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SIMULTANEOUS FLOW OF WATER AND AIR ACROSS THE LAND SURFACE DURING RUNOFF

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Abstract. This paper presents an inter-compartment boundary condition for the simulation of surface runoff, soil moisture, and soil air as a coupled system of partial differential equations. The boundary condition is based on a classic leakance approach to balance water between differently mobile regions such as the land surface and subsurface. Present work applies leakances to transfer water and air simultaneously through the land surface for soils, which are connected by an air flux with a steady atmosphere. Shallow flow and two phase flow in a porous medium are sequential calculated in an iteration loop. General criteria are stated to guarantee numerical stability in the coupling loop and for leakances to control inter-compartment fluid fluxes. Using the leakance approach, a numerical model captures typical feedbacks between surface runoff and soil air in near-stream areas. Specifically, displacement of water and air in soils is hampered at full-water saturation over the land surface resulting in enhanced surface runoff in the test cases. Leakance parameters permit the simulation of air out-breaks with reference to air pressures, which fluctuate in the shallow subsurface between two thresholds.

1 BACKGROUND

Fluid mass flows between partial differential equations of surface and subsurface flow via inter-compartment boundary conditions at the land surface or riverbeds. Highly detailed models^[6] combine free-flow of the Stokes or Navier Stokes equations with flow in a porous medium through a transition zone, where a slip condition by Beavers and Joseph ^[1] balances momentum.

Modeling runoff of water over the land surface usually involves application of some form of hydrostatic shallow water equation, namely the Saint-Venant, diffusive or kinematic wave equation. Hydrostatic shallow flow has been coupled to flow in the subsurface in form of Darcy and Richards' flow^[7,8] and recently also to two-phase flow ^[2]. Some coupled runoff models enforce continuity between the hydrostatic pressure of surface water and the matric pressure of variably saturated soils at the land surface^[7]. Others assume the existence of a small interface (transition zone) and control the mutual mass exchange between flow compartments with an additional leakance parameter^[2,4,8].

2 COUPLING FLOW COMPARTMENTS

Flow of a liquid in the overland compartment is represented by the diffusive wave equation in our numerical model. The shallow flow equation assumes hydrostatic pressure p^{H} in a depth-integrated 1D or 2D flow field. 1D, 2D or 3D flow of a liquid (superscript l) and gas (superscript g) in the soil compartment is simultaneously calculated with a two-phase flow equation. In contrast, diffusive wave overland flow and two-phase flow are sequentially calculated in an iteration loop. Thus, the numerical model iterates between the following algebraic equation systems^[2]

$$A^{H}\mathbf{h} = \mathbf{b}^{H}, \qquad A^{p} \begin{pmatrix} \mathbf{p}^{c} \\ \mathbf{p}^{g} \end{pmatrix} = \begin{pmatrix} \mathbf{b}^{l} \\ \mathbf{b}^{g} \end{pmatrix},$$
(1)

where A are system matrices for overland flow (superscript H) and two-phase flow. Right hand side vectors **b** account for source / sink terms, which originate from intercompartment fluxes (Sect. 2.1), precipitation, outlets, etc.. Primary variables are the hydraulic head h in the surface water (Fig. 1(a)), the capillary pressure p^c , and the soil gas pressure p^g .

2.1 Fluid fluxes through the land surface

A new inter-compartment boundary condition provides liquid and gas fluxes through a transition zone at the surface of a porous medium, which is a soil in this work (Fig. 1(a)). The transition zone is constructed with a continuum approach and consists of:

1. A porosity in overland flow for homogenization of surface structure (rills, etc.). Overland flow starts, if liquid depth exceeds certain thickness of surface structure $(H > a \text{ in Fig. 1(a)})^{[8]}$.



Figure 1: Transition zone between overland and soil compartments (source: Delfs et al. $(2013)^{[2]}$): (a) Surface structure depth *a* and interfaces a^l , a^g ; (b) A flow control factor *f* in the relative liquid interface permeability k_c^l follows a hysteresis curve (top) for simulation of air out-break events (bottom).

2. An interface layer a^l for a mutual coupling flux between the liquid in the overland compartment and the liquid phase of the porous medium in the soil compartment^[8]

$$q_c^l = -\lambda^l \left(p^H + p^c - p_e^g \right), \qquad \lambda^l = \frac{k_c^l k}{\mu^l a^l}, \tag{2}$$

where λ^l is the leakance for liquid, μ^l the dynamic liquid viscosity, k_c^l the relative liquid interface permeability (Sect. 2.2), k the intrinsic soil permeability, $p_e^g = p^g - p_{atm}^g$ the atmospheric excess gas pressure, and p_{atm}^g the atmospheric pressure.

3. An interface layer a^g to connect gas of the soil and atmosphere compartments^[2]

$$q_c^g = \lambda^g p_e^g, \qquad \lambda^g = \frac{k_c^g k}{\mu^l a^g},\tag{3}$$

where λ^g is the leakance for gas, μ^g the dynamic gas viscosity, and k_c^g the relative gas interface permeability (Sect. 2.2).

The fluxes q_c^l and q_c^g are implemented as implicit source terms in the algebraic equation systems (1) for iterative coupling. Concerning stability, it is important (Sect. 4.3) that the hydrostatic surface water pressure p^H is often negligible. The atmospheric pressure p_{atm}^g can be set as zero in many practical cases.



Figure 2: Test cases: (a) Smith and Woolhiser (1971) benchmark on Horton runoff (source: Delfs et al. $(2013)^{[2]}$); (b) Flood wave over a synthetic hillslope.

2.2 Functions of leakance

The leakance approach enables the modeler to control inter-compartment fluid fluxes (2) and (3) with reference to state variables (pressures). To achieve this, leakances λ_l , λ_g are modified by relative interface permeabilities k_c^l , k_c^g , respectively. It holds $0 \leq k_c^l(p^H, p^g) \leq 1 - k_{cr}^g$, where k_{cr}^g is the residual value for the relative gas interface permeability $k_c^g \approx 1 - k_c^l$. This accomplishes:

- 1. To limit the liquid exchange flux (2) by the available liquid with depth H in the overland compartment when liquid infiltrates into dry soil with high capillary forces. k_c^l is zero for if the liquid depth H exceeds certain threshold a^s .
- 2. To disconnect soil gas from the atmosphere compartment during liquid ponding and runoff in the overland compartment. The relative gas interface permeability k_c^g becomes the residual value k_{cr}^g for $H \ge a_s^{[2]}$.
- 3. To act as a value for compressed soil gas by following a hysteresis curve (Fig. 1(b)). Gas pressure p^g in the porous medium fluctuates between two thresholds p_{break}, p_{close} where gas breaks out of a liquid-covered surface and the surface closes for gas, respectively^[9]. k_c^l is reduced by the minimum flow control factor f_{break} during air pressure counterflow through the land surface^[2].

3 TEST CASES

3.1 Classic Smith and Woolhiser (1971) benchmark on Horton runoff

A light oil was applied^[7] for 15 minutes with a rate of 4.2 cm per minute on a sand flume with a length of 12.2 meter and a slope of 1% (Fig.2(a)). Liquid infiltration was tracked inside the flume and Horton runoff recorded at an outlet. Sand properties varied only slightly. Thus, flow is simulated in 1D with vertical and homogeneous soil columns^[2].

Soil air can escape into the atmosphere at the top of columns through the gas exchange flux (3). Air pressure is enforced to equal atmospheric pressure p_{atm}^g at 30 cm soil depth.

3.2 Synthetic floodplain

An inclined plain has a length of 10 meter and a slope of 2% (Fig.2(b)). The plane is initially ponded at 1 meter length. At this part, a source term of q = 3 meter per second is assigned for 10 seconds. The water depth quickly rises and a flood wave flushes around 85% of the plaine length. Inter-compartment fluxes (2) and (3) permit water and air exchange through the land surface. The remaining boundaries are assumed as impervious for water and air. Soil parameters are chosen as in the Smith and Woolhiser (1971) benchmark to represent a homogeneous sand.

4 RESULTS AND DISCUSSION

4.1 Model verification

The coupled overland / two-phase flow model is verified with liquid data of a Horton flow experiment (Sect. 3.1). Soil air flow was not measured, although air flow effects were noticed by the experimentators^[7]. Results presented in Fig. 3(a) reveal that soil gas pressures impede the calculated infiltration of water and, consequently, amplify Horton runoff. A distinctive air out-break event (Sect. 2.2) was simulated for the early part of the hydrograph. The increase in surface runoff corresponds well with the experimental data regarding the amount. However, by using 1D soil columns (Fig. 2(b)), the coupled model was not able to capture the late rise in the experimental runoff. Obviously, a broader experimental data basis is needed to test the coupled model throughoutly.

4.2 Interface thicknesses

Interfaces (transition zones) are introduced in a leakance concept (Sect. 2.1). The extra parameters require careful examination^[5]. A parameter sensitivity study revealed^[2] that interfaces impede liquid and gas exchange between compartments if their thicknesses exceed certain thresholds

$$a^l > a^l_c, \qquad a^g > a^g_c. \tag{4}$$

Thresholds are $a_c^l = 0.1$ mm for the liquid (Fig. 3(b)) and $a_c^g = 1$ mm for the gas in the test case on Horton flow (Sect. 3.1), and independent of each other. The threshold a_c^g for the gas interface thickness linearly increases with the length of the soil column. Leakances at thresholds a_c^l and a_c^g are independent of other parameters than intrinsic permeability k and the geometry (e.g. soil column length) of the subsurface porous medium system.

4.3 Stability in the coupling loop

The inter-compartment fluxes (2) and (3) are implicitly calculated in a sequential iterative coupling algorithm. One part of a flux q_c^l , q_c^g is implemented in the matrix



Figure 3: Results of Smith and Woolhiser (1971) benchmark (source: Delfs et al. $(2013)^{[2]}$): (a) Comparison of simulated and measured surface runoff at the flume outlet; (b) Liquid coupling flux q_c^l for a range of liquid interface thicknesses a^l .

and the other part in the right hand side vector of the algebraic equation system (1) if atmospheric pressure p_{atm}^g and hydrostatic pressure in surface flow p^H have finite values. As a consequence, the capillary pressure p^c and gas pressure p^g exhibit discontinuities at the compartment interface. Fig. 4(a) shows discontinuities in atmospheric excess gas pressure p_e^g . They have a constant step size of

$$\Delta p_e^g = 10^{-12} p_{atm}^g.$$
 (5)

Thus, the gas flux (3) has discontinuities with a step size of $\Delta q_c^g = \lambda^g \Delta p_e^g = 10^{-12} \lambda^g p_{atm}^g$. In the use of inter-compartment coupling fluxes q_c^l and q_c^g with surface pressure terms p^H , p_{atm}^g , it is important to ensure stability by selecting low leakances λ^l and λ^g without impeding fluid exchange. The criteria (4) and (5) guide the model applier to proper ranges for leakances λ^l and λ^g in practice, e.g. $a^l > 10^{-6}$ m and $a^g > 10^{-10}$ m for stability in the test case on Horton flow (Sect. 3.1).

4.4 Soil air entrapment

Flooded soils exhibit a reduced infiltration capacity, if a near-surface water table prevents compressed soil air from disappearing into deeper subsurface regions. Thus, Fig. 4(b) illustrates the capability of the coupled model to produce soil air entrapment in a 2D floodplain test case (Sect. 3.2). Infiltration of flood water is strongly retarded and occurs mainly adjant to the water-free part of the pervious plain ($x \approx 17$ m). As a consequence, the infiltrating water isolates an air cell of high soil air pressures.



Figure 4: (a) Discontinuities in iterative coupling $(p_{atm}^g = 101325 \text{ Pa} \text{ in the Horton flow benchmark}, source: Delfs et al. (2013)^[2])); (b) Snapshots of a synthetic floodplain for 2 h simulation time (vertical axis exagerated).$

5 SUMMARY AND CONCLUSIONS

in the numerical study, leakances controlled the mutual fluid mass transfer through an inter-compartment transition zone (Fig. 1) in a unique hydrostatic shallow / twophase flow model. The numerical stability is ensured when the boundary condition is used in combination with a sequential iterative coupling algorithm (Fig. 4(a)). Soil gas pressures impeded surface runoff from infiltrating in a liquid-covered soil flume (Fig. 3(a)) and a synthetic floodplain (Fig. 4(b)). Thus, our results suggest that air entrapment below pervious land surfaces amplifies stream flow considerably during high precipitation besides other principal stream flow generation mechanisms by Horton, Dunne, etc.. Insitu measurements of surface runoff and soil air pressures are needed for further testing of the air counterflow algorithm (Fig. 1(b)).

Various chemical and physical clogging mechanisms at land surfaces can be simulated by modifying leakances with state variables in future work (e.g. biofilms, unsaturated zones below riverbeds). The sequential coupling algorithm enables developers to couple the presented model with a dynamic atmosphere model to include soil air / atmosphere interactions^[3]. The implementation is available via the open source scientific software project OpenGeoSys (www.opengeosys.net) and can be combined with various model components, e.g. for non-isothermal flow, deformation processes, and transport of multiple reactive components.

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REFERENCES

- Beavers, G.S. and Joseph, D.D. Boundary conditions at a naturally permeable wall. J. Fluid. Mech. (1967) 30:197–207.
- [2] Delfs J.-O., Wang W., Kalbacher T., Singh A.K. and Kolditz O. A coupled surface / subsurface flow model accounting for air entrapment and air pressure counterflow. *Environ. Earth Sci.* (2013) 69(2).
- [3] Elberling B. and Larsen F., Christensen S. and Postma D. Gas transport in a confined unsaturated zone during atmospheric pressure cycle. *Water Resour. Res.* (1998) 34(11):2855–2862.
- [4] Hantush M.S. Wells near streams with semi-pervious beds. J. Geophys. Res. (1965) 70(2):2829–2838.
- [5] Liggett J., Werner A.D. and Simmons C.T. Influence of the first-order exchange coefficient on simulation of coupled surface-subsurface flow. J. Hydrol. (2012) 414-415:503-515.
- [6] Mosthaf K., Baber K., Flemisch B., Helmig R., Leijnse A., Rybak I. and Wohlmuth B. A coupling concept for two-phase compositional porous-medium and single-phase compositional flow. *Water Resour. Res.* (2011) 47:doi:10.1029/2011WR10685.
- [7] Smith R.E. and Woolhiser D.A. Overland flow on an infiltrating surface. Water Resour. Res. (1971) 7(4):899–913.
- [8] van der Kwaak J.E. and Loague K. Hydrologic-response simulations for the R-5 catchment with a comprehensive physics-based model. *Water Resour. Res.* (2001) 37(4):999–1013.
- [9] Wang Z., Feyen J., Nielsen D.R. and van Genuchten M.T. Two-phase flow infiltration equations accounting for air entrapment effects. *Water Resour. Res.* (1997) 33(12):2759–2767.