Physically-based distributed model for coupled surface runoff and subsurface flow simulation at the catchment scale

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ABSTRACT: The interactions between surface and subsurface hydrologic processes are important in many water resource applications and require modeling approaches capable of treating these processes in an integrated manner. We describe a distributed, physically-based model that couples a three-dimensional subsurface flow module to a DEM-based one-dimensional surface routing module and resolves in a detailed manner the exchange of flux and head information between the two regimes. The coupled model can treat flow in saturated and variably saturated porous media, surface runoff, channel flow, and storage in lakes and other topographic depressions. The algorithm that handles the exchange between the surface and subsurface components is described in detail, and an illustrative test case is presented.

1 INTRODUCTION

Distributed catchment scale models are becoming increasingly important in engineering practice for their ability to determine the detailed flow characteristics that are needed in the accurate description of spatially distributed phenomena such as water table dynamics and contaminant migration (Abbott, Bathurst, Cunge, O'Connell, & Rasmussen 1986).

Precipitation fluxes during storm events and potential evapotranspiration during interstorm periods are the driving forces of catchment dynamics. The catchment partitions this atmospheric forcing into surface runoff, groundwater flow, actual evapotranspiration, and changes in storage. Surface runoff involves different phenomena such as hillslope and channel flow and retardation and storage effects due to pools and lakes. Groundwater flow processes include infiltration to and exfiltration from the vadose zone. Typical catchment simulation models do not consider exfiltration and use simple one-dimensional infiltration equations, neglecting lateral flow in the subsurface. These approximations, however, are not acceptable when exfiltration or seepage from the subsurface is important. This may occur, for example, in relatively flat areas characterized by the presence of shallow aquifers, where local depressions play an important role in retarding the routing of the surface (ponding) water.

In this paper we present a physically-based distributed catchment-scale model for the simulation of coupled surface runoff and subsurface flow. The model is based on coupling Richards' equation for variably saturated porous media and a diffusion wave approximation for surface water dynamics. The numerical scheme uses a finite element Richards' equation solver, FLOW3D (Paniconi & Wood 1993; Paniconi & Putti 1994) and a surface DEM-based finite difference module, SURF_ROUTE (Orlandini & Rosso 1996). Retardation and storage effects due to lakes or depressions are also implemented, to give a complete description of the catchment flow dynamics.

Starting from a DEM (digital elevation model) discretization of the catchment surface and a corresponding three-dimensional grid of the underlying aquifer, atmospheric input (precipitation and evaporation data) is partitioned into surface and subsurface components by the FLOW3D module. The overland flux values calculated by FLOW3D at the grid nodes are transferred to the DEM cells and implemented as sink or source terms in the SURF_ROUTE module, which routes this surface water and calculates the resulting ponding head values that are in turn used as boundary conditions in FLOW3D. This interaction and exchange between the subsurface and surface components will be described in some detail.

A preliminary numerical test on a hypothetical catchment, characterized by the presence of a central depression, is used to illustrate the model and to highlight the importance of simulating as completely as possible both surface and subsurface processes, including lateral groundwater flow and exfiltration.

2 MATHEMATICAL MODEL

The mathematical model of coupled subsurface flow and surface routing phenomena can be described by a system of two partial differential equations, one describing the flow of water in the vadose and groundwater zones (Richards' equation) and the other describing the surface hydrologic response of the catchment (hillslope and channel flow). In formulating the mathematical model, we assume that hillslope flow concentrates in rills or rivulets. As such, both channel and hillslope flow can be described by a one-dimensional convection-diffusion equation defined on the rill or channel network using different parameter values to distinguish between the two flow regimes.

The system of partial differential equations can be written as

$$\sigma(S_w)\frac{\partial\psi}{\partial t} = \nabla\cdot[K_s K_{rw}(S_w)(\nabla\psi+\eta_z)] + q_s(h) \quad (1)$$

$$\frac{\partial Q}{\partial t} + c_k\frac{\partial Q}{\partial s} = D_h\frac{\partial^2 Q}{\partial s^2} + c_k q_L(h,\psi) \quad (2)$$

The parameters have the following meaning: $\sigma(S_w) = S_w S_s + \phi\frac{\partial S_w}{\partial\psi}$, $S_w(\psi)$ is water saturation, S_s is the aquifer specific storage coefficient, ϕ is porosity, ψ is pressure head, t is time, ∇ is the gradient operator, K_s is the saturated hydraulic conductivity tensor, $K_{rw}(S_w)$ is the relative hydraulic conductivity function, $\eta_z = (0,0,1)^T$, z is the vertical coordinate directed upward, and q_s represents distributed source or sink terms (volumetric flow rate per unit volume). The surface water is routed using (2) along each single hillslope or channel link using a one-dimensional coordinate system s defined on the drainage network. In this equation, Q is the discharge along the channel link, c_k is the kinematic wave celerity, D_h is the hydraulic diffusivity, and q_L is the inflow (positive) or outflow (negative) rate from the subsurface into the cell, i.e., the overland flow rate. We note that q_s and q_L are both functions of the ponding head h, and that h can be easily derived from the discharge Q via mass balance calculations.

This system of equations must be solved simultaneously for the unknown vector (Q,ψ) or (h,ψ). Nonlinearities arise in the $S_w(\psi)$ and $K_{rw}(S_w)$ characteristic curves in Richards' equation, in the nonlinear dependence of q_s on the ponding head, and in the nonlinear dependence of q_L on ψ.

2.1 *FLOW3D subsurface module*

FLOW3D is a three-dimensional finite element model for flow in variably saturated porous media, applicable to both the unsaturated and saturated zones. The characteristic relationships $K_{rw}(S_w)$ can be specified using the van Genuchten & Nielsen (1985) , Brooks & Corey (1964) , or Huyakorn, Thomas, & Thompson (1984) expressions. Equation (1) is highly nonlinear due to the pressure head dependencies in the storage and conductivity terms, and is linearized in the code using either Picard or Newton iteration (Paniconi & Putti 1994). Tetrahedral elements and linear basis functions are used for the discretization in space, and a weighted finite difference scheme is used for the discretization in time. The code handles temporally and spatially variable boundary conditions, including seepage faces and atmospheric inputs, and heterogeneous material properties and hydraulic characteristics.

For the treatment of the atmospheric boundary conditions, the input flux values are considered "potential" rainfall or evaporation rates, and the "actual" rates, which depend on the prevailing flux and pressure head values at the surface, are dynamically calculated by the code during the simulation. Overland flow, defined as the flow rate that is present at the surface and that can be routed via the surface model, is calculated at every time step from the balance between potential and actual fluxes.

Automatic switching of surface boundary conditions from a specified flux (Neumann) to a constant head (Dirichlet) condition, and vice versa, is implemented to correctly reproduce the physical phenomena occurring at the surface. This automatic switching is illustrated here by example, and is described in more detail later in the context of the coupled model. In the case of precipitation, if a surface node becomes saturated because of infiltration excess, the fraction of precipitation that does not infiltrate and remains at the surface (ponding head) becomes the overland flow to be routed via the surface module. The boundary conditions in this case switch from Neumann (atmosphere-controlled) to Dirichlet (soil-controlled) type. If precipitation intensity decreases, so that the magnitude of actual (computed) flux across the soil surface exceeds the magnitude of the atmospheric flux, the boundary condition switches back to a Neumann type. If a surface node becomes saturated because of saturation excess (the water table reaches the surface), and there is an upward flux across the soil surface (return flow), the overland flow is calculated as the sum of precipitation and return flux. The entire amount of water that remains at the surface or exfiltrates from the subsurface is then transferred for routing to the DEM-based surface runoff module, which in turn returns, after surface propagation, the ponding head distribution to FLOW3D.

2.2 *SURF_ROUTE surface runoff module*

The surface hydrologic response of a catchment is considered as determined by the two processes of hillslope and channel transport, operating across all the hillslopes and stream channels forming a watershed and including storage and retardation effects of pools or lakes and infiltration/evapotranspiration and exfiltration effects from subsurface soils.

Hillslope and channel processes. We assume that hillslope flow concentrates in rills or rivulets that form because of topographic irregularities or differences in soil erodibility and that deepen and widen during the runoff event as a function of slope, runoff characteristics and soil erodibility. To minimize the computational effort and economize on the number of model parameters, the rill formations are lumped at the DEM elemental scale into a single conceptual channel. The drainage system topography and composition are described by extracting automatically a conceptual drainage network from the catchment DEM. Each elemental hillslope rill and network channel is assumed to have bed slope and length that depend on location within the extracted transport network, and a rectangular cross section whose width varies dynamically with discharge according to the scaling properties of stream geometry as described by the "at-a-station" and "downstream" relationships first introduced by Leopold & Maddock (1953) .

The distinction between hillslope and channel flow is based on the "constant critical support area" concept as described by Montgomery & Foufoula-Georgiou (1993) . Rill flow is assumed to occur for all those cells for which the upstream drainage area A does not exceed the constant threshold value A^*, while channel flow is assumed to occur for all those cells for which A equals or exceeds A^*.

A routing scheme developed on the basis of the Muskingum-Cunge method with variable parameters is used to describe both hillslope rill and network channel flows, with different distributions of the Gauckler-Strickler roughness coefficients to take into account the different processes that characterize the two physical phenomena (Orlandini & Rosso 1998). The model routes surface runoff downstream from the uppermost DEM cell in the basin to the outlet, following the previously determined drainage network. A given grid cell will receive water from its upslope neighbor and discharge it to its downslope neighbor, with the inflow or outflow rate q_L at any catchment cell given by:

$$q_L = q\Delta x \Delta y / \Delta s$$

where q is the local contribution to surface runoff, as calculated by FLOW3D, Δx and Δy are the cell sizes, and Δs is the channel length within the cell. Inflow hydrographs and overland fluxes q_L are routed into each individual channel via the convection-diffusion flow equation (2), discretized by the Muskingum-Cunge method to yield:

$$Q_{i+1}^{k+1} = C_1 Q_i^{k+1} + C_2 Q_i^k + C_3 Q_{i+1}^k + C_4 q_{L_{i+1}}^k \quad (3)$$

where Q_{i+1}^{k+1} is discharge at network point $(i+1)\Delta s$ and time $(k+1)\Delta t$, $q_{L_{i+1}}^k$ is the overland flow rate at the $(i+1)$st space interval and time $k\Delta t$, and the routing coefficients C_i depend on c_k, on the temporal interval Δt, on the channel length Δs, and on the numerical scheme. Once the in and out discharge at each cell is determined, the cell water depth, or ponding head h, can be calculated from simple mass balance considerations, as mentioned earlier.

Topographic depressions. Isolated topographic depressions ("pits") in the catchment DEM can be attributed to the presence of pools or lakes, or can be interpreted as erroneous or missing data. Depressions cannot be handled by automatic drainage network extraction procedures, and depitting techniques are generally used to modify the elevation values and to regularize the DEM. These depitting schemes correct DEM errors and can also be used in steep basins, where the flow is mainly driven by slope and where slight artificial modifications of topography will not significantly change surface flow patterns. However, when depressions play an important role in the formation of surface and subsurface fluxes these procedures introduce inconsistent flow directions and do not correctly reproduce the storage and retardation effects of pools and lakes on the catchment response. This typically happens in relatively flat areas where flow patterns are strongly influenced by small slope changes.

In this work topographic depressions are treated as follows. Initially the location of the pits is identified from the DEM and from prior field information. A "lake boundary-following" procedure (Mackay & Band 1998) is employed to isolate and correct for potential breakdown in the subsequent drainage network extraction process. By this procedure, each cell along the boundary of the pit (also called "buffer cells") acts as a depression point for all the catchment cells draining into the pit. To ensure correct flow paths in the area, the drainage direction in all the buffer cells is forced to form a circulation path that drains into a single cell (the lake outlet cell). A flow path algorithm, in combination with a "slope tolerance" based correction procedure to account for the remaining erroneous depressions, is then applied to the modified DEM that excludes the central cells of the depression. The storage and retardation effects of the pit are accounted for by transferring with infinite celerity all the water drained by the buffer cells to the lake outlet cell, which is now treated as a reservoir. All the geometrical and physical characteristics of the depression are thus attributed to this cell. Outflow from this cell is calculated by solving, by a level pool routing procedure, the continuity equation for the reservoir:

$$\frac{\partial V}{\partial t} = I(t) - O(h^*) \quad (4)$$

where V is the storage volume of the reservoir, I and O are the incoming and outgoing discharges, functions of time and of water elevation (above a reference level) in the reservoir h^*, respectively. The reservoir water elevation thus determined is then assigned to all the lake cells and used in FLOW3D as ponding head, while the discharge from the reservoir is the outgoing flux at the cell to be used in SURF_ROUTE.

3 COUPLING BETWEEN THE SURFACE AND SUBSURFACE MODELS

The explicit in time nature of the Muskingum-Cunge discretization scheme allows the construction of the following non-iterative algorithm for the solution of equations (1) and (2):

for $t_k = 0$ to t_{max} with step Δt do:

- solve (2) using q_L^k as input to the SURF_ROUTE model, obtaining Q^{k+1} and from this the distribution of ponding heads h^{k+1};
- use h^{k+1} and precipitation/evaporation input at time t^{k+1} to set up boundary and initial conditions for FLOW3D, and solve (1) for ψ^{k+1}
- calculate (again with FLOW3D) the overland flux q_L^{k+1} using ψ^{k+1} and the balance between atmospheric inputs and actual fluxes.

The algorithm needs to be initialized, and this is done by setting an initial condition in terms of q_L for equation (2). If this condition is not known a priori, it can be calculated from an initial run of FLOW3D that will evaluate a first guess for the overland flow based on the actual atmospheric input. In this case an initial distribution of ψ needs to be specified.

Coupling between the subsurface flow and surface routing modules is such that at every time step exchange of information regarding the subsurface flux contributions to surface ponding (calculated by FLOW3D and passed on to SURF_ROUTE) and the nodal pressure head values corresponding to ponded surface cells (SURF_ROUTE to FLOW3D) occurs. This exchange is strongly linked to the control algorithm in the subsurface module that checks for and switches surface boundary conditions from soil-driven to atmosphere-driven regimes and vice versa. It is this algorithm that flags each surface node according to whether it is currently ponded, saturated, or below saturation.

Physically, the distinction between a surface node or cell being "saturated" or "ponded" is made via the input parameter "pond_head_min" that is assigned the threshold pressure head value a surface node must attain to be considered ponded, in the sense of having water available for routing by the overland flow module. The value of pond_head_min can be set to account for the amount of water that can remain trapped in microtopographic features of the surface.

Algorithmically, the distinction between a saturated and ponded node is that, within iterations of FLOW3D, the saturated node may become unsaturated depending on the balance between the potential (atmospheric) and actual (back-calculated) fluxes, whereas the ponded node will remain ponded until the next call to SURF_ROUTE, where it may then become unponded depending on the balance between overland fluxes and upslope and downslope discharges. In other words, we assume that only SURF_ROUTE can alter the state of a ponded node.

In the case of rainfall, unsaturated surface nodes that have become saturated or ponded are assigned a fixed head (Dirichlet) boundary condition, and in the subsequent iteration or time step of the subsurface flow module the soil-driven infiltration rate is back-calculated by the code after obtaining the pressure head solution. In the case of evaporation, an unsaturated surface node that has become saturated is assumed to represent subsurface return flow and is maintained in atmosphere-driven mode, assigning to the node a specified flux (Neumann) boundary condition with the flux equal to the potential (input) rate of evaporation, whereas an unsaturated surface node that has become ponded is switched to soil-driven Dirichlet mode where it will remain for subsequent surface routing as described above.

In the case of rainfall, a saturated Dirichlet surface node is switched to atmosphere-driven Neumann mode whenever the back-calculated flux exceeds the input potential rate, normally a signal that the rainfall rate has fallen below the infiltration capacity of the soil. In the case of evaporation, we again have a situation where subsurface return flow is possible, and a saturated Dirichlet surface node is switched to an atmospheric flux condition only if the magnitude of the back-calculated flux is smaller than the magnitude of the potential evaporation rate; no switching is done if the back-calculated flux magnitude is larger than the potential rate, since in this situation there is return flow in excess of atmospheric demand that will contribute to ponding.

Switching between soil-controlled and atmosphere-controlled boundary conditions is analogous but simpler in the case where the pressure head at the surface node is or has reached its lower limit or "air dry" value. An atmosphere-driven surface node that has become air dry is fixed at the air dry pressure head (Dirichlet condition) only in the case of evaporation. An air dry Dirichlet node becomes atmosphere-driven when it is raining, or, under evaporation conditions, when the magnitude of the back-calculated flux becomes larger than the magnitude of the input potential rate.

Having in this way determined the current status of each surface node (ponded, saturated, below saturation, air dry) and knowing for each of these nodes whether the potential atmospheric forcing is positive (rainfall) or negative (evaporation) and, in the case

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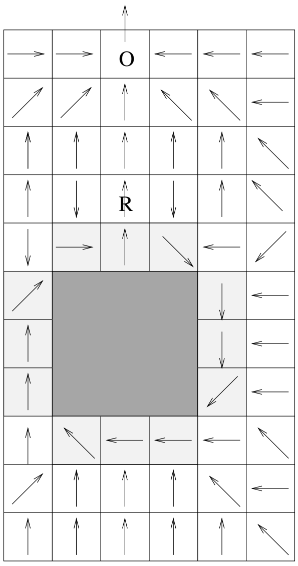

Figure 1: The catchment DEM with elevations (m a.s.l.) (left) and a schematized representation of the catchment with flow paths as calculated by the "depitting" procedure (right). The interior area of the depression is displayed in dark grey and the buffer cells with forced flow directions in light grey. The reservoir cell is identified by the letter "R", while "O" is the outlet cell.

of a Dirichlet boundary condition whether the actual, back-calculated flux represents infiltration or exfiltration and also its magnitude relative to the potential flux, we can calculate the overland fluxes to be passed to SURF_ROUTE, partition the atmospheric and soil surface components of the hydrograph into its various contributions (infiltration, actual evaporation, return flow, direct runoff), and flag any anomalous events (e.g., infiltration at a saturated node with evaporative potential flux, surface runoff at an air dry node).

4 APPLICATION

The coupled surface–subsurface model has been tested on the basin shown in Figure 1. The basin is formed by 6×11 surface cells 50×50 m wide, with elevations varying between 15 and 10 m a.s.l., and is characterized by a depression in its central part with a minimum elevation of 11 m a.s.l. During drainage network extraction the 9 central cells of the depression have been eliminated from the surface DEM. In the surrounding cells ("buffer cells") the flow direction has been imposed so that the water is drained by the depression towards the reservoir, indicated by the letter R in Figure 1, in which the geometrical characteristics of the whole depression are concentrated. Water is allowed to flow out from the reservoir when the level rises above 14 m, which is the real elevation of the lowest cell surrounding the depression. For the runoff simulation, no channel flow has been allowed, assigning a high value to the threshold area A^*. A constant value of 10 m$^{1/3}$s^{-1} has been imposed for the Gauckler-Strickler surface roughness coefficient.

The underlying aquifer is assumed to have a constant thickness of 10 m, and is divided into ten parallel layers with thickness varying from 0.1 m in the first three layers, 0.5 m in the subsequent two layers, 1.0 m in the sixth and seventh layer, to 2.2 in the final three layers. The saturated conductivity was assumed isotropic with a constant value of 10^{-5} m/s. The specific storage coefficient is $S_s = 0.01$ m^{-1} while porosity is $\phi = 0.35$. The van Genuchten and Nielsen characteristic curves were used with the following parameters: $n = 5$, $\theta_r = 0.08$, $\psi_s = -1$ m. Hydrostatic distribution of pressure head has been assigned as boundary condition along the vertical boundaries of the 3D domain, while the bottom layer is impermeable. Initial conditions of hydrostatic pressure with zero pressure head at the surface are imposed.

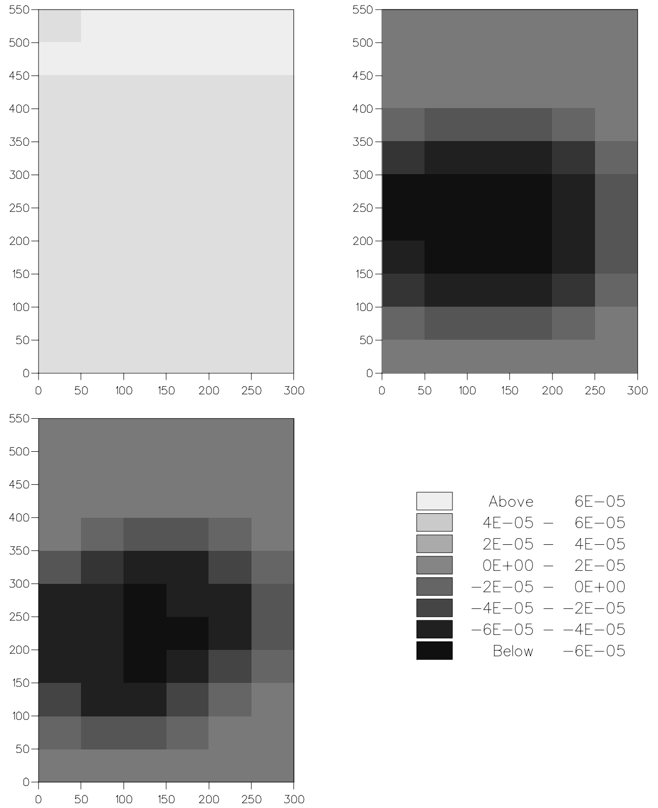

Figure 2: Overland flow rates (m^3/s) as calculated by FLOW3D at $t = 160$ min (top left), 500 min (top right) and 600 min (lower left).

The catchment is subjected to the following atmospheric forcing event. Constant precipitation occurs from $t = 0$ until $t = 360$ min with intensity 6×10^{-5} m/s. From $t = 360$ min the precipitation intensity decreases linearly to zero at $t = 415$ min. At this time evaporation begins with linearly increasing intensity up to -6×10^{-5} m/s at $t = 500$ min. For $t \geq 500$ min, evaporation continues at constant rate until the final time of simulation at $t = 600$ min. The value of pond_head_min is set to 0.01 m.

The results of the simulation are reported in Figures 2 to 4. Figure 2 illustrates the overland flow rates (positive indicates a source) as calculated from the FLOW3D module at $t = 160$, 500, and 600 min. The corresponding distribution of water elevation at the

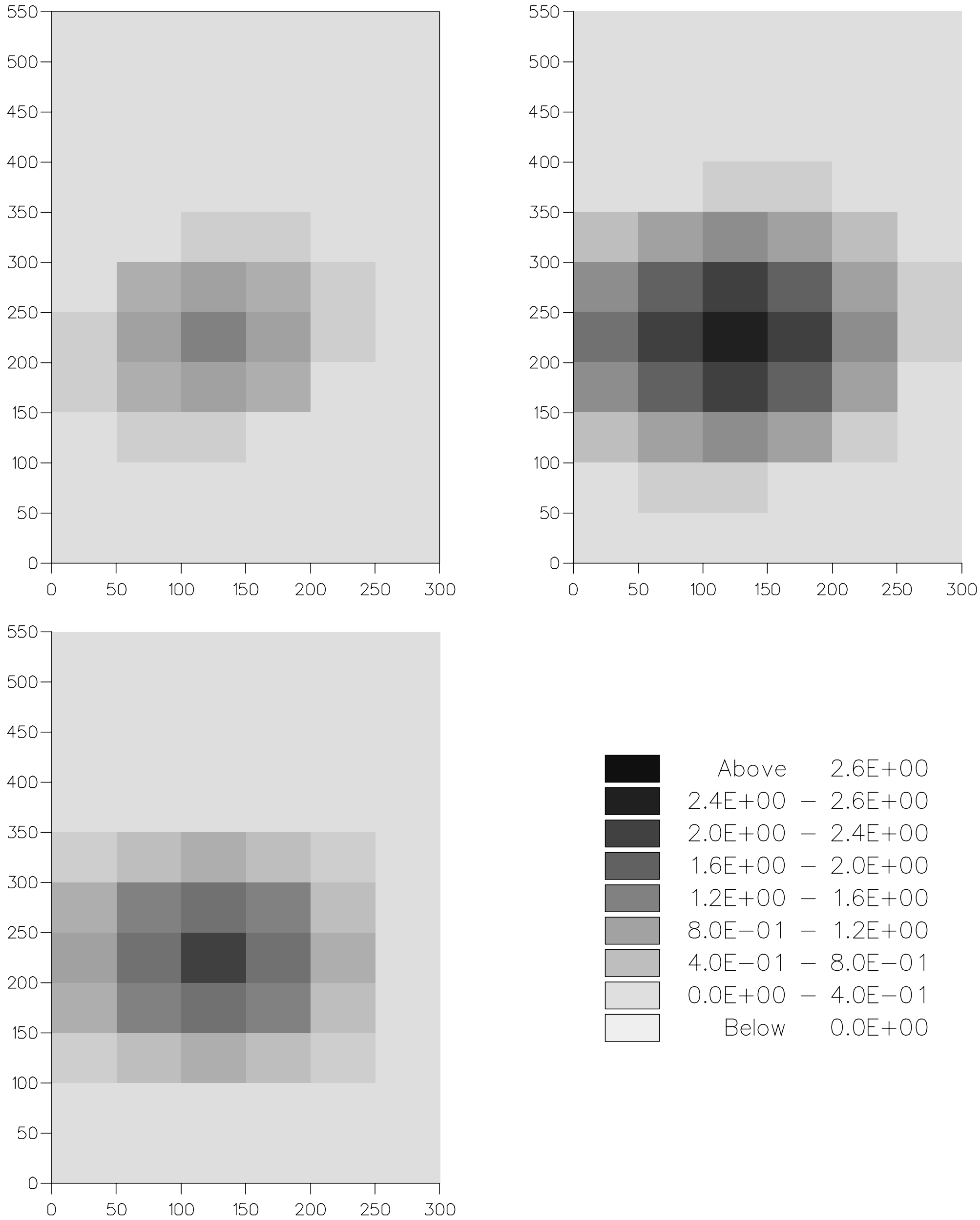

Figure 3: Ponding heads (m) as calculated from SURF_ROUTE at $t = 160$ min (top left), 500 min (top right) and 600 min (lower left).

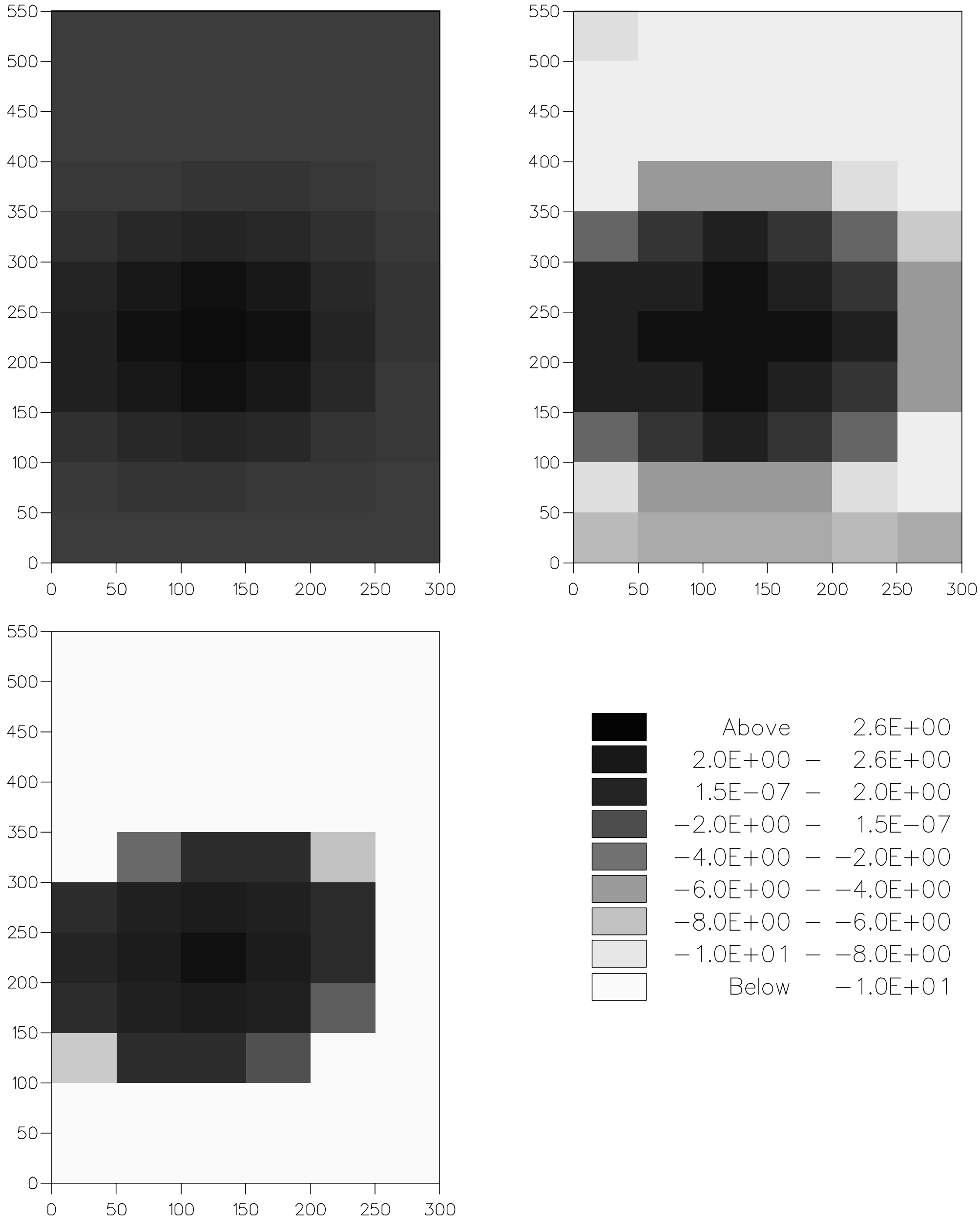

Figure 4: Pressure heads (m) as calculated from FLOW3D at $t = 160$ min (top left), 500 min (top right) and 600 min (lower left).

surface (ponding heads) calculated by SURF_ROUTE is shown in Figure 3, while Figure 4 shows pressure head values at the soil surface. Note that the soil surface is saturated at the early times, but becomes highly unsaturated even before the inception of evaporation. This is due to the fact that the aquifer is rapidly draining the system from the vertical boundary face along the catchment outlet cell.

Ponding occurs in the depression almost from the beginning of the simulation, and reaches a maximum value of $h = 2.8$ m in the central cell of the lake at the end of the precipitation period ($t = 415\ min$) to decrease to $h = 2.6$ m at $t = 500$ min and to $h = 2.1$ m by the end of the simulation. At this time, 6% of the outgoing flux is leaving the aquifer domain through its lower boundary (vertical face containing the outlet cell), 5% is going into the depression, and 89% is evaporating. Correspondingly, 85% of the volume is entering the aquifer through its upper boundary (vertical face opposite to the outlet cell), and 15% through infiltration from the lake.

5 CONCLUSIONS

A physically-based distributed catchment-scale model for the simulation of coupled surface runoff and subsurface flow is developed. The subsurface module is based on a finite element solution of the three-dimensional Richards' equation for variably saturated flow in porous media, and can handle complex boundary conditions and heterogeneous parameters. The surface runoff module is a DEM-based Muskingum-Cunge finite difference solution of the one-dimensional convection-diffusion equation describing overland flow, and treats in an integrated manner hillslope runoff, channel flow, and storage in lakes and other topographic depressions. The interaction and exchange of flux and head information between the two modules is described in detail, and some preliminary simulations on a simple catchment are illustrated. Future work will involve additional code development and test simulations to examine more carefully the interplay between coupling, iteration, and boundary condition switching, to assess the sensitivity of the model to control parameters such as the minimum ponding head value, to improve the post-processing of hydrograph output from the model, and to implement more efficient time stepping that accounts for the different numerical and physical characteristics of the surface and subsurface components.

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