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COUPLING WATER FLOW AND SOLUTE TRANSPORT IN A CATCHMENT SCALE HYDROLOGICAL MODEL

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Summary. A physically-based distributed hydrological model simulating complex surface–subsurface flow and transport interactions is presented. The subsurface component is modeled by the three-dimensional Richards equation for flow and the classical advection-dispersion-reaction equation for transport, solved using finite element/finite volume techniques. The surface model is based on a path-based (rill flow) diffusion wave equation for both flow and transport, solved using a Muskingum-Cunge scheme. The path-based paradigm, together with Leopold and Maddock scaling relations for hydraulic parameterization, allow the same surface model to be used for both overland and channel dynamics. A novel approach for resolution of the interactions of water across the land surface, based on a boundary condition switching algorithm, is extended to the solute flux exchanges. The use of a high resolution finite volume scheme for the advective component of subsurface transport introduces minimal numerical diffusion even in the absence of physical dispersion. An application to the Abdul and Gillham sandbox experiment [1] is presented to illustrate the abilities of the model and to demonstrate the influence of surface–subsurface diffusive exchanges on the tracer dynamics of this particular system.

1 INTRODUCTION

Critical exchanges of water and solutes between the atmosphere, the land surface, and the subsurface occur at all scales. At the smaller scale representing hillslopes and small catchments, it is possible to resolve these exchanges using detailed physically-based models. In the last decade, process-based distributed models that couple in a physical way surface and subsurface processes have emerged (e.g., [4],[7],[10] and papers cited therein), and constitute useful tools to investigate various hydrological problems coupling flow and transport. In addition to their importance in general water quality applications, such models allow determination of flow paths and travel time distributions, important

in addressing open issues related to coupled water and solute transport dynamics such as the role of subsurface water in runoff generation and the relative contributions of "'old water"' and "'new water"' in streamflow hydrographs. Appropriate mathematical equations governing surface and subsurface flow and transport as separate components exist, but their coupling is still a challenge. Moreover, these equations can be very difficult to solve, owing to nonlinearities, sharp propagation fronts, and heterogeneities. In this work we consider the implications of these complexities on solving flow and transport in a coupled surface–subsurface model. The model used is based on the coupling of the three-dimensional Richards equation for flow in variably saturated porous media, a path-based (rill flow) diffusion wave approximation to the Saint-Venant equations for surface dynamics on hillslopes and in stream channels, and the classical advection-dispersion-reaction equation with first-order mass transfer. Numerical solution schemes include finite elements for discretization of the flow equations and coupled finite elements-finite volumes for the transport equation. An application on the Abdul and Gillham sandbox experiment [1] is used to illustrate the ability of the model to describe complex surface–subsurface flow and transport interactions.

2 FLOW MODEL

The diffusive wave equation and the Richards equation respectively describe surface flow propagation and variably saturated flow in the subsurface porous media:

$$\frac{\partial Q}{\partial t} + c_k \frac{\partial Q}{\partial s} = D_h \frac{\partial^2 Q}{\partial s^2} + c_k q_s \tag{1}$$

$$S_w S_s \frac{\partial \psi}{\partial t} + \phi \frac{\partial S_w}{\partial t} = \vec{\nabla} \cdot [K_s K_r (\vec{\nabla}\psi + \vec{\eta_z}] + q_{ss} \tag{2}$$

where s is the longitudinal coordinate used to describe the channel network [L], Q is the surface discharge $[L^3/T]$, c_k is the kinematic celerity $[L/T]$, D_h is the hydraulic diffusivity $[L^2/T]$, and q_s is the inflow (positive) or outflow (negative) rate from the subsurface to the surface $[L^3/LT]$. In the subsurface flow equation (2), $S_w = \theta/\theta_s$ is water saturation [-], θ is the volumetric moisture content [-], θ_s is the saturated moisture content (generally equal to the porosity Φ), S_s is the aquifer specific storage $[L^{-1}]$, ψ is pressure head [L], t is time [T], $\vec{\nabla}$ is the gradient operator $[L^{-1}]$, K_s is the saturated hydraulic conductivity $[L/T]$, $K_r(\psi)$ is the relative hydraulic conductivity [-], $\vec{\eta_z} = (0, 0, 1)'$, z is the vertical coordinate upward [L], and q_{ss} is the source (positive) or sink (negative) terms $[L^3/L^3T]$. The surface–subsurface flow coupling is handled through appropriate definiton of the exchange fluxes q_{ss} and q_s.

Both the 3D subsurface flow and 1D surface flow equations are solved using classical numerical formulations, i.e., Galerkin finite elements for the subsurface and a finite difference explicit in time Muskingum-Cunge algorithm for the surface. More details on both subsurface and surface flow solvers, and their relative features can be found in [2, 8].

3 TRANSPORT MODEL

A diffusive wave equation and the classical advection-dispersion equation respectively describe transport processes at the land surface and in subsurface porous medium:

$$\frac{\partial Q_m}{\partial t} + c_t \frac{\partial Q_m}{\partial s} = D_c \frac{\partial^2 Q_m}{\partial s^2} + c_t q_{ts} \tag{3}$$

$$\frac{\partial \theta c}{\partial t} = \vec{\nabla} \cdot [-\vec{U} c + D \vec{\nabla} c] + q_{tss} \tag{4}$$

where Q_m is the mass discharge $[M/T]$, c_t is the kinematic solute celerity $[L/T]$, D_c is the solute surface diffusivity $[L^2/T]$, and q_{ts} is the mass inflow (positive) or outflow (negative) rate from the subsurface to the surface $[ML^3/LT]$. In the subsurface transport equation (4), c is the solute subsurface concentration $[M/L^3]$, $\vec{U}$ is the Darcy velocity $[L/T]$, D is the tensor accounting for both mechanical dispersion and molecular diffusion $[L^2/T]$, and q_{tss} is the mass source (positive) or sink (negative) terms $[M/L^3T]$. Both the volumetric water content θ and the subsurface velocity field $\vec{U}$ are computed by the subsurface flow model. The surface–subsurface transport coupling is handled through the definiton of the exchange fluxes q_{tss} and q_{ts}.

For consistency with the flow solver, the surface transport equation is solved with the same formulation as the one used to solve for flow. A finite difference explicit in time Muskingum-Cunge algorithm is thus used to compute ingoing and outgoing mass discharge for every cell of the surface domain.

The subsurface transport solver uses a time-splitting technique combining both finite volumes and classical finite elements. The method used is similar to the one presented in [5, 6] except that classical finite elements are used instead of mixed hybrid finite elements. Following this approach, the advection-dispersion equation is solved via a time-splitting approach that solves separately the dispersion and advection parts. The advection equation is first solved using an explicit in time finite volume formulation. The resulting concentration is used as an initial condition for the finite elements resolution of the diffusive part of the equation. This method allows the use of multiple advective time steps per dispersive time step and has been shown to yield accurate results also when dealing with advection-dominated transport processes. We refer the reader to reference and to [9] for more details.

4 surface–subsurface COUPLINGS

The coupling for both the flow and transport surface-subsurface exchanges is based on a surface boundary condition switching algorithm. Boundary condition switching is necessary because of the way soil surface conditions evolve over time in response to atmospheric forcing. Mass balance equations are used to compute relevant exchange fluxes between the surface and subsurface - i.e. q_{ss} and q_s of equations (1) and (2) for flow and q_{tss} and q_{ts} of equations (3) and (4) for transport.

4.1 Flow coupling

As atmospheric forcing constitutes a boundary condition for the subsurface flow equation, the partitionning between surface and subsurface flow processes is controlled by the subsurface flow model. Depending on whether the surface is ponded or unsaturated, either a Dirichlet-type (prescribed head) or a Neumann-type (prescribed flux) boundary condition is imposed for the subsurface flow resolution. For surface nodes where ponding occurs, the actual flux that can infiltrate or exfiltrate is evaluated after the subsurface flow solution using the pressure field computed using the Dirichlet boundary condition. The switching algorithm then performs a mass-balance calculation between the potential flux (i.e., the atmospheric forcing), the actual flux, and the ponding water (when existing) to determine (i) if the surface is ponded or not and (ii) the amount of water that is partitioned to surface runoff if ponding occurs. A switching check between Neumann and Dirichlet conditions is performed at every non-linear iteration of the Richards equation solver. More details on the flow coupling algorithm can be found in [2].

4.2 Transport coupling

Transport exchanges across the land surface are strongly coupled to water exchanges. The transport interactions between surface and subsurface are directly controlled by the corresponding flow dynamics computed with the flow model, i.e., by the ponding situation, the actual flux (infiltration or exfiltration) and the potential flux (rainfall or evaporation). Depending on the flow situations, either a total Cauchy or a zero-Neumann boundary condition is imposed on the subsurface transport module. For surface nodes where infiltration occurs, a total Cauchy boundary condition is imposed. In the case of rainfall, at a given time a surface node evaluated by the flow module as unsaturated signals that all the potential rainfall and the ponding head at the surface (if existing) have infiltrated and the total flux imposed at the surface is the sum of the rainfall and the contributions as calculated by the flow equation:

$$(D\vec{\nabla}c - \vec{U}c) \cdot \vec{n} = q_{Cauchy} = Rc_r + (q_{act} - R)c_{surf} \tag{5}$$

where the LHS indicates the total Cauchy boundary condition to be imposed in the subsurface transport module, R is rainfall rate and c_r its input concentration, q_{act} is the infiltration flux already calculated by the flow code, and c_{surf} is the concentration at the surface node (imposed or calculated at the previous time step).

If the node is ponded, the infiltration capacity is smaller than the total amount of water available for infiltration (i.e., potential rainfall plus ponding water) and thus some water remains at the surface. In this case, the surface concentration is updated using a mass-balance calculation to account for the effect of rainfall (for instance dilution) on the surface concentration. The total flux imposed is then calculated using this updated concentration and the actual flux computed by the flow model. For surface nodes where exfiltration occurs, a zero-Neumann boundary condition is imposed. The flow model indeed computes

an outgoing water flux across the land surface and the concentration of this water is part of the unknowns of the subsurface transport equation. The zero-Neumann boundary condition allows to model a solute exchange flux controlled by advection only. Note that in the transport coupling algorithm no diffusive solute exchanges between surface and subsurface are modeled. The effect of this assumption will be illustrated in the section describing the application example. More details on the transport coupling algorithm can be found in [9].

5 SOLUTION PROCEDURE

The explicit nature of the surface flow formulation allows the use of a noniterative sequential procedure for the resolution of the coupled flow and transport problem. The different steps between time t^k and t^{k+1} can be described as follow: (i) solution of the surface flow equation using q_s^k as source term to compute discharge Q^{k+1} and the ponding head h^{k+1}; (ii) solution of the surface transport using q_{ts}^k as source term to compute Q_m^{k+1} and its equivalent in surface concentration c_{surf}^{k+1}; (iii) definition of the surface boundary condition for the subsurface flow equation using h^{k+1} and atmospheric inputs; (iv) solution of the subsurface flow equation to compute the pressure field ψ^{k+1}, the velocity field $\vec{U}^{k+1}$, and the moisture content θ^{k+1}; (v) calculation of the subsurface-to-surface water source/sink term q_{ss}^k using ψ^{k+1} and the balance between atmospheric inputs and actual fluxes; (vi) definition of the surface boundary condition for the subsurface transport equation using c_{surf}^{k+1}, h^{k+1}, and potential and actual water fluxes; (vii) solution of the subsurface transport equation to compute the subsurface concentration c^{k+1}; and (viii) calculation of the subsurface-to-surface transport source/sink term q_{tss}^k using all the flow and transport variables needed to perform a consistent solute mass-balance.

The time step strategy is controlled by the subsurface flow model. During the simulation, the time step size grows and decreases as a function of the number of nonlinear iterations needed to reach convergence for the subsurface flow equation. Nevertheless, multiple time steps for both the flow and transport surface equations can be executed per single subsurface flow time step. For the transport solution, the dispersive time step is chosen to be equal to the one used for the subsurface flow resolution. Multiple advective time steps per dispersive time step can be used if needed to ensure an appropriate CFL number and to properly capture the advective processes. This elaborate time step strategy adapts automatically to the complex surface–subsurface flow and transport dynamics in an accurate and efficient way.

6 APPLICATION EXAMPLE

The Adbul and Gillham sandbox experiment [1] has been used in several previous studies on integrated flow and transport modelling to assess the quality of surface–subsurface coupled models. Nevertheless, it is widely recognized that theflow and transport dynamics of this experiment cannot be accurately reproduced because of the strong influence of

the air phase on the infiltration process in the system. The model presented in this paper was thus validated using synthetic hillslope tracer experiments. The results presented in [9] demonstrate that the model properly describes the main runoff generation processes. Simulations on the Abdul and Gillham system are here performed not to validate the model but rather to illustrate the role of surface–subsurface tracer diffusive exchanges on transport dynamics at a small scale.

6.1 Experimental setup

The geometry of the domain and the surface and rainfall parameters are described in Figure 1a. The soil parameters (including van Genuchten parameters - see [2] for their definition) are described in Table 1. The domain is triangulated starting from a 5 x 100 x 100 grid. The rainfall is tagged with a virtual tracer whose concentration is set to one. The initial concentration in the subsurface domain is equal to zero. Both the lateral and longitudinal dispersivities are set to zero and only the molecular diffusion is considered, at a value equal to $1.2 \times 10^{-9}\ m^2/s$.

n	p_{sat}	K_s	S_s	Porosity
5.5	-0,44 m	3.5×10^{-5} m/s	$5. \times 10^{-4}\ m^{-1}$	0.34

Table 1: Soil parameters used to simulate the Abdul and Gillham system.

Two different simulations were performed. The first uses the transport coupling algorithm presented previously. This algorithm only accounts for advective solute exchanges; diffusives exchanges are not modeled. In the second simulation we modify the coupling algorithm to account for diffusive solute exchanges in a simple way, by adding an exchange term proportional to the concentration difference between surface and subsurface. The proportionality coefficient characterizing these exchanges is then calibrated ad hoc to obtain a reasonably good fit between measured and simulated transport responses. Note that the aim of this modelling exercise is not to obtain a perfect fit, not to adress the complex issues of the influence of hydrodynamic mixing on tracer experiments (see [3]), but rather to illustrate the possible influence of these diffusive exchanges on the simulated transport dynamics, and to show the capabilities of the proposed modeling approach to simulate flow and transport at a laboratory or small catchment scale.

6.2 Results and discussion

The comparison between the relative contributions of event and pre-event water simulated with (blue) and without (red) surface–subsurface diffusive solute exchanges and measured by Abdul and Gillham is presented in Figure 1b. Normalized total outflow, normalized event contributions, and normalized pre-event contributions are plotted. The normalization is achieved by dividing the fluxes by the rainfall rate so that the plotted

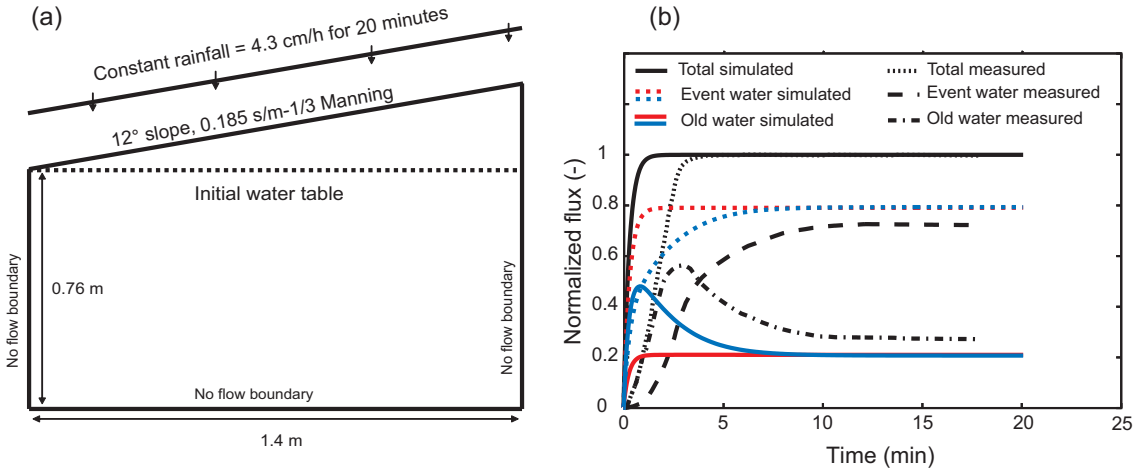

Figure 1: (a) Geometry and boundary conditions for the Abdul and Gillham system; (b) Comparison between simulated and measured fluxes. For the simulated ones: red = without surface–subsurface diffusive exchange for solute and blue = with surface–subsurface diffusive exchanges for solute.

values are bounded between 0 and 1. As mentioned previously, the flow dynamics cannot be reproduced properly as a steady state is reached in the simulations at an earlier time compared to the measurments. The transport results suggest that representation of the diffusive solute exchanges is needed to simulate an early peak of pre-event water. Indeed the results obtained with only advective coupling do not show the pre-event water peak, confirming the results presented in [3] that suggest that hydrodynamic mixing may have a stong impact on hydrograph separation, at least at the laboratory scale.

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