MODELING COUPLED SURFACE AND SUBSURFACE FLOW AT THE CATCHMENT SCALE

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June, 2001

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 et al.* 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.

We will describe a physically-based distributed catchment-scale model for the simulation of coupled surface runoff and subsurface flow [*Bixio et al.* 2001]. 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 and Wood* 1993; *Paniconi and Putti* 1994] and a surface DEM-based finite difference module, SURF_ROUTE [*Orlandini and 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. The state of the art in handling this interaction and exchange between the subsurface and surface components will be described in some detail.

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 and Nielsen* [*1985*], *Brooks and Corey* [*1964*], or *Huyakorn et al.* [*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 and 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.

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.

2.2.1 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 and Maddock* [*1953*].

The distinction between hillslope and channel flow is based on the "constant critical support area" concept as described by *Montgomery and 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 and 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:

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

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.

2.2.2 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 the model 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 and 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:

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

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 Surface–subsurface interactions

The factors determining the water balance of a catchment are soil, topography, vegetation, and climate [*Eagleson* 1978]. Of these, soil and topography are internal and thus discretized and parameterized as part of the model; vegetation is not being considered in this version of the model; and atmospheric forcing, as represented by rainfall and evaporation, functions as the key external driver of surface and subsurface flow processes. It is natural and common in mathematical models to treat these external forcing terms as surface boundary conditions, but because the soil does not act as an infinite store (rainfall) or supply (evaporation) of water, which implies that incoming water gets partitioned into infiltration and surface runoff while, during interstorm periods, water demand by the atmosphere is not always satisfied at the potential rate, these boundary terms cannot in practice be implemented as straightforward Neumann (flux) conditions.

Standard treatment [*Huyakorn et al.* 1986] in an uncoupled (subsurface only) flow model is to consider both atmospheric rainfall and evaporation inputs as *potential* rates. During a rainfall episode on an initially unsaturated soil, the surface boundary condition is of Neumann type until the pressure head at the surface, computed by the model, becomes zero, signalling saturation. At this time the boundary condition is "switched" to a Dirichlet type (specified fixed head), allowing the model to compute or back-calculate the *actual* rate at which water enters the soil, which will initially be lower than the potential rate. If during the course of the rainfall period the actual flux should become larger than the potential rate (as could happen for instance if there is a fall in precipitation intensity), we have a signal that the soil can take in more water than is suggested by the Dirichlet boundary condition and that this extra water is physically available in the form of potential rainfall, so the boundary condition is switched back to a Neumann type and the surface pressure head is again free to vary and should drop below zero.

Analogously, during an interstorm period when the atmospheric input represents a potential evaporation rate, the boundary condition is of Neumann type until soil drying causes the surface pressure head to drop to a threshold "air-dry" value ψ_{min} at which stage a Dirichlet condition is imposed and the actual evaporation rate (lower in magnitude than the potential rate) is calculated from the model. If the actual flux later becomes larger in magnitude than the potential rate (for instance due to an evening drop in potential evaporation), then the boundary condition is switched back to Neumann type and the soil satisfies the full atmospheric demand for water.

It seems reasonable that there should be a similar mechanism for managing the supply and demand of water between soil and atmosphere for both rainfall and evaporation events, however the definition of the threshold value ψ_{min} in the latter case is not as unambiguous as its counterpart $\psi = 0$ in the former case. Not many values for ψ_{min} have been reported in the literature, although *Hollinger and Isard* [*1994*] cite some studies that have been conducted to measure the "air-dry volumetric water content" and its relationship to the permanent wilting point for vegetation. Indeed it may make more sense to base the threshold concept on a moisture content rather than a pressure head, given that under very dry conditions large changes in pressure head are often accompanied by only small changes in moisture content. More field data is required however to test this threshold hypothesis for interstorm periods. It would also be interesting to compare the actual fluxes computed by the model after ψ_{min} is reached to some of the expressions for actual evaporation rate that have been proposed, for instance a linear relationship between this flux and the relative saturation of the soil profile as this saturation value drops in time [*Simmons and Meyer* 2000], and to compare, in field applications, the computed time that elapses between the start of an interstorm period and the attainment of ψ_{min} to analogous measures such as the "time to stage-two drying" estimated from albedo, surface temperature, or surface soil moisture data [*Salvucci* 1997].

The boundary condition switching mechanism has some interesting features with important implications for the coupled surface–subsurface model:

- The switching check is done surface node by surface node, so not only is spatial variability in rainfall/evaporation readily handled, but soil and topographic controls that are as important as atmospheric forcing in determining the spatial patterns of runoff and infiltration are accounted for as well.
- The switching check is done at every time step (in reality since the subsurface model is nonlinear and solved iteratively, we perform the check at each iteration) so temporal variability in rainfall/evaporation is handled, alternating storm and interstorm periods can be simulated, and no assumptions or parameterizations are needed to determine the time to stage-two drying and the time to saturation (or ponding) and the subsequent actual exfiltration and infiltration rates.
- A Neumann boundary condition at the surface corresponds to an atmosphere-controlled infiltration or exfiltration process while a Dirichlet condition represents a soil-limited

process, so these land–atmosphere interactions are easily monitored.

- During a rainfall event at a Dirichlet surface node the difference between the potential and actual fluxes represents "excess" water that, when we introduce a surface routing model, provides the key exchange variable between the surface and the subsurface and allows determination of rainfall-infiltration-runoff partitioning and the activation of surface saturation, overland flow, partially contributing areas, and seepage.

- A single criterion, attainment of zero pressure head at the surface during a rainfall event, accounts for both of the possible mechanisms for overland flow generation, Horton runoff (infiltration excess) and Dunne runoff (saturation excess). The distinction between the two mechanisms can then be made by examining the vertical soil moisture or pressure head profile: if the profile is not completely saturated then the runoff event is of Horton type.

- The balance of water fluxes across the land surface contributes in a significant way to the numerical mass balance over the catchment and to the outflow hydrographs, and the boundary condition switching check provides a straightforward means of computing these components.

In introducing the surface routing model, boundary condition switching performed by the subsurface module is extended to allow excess water to accumulate at the surface as ponding. This ponded water, converted to a flux q_L, constitutes a forcing term input to the routing model at each new time step. The routing model redistributes this water (or accumulates it if the node is part of a partially filled lake or reservoir), and returns with updated surface discharge values into and out of each cell, from which updated ponding head values for the new time step are calculated for input to the subsurface module. A surface node at any point in time can thus be in one of four states: air-dry, unsaturated, saturated, and ponded. Processing for the new fourth state requires balancing not just of actual and potential fluxes as is done for the other three states, but also of ponding heads (or their equivalent in terms of fluxes).

Physically, the distinction between a surface node being "saturated" or "ponded" is made via the model input parameter "pond_head_min" to which 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 (height) of water that can remain trapped in microtopographic features of the surface. Algorithmically, the introduction of the parameter pond_head_min allows us to activate the SURF_ROUTE module only when there is surface water available for routing, rather than at every time step. The sensitivity of the model (e.g., hydrograph response) to pond_head_min remains to be investigated.

In treating the fourth case (ponding) as an extension of the other three, where water balance "accounting" and boundary condition switching continues to be managed by the subsurface module, structural changes to the code in introducing the surface routing model were kept to a minimum. The program logic remained unchanged, even if the ponding case is considerably more intricate than the non-ponded cases, as is documented in Figure 1. Subsurface module accounting also means that what is passed from the subsurface to the surface module at each time step is not the (back-calculated) flux at a given node, but the incremental change in this flux between the previous time step and the current one. That is, the subsurface module updates the surface module, but at the end of its time step the surface module, which converts its updated discharge fluxes to ponding heads to be passed back to the subsurface module, does so without removing this water from the storage amount represented in its discharge fluxes, since this accounting is left to the subsurface module.

The treatment of the ponding case is schematized in Figure 1, which we subdivide into four scenarios: positive potential and actual fluxes, positive potential and negative actual fluxes, negative potential and positive actual fluxes, and negative potential and actual fluxes. In this figure x, $2x$, and $3x$ should be considered flux-converted heads ("surface" axis) or head-converted fluxes ("potential" and "actual" axes). For each scenario the figure explains what is the result (in terms of ponding, saturation status, runoff generation, boundary condition, and actual flux into or out of the soil) at the end of a time step if at the beginning of the time step the potential, actual, and ponding fluxes acting on a surface node during subsurface module execution are as indicated. The resulting flux and saturation status of the surface is that which gets passed to the surface module at the next time step.

Of the four scenarios, the second one, where potential flux is positive (rainfall) and the actual flux is negative, is the simplest. In this case, since the surface is ponded and there is atmospheric supply rather than demand for water, both the potential and actual fluxes contribute entirely to the ponding level, irregardless of the relative magnitudes of the potential, ponding, and actual fluxes. It is clear that the actual flux in this case represents return flow or seepage.

A more complex scenario is the fourth one, where potential and actual fluxes are again opposite in sign, but in this case the atmospheric event is evaporation and there is ponding and infiltration occuring at the surface. This is a scenario which may typically arise just after a rainfall event. If we examine the fourth case in this scenario, where potential flux is $-x$, ponding flux is x, and actual flux is $2x$, the net result indicated in Figure 1 is that the ponding level drops to zero, so that no runoff is generated and the boundary condition switches to Neumann type (atmosphere-controlled) for the next time step, the actual infiltration is x rather than $2x$ since there is not actually $2x$ units of water available for infiltration, and there is no water lost to the atmosphere to satisfy evaporative demand.

Two general rules that are applied in this water balance accounting procedure are:

- Under ponding or saturated conditions, precedence in water redistribution is given to what is (back-)calculated by the code, and then to what is suggested by the potential rainfall/evaporation rate.
- Under saturated or ponded conditions, any exfiltration (negative actual flux) is always taken to be return flow/seepage. This flux contributes to surface runoff, but also contributes to satisfying (potential) atmospheric demand in the case of evaporation.

4 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:

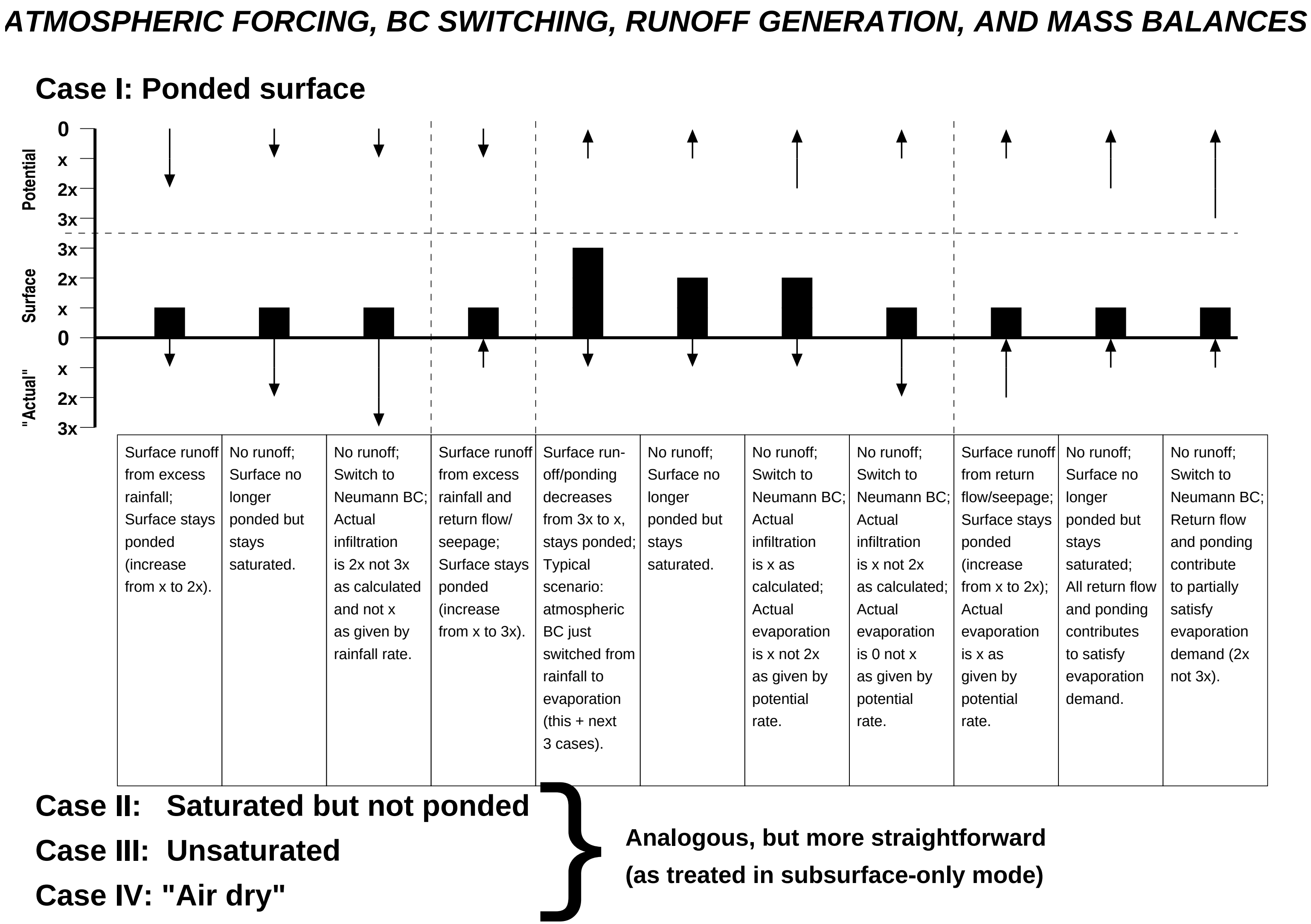

Figure 1: Schematic depiction of atmosphere-surface-subsurface interactions in the coupled model.

- 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, as described previously.

Acknowlegments This work has been supported in part by the European Commission (contract ERB-IC15-CT96-0211), by the Italian Ministry of the University (project ISR8, C11-B), and by the Sardinia Regional Authorities.

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