Implementing Hydrologic Boundary Conditions in a Multiphysics Model

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Abstract: Modeling of hydrologic processes using multiphysics modeling packages shows significant promise in a number of applications. However, these packages have not yet developed a complete set of implementations for boundary conditions important in hydrologic modeling. Three such boundary conditions—rainfall infiltration, seepage faces, and evapotranspiration fluxes—are implemented using the generic boundary condition and internal sink routines provided in one multiphysics package, COMSOL multiphysics. Comparison with results from previous simulations using dedicated hydrologic models demonstrates that with care and creativity these boundary conditions can be implemented accurately and efficiently. Boundary condition implementation should not limit the applicability of multiphysics models to a broad set of problems of interest to the hydrologic community.

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Introduction

Modeling of hydrologic processes using multiphysics modeling packages, e.g., Abaqus, ANSYS Multiphysics, COMSOL Multiphysics, or LS-DYNA, shows significant promise in a number of applications (e.g., Balážová et al. 2002; Chui and Freyberg 2007; Burbey 2008; Cardiff and Kitanidis 2008). These flexible relatively easy-to-use computing environments provide robust numerical solvers for user-assembled coupled partial and ordinary differential equations, mesh generation tools, and a unified graphical modeling environment for model formulation, parameter and initial condition specification, and postprocessing. While at least one of these packages has provided modules designed for hydrologic applications, e.g., COMSOL's Earth science module (COMSOL 2005a), they have not yet developed a complete set of implementations for boundary conditions important in hydrological modeling. In this paper we examine the feasibility of implementing three such boundary conditions—rainfall infiltration, seepage faces, and evapotranspiration fluxes—through the generic boundary condition and internal sink routines provided in the multiphysics package, COMSOL multiphysics (COMSOL 2005a,b).

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Boundary Condition Development and Testing

Variably saturated flow is modeled using the Richard's equation, whose approximate solutions are implemented within the Earth science module of COMSOL multiphysics using finite elements (COMSOL 2005a,b). We describe the implementation of three common hydrologic boundary conditions—rainfall infiltration, seepage faces, and evapotranspiration fluxes—and test them in one- and two-dimensional steady and transient simulations.

Rainfall Infiltration Boundary Condition

Rainfall infiltration boundary conditions involve switching between Dirichlet and Neumann boundary conditions depending on the solution at the soil surface. An algorithm governing such switches is not explicitly available in COMSOL. However, COMSOL's general mixed (Cauchy) boundary condition, together with conditional statements, allows implementation of these switches. Introducing complementary smoothing functions into the general mixed boundary condition defined in COMSOL (COMSOL 2005a) gives

$$n \times \frac{\kappa_s}{\eta} k_r \nabla (p + \rho_f g z) = \alpha N_0 + \beta R_b (H_b - H) \quad (1)$$

where n=normal to the boundary; κ_s=intrinsic permeability (m^2); η=fluid viscosity (Pa s); k_r=relative permeability (-); p=fluid pressure (Pa); ρ_f=fluid density (kg/m^3); g=gravitation acceleration (m/s^2); z=vertical coordinate (positive upward) (m); α,β =complementary smoothing functions; N_0=nonhead dependent flux (m/s); R_b=external resistance (s^{-1}); $H_b = z_b + p_b/(\rho_f g)$ =external total head (m); z_b=external elevation (m); p_b =external pressure (Pa); and $H = z + p/(\rho_f g)$=total head at the boundary (m).

This general boundary condition reduces to a Neumann condition when R_b=0 and to a Dirichlet condition when R_b is infinite

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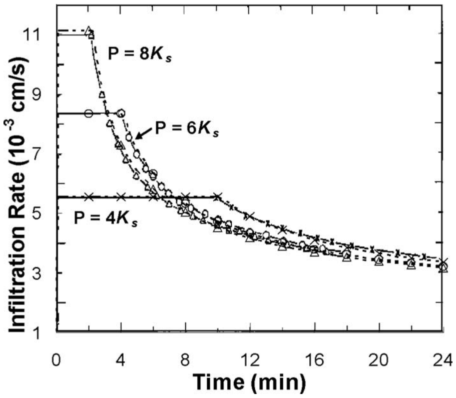

Fig. 1. Infiltration curves from Mein and Larson (1973) (solid lines) and COMSOL (dotted lines) at different constant precipitation rates (P)

(very large) (Forsyth 1988) and $N_0=0$. Therefore, we can use the mixed boundary condition to represent solution-dependent switching of Neumann or Dirichlet conditions through the specification of R_b and conditional statements. At the start of rainfall, we set

$$N_0 = P, \quad \text{and} \quad R_b = 0 \tag{2a}$$

where P=precipitation rate (m/s). This gives a specified flux at the precipitation rate on the boundary. When the pressure head on the boundary becomes greater than 0 gauge (i.e., $p>0$ or $H>z$), we set

$$N_0 = 0, R_b = \text{large number, and } H_b = z + h_{\text{ponded}} \tag{2b}$$

This provides a ponded Dirichlet condition at h_{ponded} ($h_{\text{ponded}}=0$ at incipient ponding) which can either be a prespecified value or a solution from a coupled surface model. However, if the resulting flux from the Dirichlet condition exceeds the precipitation rate [i.e., $R_b(H_b-H)>P$], the boundary reverts to the Neumann flux using the parameters listed in Eq. (2a). To minimize the number of switches during iterative solution, we turn on/off the boundary conditions gradually over a small range of boundary pressure using complementary smoothing functions, α and β, for the non-head dependent specified flux, N_0, and the external resistance, R_b.

To test the rainfall infiltration boundary condition implementation described above, we reproduce several simulations from Mein and Larson (1973). Mein and Larson computed numerical solutions of a Richard's equation model of infiltration under a constant intensity precipitation into a homogeneous soil with uniform initial moisture content of 0.125. The medium is a sandy loam with a saturated hydraulic conductivity of 1.39 $\times 10^{-3}$ cm/s and a porosity of 0.518. We visually fit a van Genuchten model to the soil moisture retention and relative permeability curves provided by Mein and Larson to obtain a residual moisture content of 0.119 and van Genuchten parameters of 0.026 8 cm^{-1} and 4.36. Mein and Larson did not specify the depth of their simulated soil column. We assume a depth of 2 m, which is deep enough to avoid any interaction with the wetting front during the simulation period of 24 min. Fig. 1 compares our infiltration curves with the numerical results of Mein and Larson, showing very good agreement. There are minor disparities between the two sets of results, which are the result of the fitted van Genuchten model and some distortion in the scanned image from the original paper.

Seepage Face Simulation

The pressure along a seepage face is atmospheric and the ground surface above a seepage face is typically no flow or is subjected to a specified evaporative or infiltration flux. Adopting an approach similar to that used for the rainfall infiltration boundary condition, a mixed boundary condition can be used to split a boundary into a Dirichlet portion for the seepage face and a Neumann portion for the region above the seepage face. First, we set

$$N_0 = I, \quad \text{and} \quad R_b = 0 \tag{3a}$$

where I=infiltration or evapotranspiration rate (m/s). However, if the pressure head on the boundary becomes greater than 0 gauge (i.e., $p>0$ or $H>z$), we set

$$N_0 = 0, R_b = \text{large number, and } H_b = z \tag{3b}$$

This gives a Dirichlet condition at a pressure head of 0, which then correctly represents a seepage face. It is convenient to express R_b in terms of the saturated hydraulic conductivity, K_{sat}, and a coupling length scale, L

$$R_b = \frac{K_{\text{sat}}}{L} \tag{4}$$

We test the mixed boundary condition formulation by comparing with Clement et al. (1996). They simulated steady-state flow through a 1-m^2 domain. The top and the base of their domain are no-flow boundaries. The water levels on the left and on the right are at 1.0 and 0.2 m, respectively. K_{sat} is 1.0 m/day and the van Genuchten parameters are 0.64 m^{-1} and 4.65. Table 1 shows that the results from COMSOL match those of Clement et al. (1996) as long as L is small enough. Given the convergence challenges for smaller values of L (e.g., L=0.1 and 0.001 m) and the reasonable accuracy achieved with L=1 m, we set L to be 1 m for a subsequent transient simulation.

Table 1. Results for 1-m^2 Domain with Different Coupling Length Scales

L (m)	Inflow (m^2/day)	Total outflow (m^2/day)	Outflow below tailwater elevation (m^2/day)	Seepage outflow (m^2/day)	Seepage face length (m)
Clement et al.	NA	0.55	NA	NA	0.32
1,000	0.521	0.515	0.181	0.334	0.389
10	0.545	0.544	0.269	0.275	0.319
1	*0.545*	*0.545*	*0.273*	*0.272*	*0.317*
0.1	0.545	0.545	0.272	0.273	0.317
0.001	0.545	0.545	0.272	0.273	0.317

Note: Data in italic font contains results for L=1 which is the coupling length scale used for a subsequent transient simulation. NA=not applicable.

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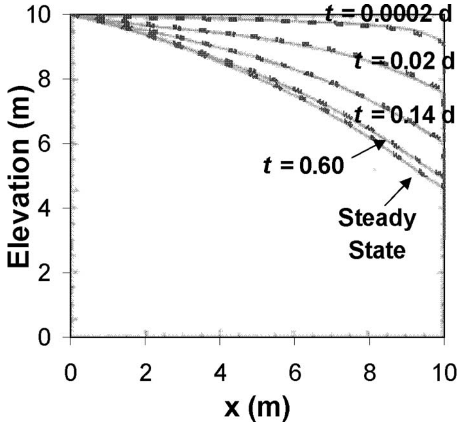

Fig. 2. Water table elevations at different times from Wise et al. (1994) (solid lines) and COMSOL (dotted lines)

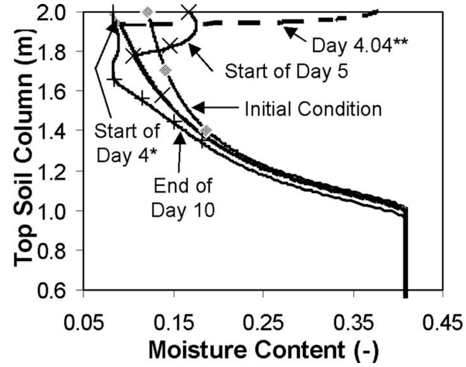

Fig. 4. Soil column moisture profiles during the 10-day simulation. Day 3 is almost on top of Day 3.04 except the upper 10 cm (* immediately before the rainfall and ** immediately after the rainfall).

The transient simulation in Wise et al. (1994) uses a 10 m $\times 10$ m square domain with no-flow boundaries along the top and the base. The initial total head throughout the domain is at 10 m, i.e., water table is at the top of the domain. Wise et al. kept the water table on the left at the top of the domain while they instantaneously lowered the head on the right boundary at $t=0$ to an elevation of 3 m. The homogeneous and isotropic K_{sat} is 5.1 m/day and the specific storage is 5×10^{-5} m^{-1}. The residual moisture content is 0.01 and the porosity is 0.46. The van Genuchten parameters are 2.0 m^{-1} and 2.8. Fig. 2 shows a good match between the water table elevations from COMSOL and from Wise et al.

Interception and Evapotranspiration

To simulate interception and evapotranspiration, we implement an algorithm presented in Panday and Huyakorn (2004). Interception storage is the mass balance between rainfall onto interception storage and canopy evaporation (E_{can}). If E_{can} does not meet the reference evapotranspiration rate (E_p), transpiration (T_p) occurs over a prescribed effective root length at a rate that accounts for leaf area index, moisture availability, and root distribution. If the E_p still has not been met by both E_{can} and T_p, evaporation (E_s) then occurs over a prescribed extinction depth below the soil surface at a rate that accounts for moisture availability. The above algorithm will always produce an actual evapotranspiration (E_a) equal to or less than E_p.

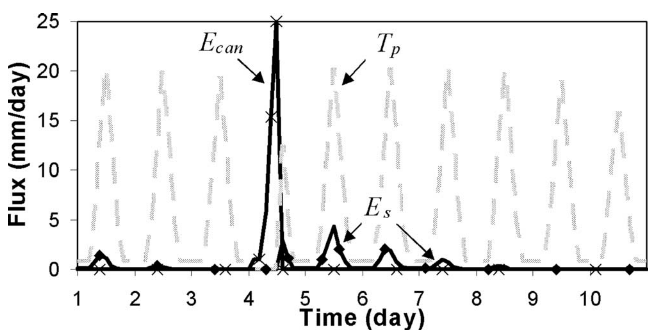

Fig. 3. Canopy evaporation (E_{can}), transpiration (T_p), and evaporation (E_s) from the soil during the 10-day simulation

We implement this complex boundary using coupled equations, along with generic internal sinks, which permits conditional expressions. For testing, we simulate a hypothetical 10-day scenario involving a diurnal E_p and a single rainfall event. The modeling domain is a one-dimensional homogeneous vertical column of sandy loam 2 m long. The porosity and the residual moisture content are 0.41 and 0.065, respectively. K_{sat} is 1.23×10^{-5} m/s and the specific storage is 0. The van Genuchten parameters are 7.5 m^{-1} and 1.89. The interception storage is initialized to 0 and the initial head is 1.0 m throughout the soil column. A single rainfall event of uniform intensity 2 cm/h starts at the beginning of Day 4 and lasts for 1 h. Fig. 3 shows the three components of $E_a - E_{\mathrm{can}}$, T_p, and E_s—over the 10-day period. Fig. 4 shows the evolution of the moisture profile during the simulation.

The simulated behavior shows insignificant mass balance errors and is consistent with hydrologic expectations. While there is a computational cost in implementing such a complex condition, for this one-dimensional example the overall computational speeds were high and there were no instabilities introduced by the conditional expressions.

Conclusions

Simulating hydrologic processes requires challenging boundary conditions that are not necessarily available in multiphysics modeling packages. However, with care and creativity one can use generic boundary condition routines in such packages to craft good representations of important hydrologic boundary conditions. Given the versatility and integrated nature of multiphysics packages, they are becoming important tools for simulating coupled atmospheric-hydrologic-ecologic systems. The approaches developed and demonstrated here are extensible to many other settings, suggesting that boundary condition implementation should not limit the applicability of multiphysics models to a broad set of problems of interest to the hydrologic community.

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