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A comparison of mathematical models for chemical transfer from soil to surface runoff with the impact of rain

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ABSTRACT

Chemical transfer is considered as one of the main contributors to water pollution. Three physical based models (complete-, incomplete-mixing models and the equivalent model of convection) were refined and applied to describe the process of solute transport into runoff on loessial slope land. The effects of rain intensity, slope gradient and initial water content on solute transport was studied with simulated rain. Most parameters in the models can be measured directly, some parameters, for example, α (the solute concentration ratio between the infiltration and the effective mixing depth), β (the solute concentration ratio between the runoff and the effective mixing depth) and S (the soil adsorptivity) in the incomplete-mixing model were determined by curve fitting method based on the experimental data. And, h_m (the effective mixing depth in the complete-mixing model), $h_m{}'$ (the effective mixing depth in the incomplete mixing model) and H_0 (the equivalent depth of transfer) can be expressed with a regression equation related to rain intensity, slope gradient and initial water content, respectively. Simulated results indicated that the three models are suitable to predict the amount of solute loss, and the refined equivalent model of convection fits solute transport process in runoff rather than the effective-mixing models on loessial plateau area. The complete-mixing model and the refined equivalent model of convection are convenient to use for simplified parameters, and the incomplete-mixing model was more appropriate for practical situations.

1. Introduction

The transfer of solute from soil to runoff has been recognized as a major source of contamination in receiving water bodies. The loss of nutrients from arable land has been widely studied under controlled conditions of rain intensity, slope gradient, and initial soil–water content (Heckrath et al., 1995; Chiaudani and Premazzi, 1998; Gao et al., 2004; Shigaki et al., 2007; Stutter et al., 2008; Dong et al., 2013). Extreme rains cause high nutrient losses and dissolved reactive phosphorus increases in the runoff at higher rain intensities (Shigaki et al., 2007). Soil stability, water and solute permeability have been widely studied at various slope gradients (Assouline and Ben-Hur, 2006; Donjadee and Chinnarasri, 2012). Donjadee and Chinnarasri (2012) observed that increasing the slope gradient from 3 to 30° increased the runoff volume per unit surface area from 13.4 to 21.4 mm at a rain intensity of 55 mm/h and from 46.1 to 59.6 mm at a rain intensity of 140 mm/h, indicating that slope gradient accelerated runoff. The effect of initial soil–water content on the transport of soil solute has also been investigated in many field and simulation studies. Some researchers have claimed that the initial soil–water content has a positive effect on solute runoff. Benjamin and Cruse (1985), however, found that a decrease in the matric potential from −0.2 to −4.0 kPa increased the shear strength of aggregates in clay loam and silty loam soils.

Solute transport in runoff with the impact of mentioned factors has been described with models, which are often used to predict nutrient transport and may be useful for planning good management practices for the efficient use of applied chemicals and for the effective protection of aquatic environments. The models are widely used in both laboratory and field experiments, from simple empirical formula to comprehensively distributed physically and chemically based descriptions (Beven, 1989; Novotny and Olem, 1994; Abbott and Refsgaard, 1996; Preti, 1999; Singh and Woolhiser, 2002; Singh, 2002).

In early developed models, the mixing concept is most commonly used for modeling chemical transport to the runoff (Steenhuis and Walter, 1980; Ahuja et al., 1981; Ahuja and Lehman, 1983; Wallach et al., 1988; Steenhuis et al., 1994; Zhang et al., 1997; Gao et al., 2004, 2005; Walter et al., 2007; Dong et al., 2013). Rainwater was assumed to mix completely and uniformly with a thin zone of surface soil and soil water (Steenhuis and Walter, 1980). Ahuja et al. (1981) placed ^{32}P at the soil surface and at 5-mm intervals in soil boxes and found that the interaction between rainwater and soil water was maximum at the surface and decreased rapidly with depth under free infiltration and saturated water conditions. The complete-mixing model was thus proposed

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(Ahuja et al., 1981), it hypotheses that rainwater completely mixes with soil water in the effective mixing layer (Ahuja et al., 1981), and the solute concentration in the runoff equals the concentration in the infiltrating water and in the mixing layer. Later, Ahuja and Lehman (1983) found that the concentration in runoff and in infiltration is not the same. The incomplete-mixing model was thus proposed (Ahuja, 1986), it considered that solute concentration in the effective mixing depth was in direct proportion to that in the infiltrating and runoff water. The model is also restricted to saturated water conditions without water loss, soil erosion, and soil-solute adsorption. Field runoff concentrations predicted with these models typically decreased exponentially over time (Wallach et al., 1989). Rainwater, however, mixes incompletely with soil water, Wang and Wang (2010) improved the incomplete-mixing model of solute transport and the model by introducing Philip's (1957) infiltration equation to predict solute transport in the soil of the Loess Plateau under unsaturated conditions. It was proposed that rainwater first met the water demand of the effective depth to saturation. Still, few papers have proposed the way of estimating parameters in the models.

Different from the effective-mixing models, Wallach et al. (1988) developed the effective depth of transfer model and assumed that the solute concentration in the depth was equal to the concentration at the soil surface in the absence of infiltration. The model was improved by coupling a conventional convective-dispersion equation into the mixing-depth model to describe solute transport, with the transfer coefficients varying as a function of depth (Wallach et al., 1988; Wallach and Van Genuchten, 1990). Laboratory studies by Wang et al. (1999a) proposed the equivalent model of convection based on the concept of the effective depth of transfer and assumes an equal probability of solutes being transported to the runoff from the equivalent mixing depth. This model considered that the transport of solutes from the exchange layer to the surface runoff is assumed to be dependent on the mass-transfer coefficient (Wang et al., 1999a). Dong et al. (2013) refined the equivalent model of convection based on Gao et al. (2004, 2005), proposed the solute-transport model, in which the presumed exchange layer was replaced by a mixing depth, the exchange rate was assumed to be controlled by the splashing of raindrops, and the effect of diffusion was neglected. The mass-transfer coefficient, k_m, was replaced with the variable e_r (the raindrop-induced rate of water transfer and represents the soil water ejected from the soil during rain), proposed by Gao et al. (2004), and Walter et al. (2007) also assumed that chemicals near the surface of the soil were most likely to be transported to the runoff due to the impact of raindrops. Yang et al. (2015) used the refined model with considering of the adoptive ions. The effective-mixing model and the equivalent model of convection are most popular used in solute transport simulation according to plenty of studies (Ahuja et al., 1986; Wallach et al., 1989; Dong et al., 2013; Yang et al., 2015). However, there have few studies to specify the characteristics and the applicability of each model during simulating solute transport into runoff.

The objectives of this study are to compare the feasibility and applicability of the effective-mixing models and the equivalent model of convection. And the ways of parameters determination for each model. The accuracy of models in simulating solute transport into runoff was evaluated by comparing the predicted data with the experimental data. The application condition of each model during solute transport simulation was proposed.

2. Experimental methods

The laboratory experiments were designed to test the applicability of the commonly used chemical transport models in Loess Plateau of China, and the methods of estimating corresponding parameters.

2.1. Site description

The experiments were performed at the Key Laboratory of Soil Erosion and Dryland Farming on the Loess Plateau, Yangling, Shaanxi province, China. The Yangling District is located on the western Guanzhong Plain of Shaanxi Province, north of the Weihe River (E107°59′–108°08′, N34°14′–34°20′). It is 7 km long from north to south and 16 km wide from east to west, covering a total area of 94 km^2. The area has an arid–humid monsoon climate. The annual mean precipitation and evapotranspiration are 637.6 mm and 884.0 mm, respectively (Huang et al., 2013).

2.2. Experimental set-up

The experimental set-up mainly includes two parts: rain simulator and soil flume. All experiments were performed with nozzles rain simulator as depicted in Fig. 1. The nozzles of which were placed 15 m above the test soils to simulate natural conditions and generated various computer controlled rain intensities from 0.067 to 0.2 cm/min, each simulated rain lasting for 1 h.

2.3. Soil sampling

The experimental soils were sourced from the A horizon (10–30 cm depth) of a cultivated field in the district of Yangling. The distribution of particle sizes was determined by sieving in combination with the pipette method (Hillel and Rossiter, 1981). Various chemical and physical properties of the final experimental soil are listed in Table 1. Soil

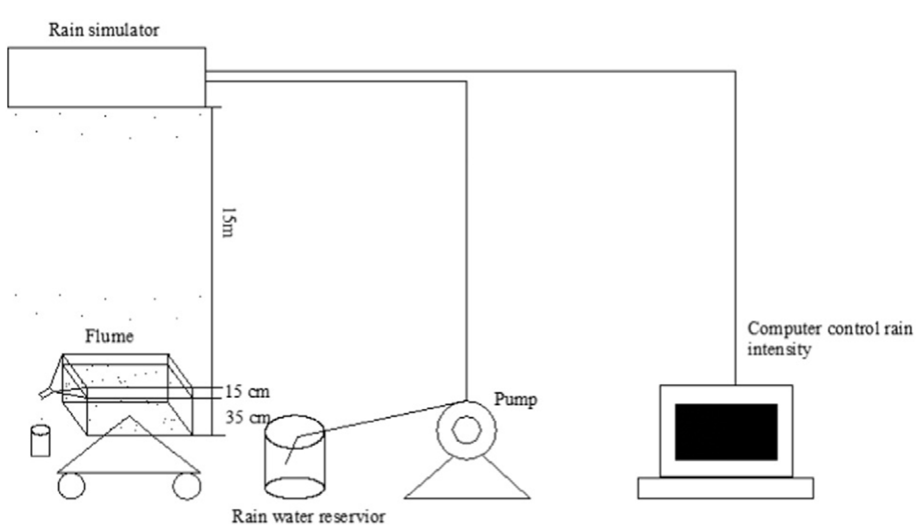

Fig. 1. Rain simulator and solute-water sampling.