Modeling Water Flow and Chemical and Sediment Transport in Watershed Systems

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Abstract

This paper presents a numerical model simulating water flow and chemical and sediment transport in watershed systems that may include a 2-D overland regime, a 1-D river/stream network, and 3-D subsurface media. The diffusion wave approach is used in modeling flow in surface systems, while the subsurface flow is described by the Richards equation. In the surface chemical system, both dissolved and particulate chemicals are taken into account. While in the subsurface systems, we include dissolved chemicals, adsorbing sites, and adsorbed chemicals. Chemical kinetics based the collision theory is used to describe interactions among chemicals. The interaction between surface and subsurface is accounted for through infiltration/seepage. We employed the backward method of characteristics to solve diffusion wave flow equations. The Picard method was applied to deal with the non-linearity of the flow equations. Richards' equation is discretized with the Galerkin finite element method. The predictor-corrector numerical scheme was employed to solve transport equations. The Newton-Raphson method was used to solve the set of ordinary differential equations describing chemical kinetics among all chemical species in the corrector step. An example is given for demonstration.

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1 Introduction

To accurately estimate the fate and transport of chemicals in a watershed system, numerical models that account for both water flow and chemical transport are needed. A complete watershed system should embrace both surface and subsurface subsystems, where the two subsystems exchange water and chemicals through infiltration and seepage processes. Without coupling the two subsystems, only can one deal with systems given infiltration/seepage information. However, infiltration and seepage are usually not known as a priori during a transient simulation. Unfortunately, numerical models which take into account complete watershed flow systems are few and models which is capable of dealing with both flow and transport is still lacking. As an initiation, we present a numerical model that account for flow and transport in a complete watershed system here.

2 Governing Equations

The diffusion wave model (Singh [1]) is employed to construct the governing equations of 1-D river/stream and 2-D overland flow, where the velocity is evaluated by the equation provided by Hergarten [2]. Subsurface flow is described with the Richard's equations (Yeh [3]). In surface transport, both chemicals and sediments are included. Chemical kinetics, based on the collision theory, is used to describe the interactions among chemicals. Any kinetic reaction can be written as

$$\sum_{j=1}^{N} a_{mj}\mathbf{C}_j \rightleftarrows \sum_{j=1}^{N} b_{mj}\mathbf{C}_j \qquad m \in [1, N_{rx}] \tag{1}$$

where where N is total number of chemicals and sediments; a_{mj} and b_{mj} are stoichiometric coefficients of reactant and product chemicals, respectively; N_{rx} is total number of reactions; $\mathbf{C}_j$ is the j^{th} species in the complete chemical/sediment list. In our model, a reaction can be an aqueous complexation, an adsorption of a dissolved chemical on to a sediments, a volatilization of a dissolved chemical, or an adsorption of dissolved chemicals onto an adsorbing site to form adsorbed chemicals. Among chemicals and sediments, bed sediments and particulate chemicals adsorbed on bed sediments are immobile and the others are mobile. Deposition, erosion, and chemical reactions are the mechanisms to change the concentrations of immobile materials. The concentrations of mobile materials are determined by solving the associated partial differential

equations that include advection, diffusion, and source/sink terms from injection, withdrawal, and reactions. It is assumed only dissolved chemicals are allowed to pass through the surface/subsurface interface.

The boundary conditions used for solving surface flow can be either of Dirichlet type with given water stage (or depth) or of flux type with time-dependent, depth-dependent, or stage-difference dependent flux (or flow rate). Boundary conditions of Dirichlet type (given head), flux type (given flux due to head gradient), and variable type (given allowed ponding depth and maximum incoming/outgoing fluxes) can be taken to undergo subsurface flow simulations (Yeh [3]). To solve transport equations for mobile materials, we may employ boundary conditions of either Dirichlet type (given material concentration), flux type (given material flux), or variable type (given material concentration for incoming flow). The details about description of governing equations, chemical reactions, and boundary conditions can be found in Yeh et al. [4].

3 Numerical Strategies

The continuity equations of 1-D river/stream flow and 2-D overland flow can be written into of advective form and then be solved with the Lagrangian approach, where the backward method of characteristics is used and water depth is the transported quantity with all source/sink terms taken into account along steam lines. During each nonlinear iteration, flow velocity is updated based on the computed water stage and is used in the next iteration. The Picard method is used to handle nonlinearity. The 3-D subsurface flow equation is approximated with Galerkin finite element method. The Picard method is employed to deal with the nonlinearity introduced by unsaturated soil characteristics (Yeh [3]). The following two issues have been addressed to handle flow through surface/subsurface interface: (1) If the flow direction is determined from subsurface to surface, seepage occurs when the pressure head at the corresponding subsurface node is positive; otherwise, evaporation happens, (2) When rainfall is given negative, it appears as a sink to the surface system when the overland is wet; otherwise, it is a sink to the subsurface system.

We have employed the predictor-corrector scheme to solve transport equations for mobile materials. The governing equation of any mobile material can be written in the following form.

$$A\frac{\partial C}{\partial t} = L(C) + RHS \qquad (2)$$

where C represents the concentration of any mobile material; $\partial C/\partial t$ is the partial time derivative of C; L is the advection-diffusion operator, A is the mass coefficient; and RHS represents source/sink terms. Hence, we can solve the above equation through the following two steps. First, we solve

$$A\frac{C^{N+1/2}-C^{N}}{\Delta t} = L(C^{N+1/2}) + (RHS)^{N} \tag{3}$$

Second, we solve

$$A\frac{C^{N+1}-C^{N}}{\Delta t} = L(C^{N+1/2}) + (RHS)^{N+1} \tag{4}$$

We can also subtract Eq. (7) from Eq. (8) to yield

$$A\frac{C^{N+1}-C^{N+1/2}}{\Delta t} = (RHS)^{N+1} - (RHS)^{N} \tag{5}$$

The advantage of solving Eq. (5), rather than Eq. (4), is that we can compute C^{N+1} node by node when $C^{N+1/2}$ is previously determined. Thus, we first solve Eq. (3) for $C^{N+1/2}$ (the intermediate value) in the so-called predictor step and perform the so-called corrector step by solving Eq. (5) to obtain C^{N+1}. The Governing equations of immobile materials and Eq. (5) of mobile materials compose a set of nonlinear ordinary differential equations that is solved by using the Newton-Raphson method.

In our model, transport is assumed not to influence flow. A one-time-lag approach is taken to deal with the interaction between surface and subsurface systems, and between 2-D overland and 1-D river/stream as well. Three time scales can be used in the model: the large one for 3-D flow; the medium one for 3-D transport, 2-D flow, and 2-D transport; the small one for 1-D flow and transport. In general, a 3-D flow time step may include many 2-D flow time steps and a 2-D flow time step can cover a number of 1-D flow time steps.

4 Example Problem

In this example, we consider a coupled 1-D/2-D/3-D flow and transport system that is discretized as shown in Figure 1. Initially, ground surface is dry and the subsurface is assumed at a steady state that is determined by the following boundary conditions: no flux on the left (x = 100 m), the right (x = 900 m), and the bottom (z = 0 m) boundaries, a constant total head of 10 m for the lower part ($z \leq 10$ m) of both the front (y = 0 m) and the back (y

= 900 m) boundaries; variable boundary condition of zero depth and zero rainfall for the surface on the top and for the rest of the front and the back boundary surfaces. The unsaturated soil characteristics are described by the following two equations.

$$\theta = 0.15 + 0.0015(h + 100) \quad \text{and} \quad K_r = \frac{h + 100}{100} \tag{6}$$

where θ is moisture content and K_r is relative conductivity. The saturated conductivities are $K_{xx} = 10^{-4}$ m/s, $K_{yy} = 10^{-5}$ m/s, and $K_{zz} = 2\times10^{-6}$ m/s. As the transient simulation begins, a rainfall of 10^{-5} m/s during the 1sthour and 1.5×10^{-5} m/s for the next 11 hours is applied to the system. Boundary conditions for solving surface flow equations are: zero water depth at the upstream river end (x = 500 m and y = 900 m) and on the top ridge of the overland domain (x = 100 m and x = 900 m); depth-dependent flux for the downstream river end (i.e., x = 500 m and y = 0 m) and for 1-D/2-D interface boundary; no-flux for the rest of the 2-D boundary.

In chemical/sediment transport there exist three dissolved chemicals (**C1**, **C**2, and **C**3), one suspended and one bed sediments (**SS1** and **BS1**), three particulate chemicals each on the suspended and the bed sediments (**PS1**, **PS2**, **PS3**, and **PB1**, **PB2**, **PB3**), one adsorbing site (**S1**), and three adsorbed chemicals (**D1**, **D2**, and **D3**). The sediment size is of cohesive type. The settling speed is 4.5×10^{-4} m/s. The critical shear stresses for deposition and erosion are 4.75 g/m/s^2 and 4.68 g/m/s^2, respectively. The following chemical reactions are taken into account.

$$\begin{aligned}
&\mathbf{C1} + \mathbf{C2} \rightleftharpoons \mathbf{C3} && k_f = 0.01, && k_b = 0.005\\
&\mathbf{C1} + \mathbf{SS1} \rightleftharpoons \mathbf{PS1} + \mathbf{SS1} && k_f = 0.0001, && k_b = 0.0\\
&\mathbf{C2} + \mathbf{SS1} \rightleftharpoons \mathbf{PS2} + \mathbf{SS1} && k_f = 0.0001, && k_b = 0.0\\
&\mathbf{C3} + \mathbf{SS1} \rightleftharpoons \mathbf{PS3} + \mathbf{SS1} && k_f = 0.0001, && k_b = 0.0\\
&\mathbf{C1} + \mathbf{BS1} \rightleftharpoons \mathbf{PB1} + \mathbf{BS1} && k_f = 0.00001, && k_b = 0.0\\
&\mathbf{C2} + \mathbf{BS1} \rightleftharpoons \mathbf{PB2} + \mathbf{BS1} && k_f = 0.00001, && k_b = 0.0\\
&\mathbf{C3} + \mathbf{BS1} \rightleftharpoons \mathbf{PB3} + \mathbf{BS1} && k_f = 0.00001, && k_b = 0.0\\
&\mathbf{C1} + \mathbf{S1} \rightleftharpoons \mathbf{D1} && k_f = 0.001, && k_b = 0.0002\\
&\mathbf{C2} + \mathbf{S1} \rightleftharpoons \mathbf{D2} && k_f = 0.001, && k_b = 0.0001\\
&\mathbf{C3} + \mathbf{S1} \rightleftharpoons \mathbf{D3} && k_f = 0.001, && k_b = 0.0
\end{aligned} \tag{7}$$

where k_f and k_b represent forward and backward reaction rate constants, respectively. Only bed sediments and adsorbing sites exist in the system initially. The initial concentrations are 10 g/m^3 for the bed sediment on

overland, 100 g/m^3 for the bed sediment in river/stream, and 2 g/m^3 for the adsorbing site. As the transient simulation starts, **C1**, **C2**, and **C3** of 1 g/m^3 come into the system through rainfall. We employ surface/subsurface variable boundary conditions for the top boundary and a variable boundary condition with a zero incoming concentration for the front and back subsurface boundaries. In addition, we apply the no-flux condition for the right, the left, and the bottom boundaries. An absolute error of 0.01 m is taken to determine 3-D flow convergence, and a relative error of 10^{-4} is used to determine convergent solutions for the other modules.

Figures 2 and 3 show the numerical results of river water depth and subsurface pressure head at various times of the 12 hour simulation. Figure 4 plots the sediment concentrations in 1-D river at the end of simulation. Figure 5 plots the concentration distribution of dissolved chemicals on the overland. We observe the removal of bed sediment in river/stream (Figure 4) but do not have change of sediment distribution on overland. In this example, infiltration exists on the surface/subsurface interface through the entire simulation. Therefore, the incoming variable boundary condition is used to account for the top boundary in dealing with 3-D subsurface transport. Because of this and because the chemistry in the surface system is the same for **C1** and **C2** (the 1st, 2nd, 3rd, 5th, and 6th reaction in Eq. (7)), we obtain identical concentration distribution for these two dissolved chemicals on the overland (Figure 5). However, their concentration distributions are not same in the subsurface because they are involved in adsorption reactions with different backward rate constants (the 8th and 9th reactions in Eq. (7)). More details about this problem can be found in Yeh et al. [4].

5 Summary

This paper presents an initial work of modeling flow and transport in a complete watershed system that accounts for 1-D river/stream network, 2-D overland, and 3-D subsurface. To make the model applicable to more problems, the following issues should be addressed in the continuing work: (1) density effect, (2) the existence of interstitial water associated with bed sediments, (3) chemical equilibrium, and (4) a hybrid surface flow scheme containing the combination of dynamic, the diffusion, and the kinematic wave models to evaluate water flow accurately and efficiently.

6 References

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[4] Yeh, G. T., H. P. Cheng, J. R. Cheng, and H. C. Lin, 1997. *A Numerical Model to Simulate Water Flow and Contaminant and Sediment Transport in WAterSHed Systems of 1-D Stream-River Network, 2-D Overland Regime, and 3-D Subsurface Media (WASH123D: Version 2.0).* A technical report of the Waterway Experimental Station, U. S. Army Corps of Engineers, U. S. A. (in press)

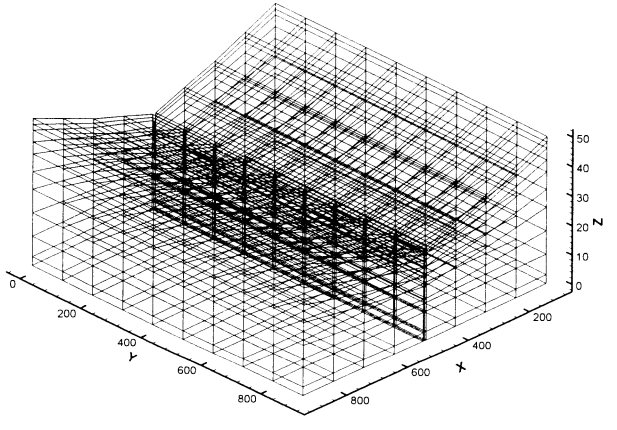

Figure 1. The discretization of the example problem.

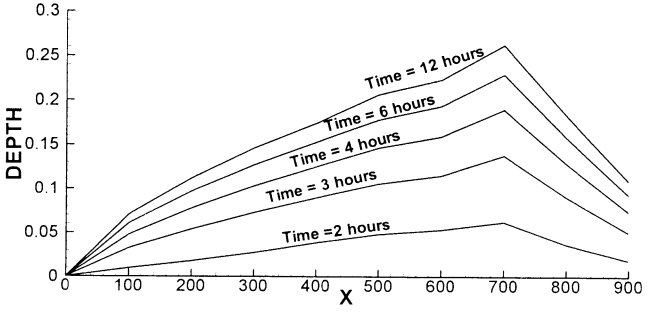

Figure 2. Water depth along the river.

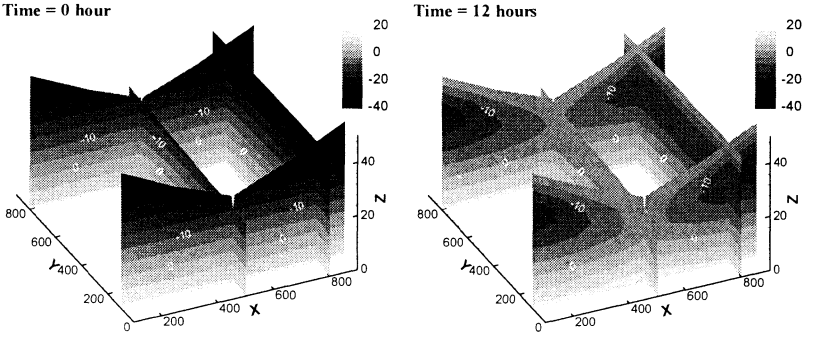

Figure 3. Pressure head in the subsurface.

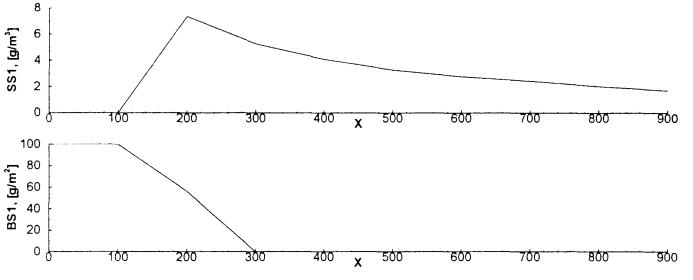

Figure 4. Sediment concentrations along the river at Time = 12 hours.

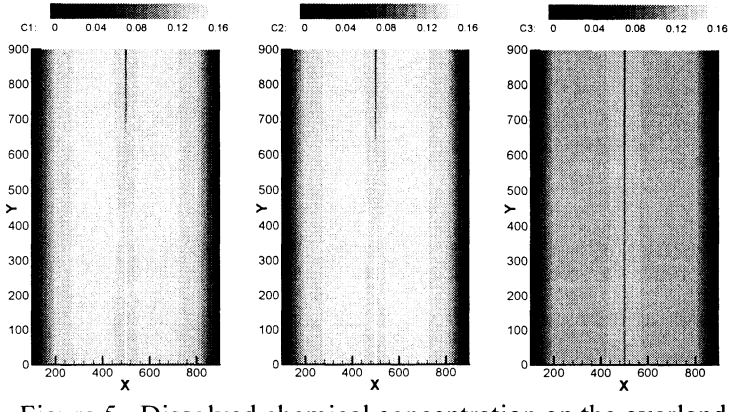

Figure 5. Dissolved chemical concentration on the overland at Time = 12 hours.