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Analysis of soluble chemical transfer from soil to surface runoff and incomplete mixing parameter identification

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Abstract

A two-layer mathematical model proposed by Tong et al. (2010) was used to predict soluble chemical transfer from soil into surface runoff with ponded water on the soil surface. Infiltration-related incomplete mixing parameter γ and runoff-related incomplete mixing parameter α in the analytical solution of the Tong et al. (2010) model were assumed to be constant. In this study, different laboratory experimental data of soluble chemical concentration in surface runoff from initially unsaturated and saturated soils were used to identify the variables γ and α based on the analytical solution of the model. The values of γ and α without occurrence of surface runoff were constant and equal to their values at the moment when the surface runoff started. It was determined from the results that γ decreases with the increase of the ponded water depth, and when the initial volumetric water content is closer to the saturated water content, there is less variation of parameter γ after the occurrence of surface runoff. As infiltration increases, the soluble chemical concentration in surface runoff decreases. The values of parameter α range from 0 to 1 for the fine loam and sand under the controlled infiltration conditions, while it can increase to a very large value, greater than 1, for the sand under the restrained infiltration conditions, and the analytical solution of the model is not valid for experimental soil without any infiltration if α is expected to be less than or equal to 1. The soluble chemical concentrations predicted from the model with variable incomplete mixing parameters γ and α are more accurate than those from the model with constant γ and α values.

Keywords: Surface runoff; Incomplete mixing parameter; Analytical solution; Soluble chemical

1. Introduction

Chemical transfer from soil to surface runoff during rainfall has become a serious agronomic and environmental problem (Wang et al., 1999; Tian et al., 2011; Yu et al., 2011). Agronomists focus on the loss of soil productivity, while environmental scientists focus on the deterioration of water quality (Wang et al., 2014). Therefore, it is necessary to study the chemical transfer from soil to surface runoff and identify the important factors helping to reduce chemical loss in surface runoff and subsequent pollution.

One of the most popular theories used in the study of soluble chemical transfer from soil to surface runoff is the mixing zone (or mixing layer) theory (Ahuja et al., 1981b). The mixing zone theory assumes that there is a region below the soil surface where the soil solution, surface water, and infiltrating water mix instantaneously; that the soil below will not supply chemicals to that region; and that the mixing zone depth is constant. The theory has been applied to experimental

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soil with ponded water on the soil surface by Gao et al. (2004). However, Zhang et al. (1997) have found that the mixing zone depth in the model for predicting soluble chemical transfer from soil into surface runoff is much less than in reality. Therefore, some researchers have developed an incomplete mixing theory (Ahuja and Lehman, 1983). Wang et al. (1999) have applied the incomplete mixing theory in the northern part of China without ponded water. The process of ponded water increasing prior to the occurrence of surface runoff has not been studied, although ponded water is very common in the southern part of China.

Using the incomplete mixing theory, Tong et al. (2010) established a two-layer model to predict the concentration of soluble chemicals, which come from soil, in surface runoff, considering an increase in ponded water. They derived an analytical solution under the assumption that the incomplete mixing parameters related to surface runoff and infiltration are constant throughout the rainfall process, and applied their model to initially unsaturated and saturated soils. Their experimental and modeled results clearly showed differences between the incomplete mixing parameters of the two soils. However, they did not analyze the experimental and modeled results with variable incomplete mixing parameters, perhaps leading to an inaccurate prediction of the soluble chemical concentration in surface runoff.

Therefore, the main objective of this study was to analyze soluble chemical transfer from soil to surface runoff and to find a way to identify and analyze the incomplete mixing parameters for the two-layer model of Tong et al. (2010), which will help provide more accurate practical predictions of the soluble chemical concentration in surface runoff from soil in the future. The mathematical model for predicting soluble chemical concentration in surface runoff from soil and the method of determining incomplete mixing parameters after surface runoff occurs is presented. An experimental study was performed of soluble chemical transfer from soil to surface runoff and the identified incomplete mixing parameters were analyzed. The results are described below.

2. Mathematical model and identification method for incomplete mixing parameters

2.1. Mathematical model and its analytical solution

The simple two-layer model from Tong et al. (2010) was used in this study (Fig. 1). The upper layer, called the whole mixing layer, includes the ponding-runoff zone and the soil mixing zone (Ahuja et al., 1981b). The lower layer is the underlying soil layer. In accordance with the assumptions of Govindaraju et al. (1996) and Ahuja et al. (1981a), chemicals in the soil mixing zone are the only source of chemicals for runoff and infiltrated water, and the chemicals are only considered to be transported vertically (Steenhuis and Walter, 1980). The chemicals in the soil mixing zone can move to the underlying soil layer with the infiltrated water. Meanwhile, the chemicals in the underlying soil layer can move to the soil mixing zone through the mass diffusion process because the

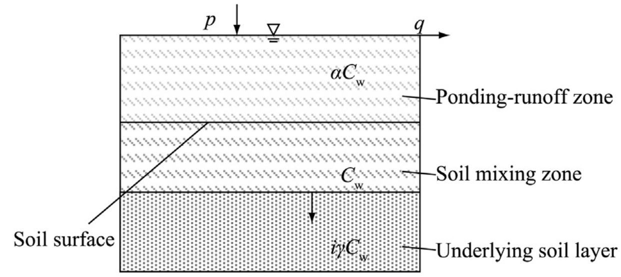

Fig. 1. Sketch of two-layer model.

chemical concentration in the underlying soil layer is higher than that in the mixing soil zone. The net chemical flux from the soil mixing zone to the underlying soil layer is expressed as $i\gamma C_{\mathrm{w}}$, where i is the soil infiltration rate, γ is the infiltration-related incomplete mixing parameter, and C_{w} is the chemical concentration in the soil mixing zone. Here, it should be noted that C_{w} is a function of time because the soil infiltration rate changes with different rainfall periods, which will be shown in the following section.

In order to describe the incomplete solute mixing in the ponding-runoff zone, a runoff-related incomplete mixing parameter α is introduced. The chemical concentration in the ponding-runoff zone is αC_{w}. In order to simplify the complicated chemical transport process near the soil surface, it is assumed that the chemical concentration is uniform in the ponding-runoff and soil mixing zones.

The mass of soluble chemicals in the whole mixing layer is written as

$$M_{\mathrm{w}}(t) = C_{\mathrm{w}}(t)\left(\alpha h_{\mathrm{p}}(t) + h_{\mathrm{mix}}\theta_{\mathrm{s}}\right) \tag{1}$$

where M_{w} is the mass of soluble chemicals per unit area in the water phase (μg/cm^2), h_{p} is the depth of ponded water on the soil surface (cm), h_{mix} is the soil mixing zone depth (cm), θ_{s} is the saturated volumetric water content in the soil mixing zone, and t is time (min).

If the chemical concentration in the rainfall is assumed to be zero, the following equation can be obtained based on mass conservation:

$$\frac{\mathrm{d}M_{\mathrm{w}}(t)}{\mathrm{d}t} = -\gamma i C_{\mathrm{w}}(t) - \alpha q C_{\mathrm{w}}(t) \tag{2}$$

where q is the specific discharge rate of the surface flow (cm/min).

Eqs. (1) and (2) can create a mass conservation model in the kinetic and static conditions in the whole mixing layer. The rainfall event is divided into four different periods, including the periods from the beginning of rainfall to the occurrence of ponded water on the soil surface, from the occurrence of ponded water to the generation of runoff, from the generation of runoff to the formation of steady runoff, and from the formation of steady runoff to the end of rainfall. The solutions to Eqs. (1) and (2) in the four periods can be obtained.

During the period from the beginning of rainfall to the occurrence of ponded water, the infiltration rate is equal to the