agricultural University

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 can not 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
  \[
  \frac{\partial C}{\partial t} = \frac{\partial}{\partial x}\left(D \frac{\partial C}{\partial x}\right) + \frac{\partial}{\partial z}(\beta C)
  \]
  Upper Boundary Condition
  \[
  \left. C \right|_{z=0} = C_0
  \]
  - Overland flow
  \[
  \frac{\partial C}{\partial t} + \frac{\partial q C}{\partial x} = E_r(C_0 - C) + K_i(C - C_i - IC) + kl
  \]
  The mass transfer coefficient, \(K_iLT_1\), is the rate of chemical transfer at the interface induced by concentration gradient. It can be calculated approximately based on channel flow parameters.

- Mixing Layer-Raindrop Dispersion Model
  - Overland flow
  \[
  \frac{\partial C}{\partial t} + \frac{\partial q C}{\partial x} = E_r(C_0 - C) + K_i(C - C_i - IC) + kl
  \]
  - Mixing layer
  \[
  \frac{\partial C}{\partial t} + \frac{\partial}{\partial z}(\beta C + \frac{1}{\rho} \frac{\partial q C}{\partial x} + E_r(C_0 - C) + K_i(C - C_i - IC))
  \]
  \(E_rLT_1\) is the rate at which soil-water is ejected into the runoff;
  \(E_r = mW PF \rho_f\)
  \(E_r\) is related to soil detachability \(m\), rainfall intensity \(P\), and soil dry bulk density \(\rho_f\)

- Modified model
  - \(K_T\): 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
  \(T_1 = K_T = E_r\)
  Here, \(T_1\) represents the rate of mass transfer from soil surface to overland flow induced both by raindrop dispersion and by interfacial diffusion of dissolved chemicals. \(T_1\) is affected by rainfall, slope and roughness of soil surface, and hydraulic properties of soil.
  The modified model with new coefficient is:
  - Soil solution
  \[
  \frac{\partial C}{\partial t} = \frac{\partial}{\partial x}\left(D \frac{\partial C}{\partial x}\right) + \frac{\partial}{\partial z}(\beta C)
  \]
  Upper Boundary Condition
  \[
  \left. C \right|_{z=0} = C_0
  \]
  - Overland flow
  \[
  \frac{\partial C}{\partial t} + \frac{\partial q C}{\partial x} = T_1(C_0 - C) + K_i(C - C_i - IC)
  \]

Results

- Model Parameter Optimization
  The least square method was employed to optimize the model parameters using the average Br\textsuperscript{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).
2. 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 rainfall splash so that there is less resistance for the solute 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.

- Experimental Measurement vs. Model Prediction
  The chemical concentration in runoff decreased rapidly in the first 5 min. After that, it was reduced to less than 0.1C\textsubscript{0}. The model prediction agreed well with the experimental data (\(R^2 = 0.9875\)) and the relationship is significant at a level of 0.05 by Wilconxon Rank Sum (WRS) test with \(P = 0.164\).

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.