Modélisation numérique des interactions eaux souterraines / eaux de surface: défis et progrès récents

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Proper understanding and representation of hydrosphere interactions (between the atmosphere, land surface, soil zone, aquifers, rivers/lakes, and vegetation) is increasingly relevant to climate prediction, environmental protection, and water management.

We are at a crossroads in hydrological modeling:

- models (of all flavors) are being integrated across many disciplines and over multiple scales, and they are being intercompared
- better datasets are increasingly being made available (for hypothesis testing and model validation) that provide observations (on the ground, airborne, and from space) of more processes, in more detail, and at higher accuracy
- computational boundaries are continually being pushed (cost and capabilities of systems, efficiency and robustness of algorithms), for easier and more effective data analysis and process simulation
Outline

CATHY (CATchment HYdrology) model description

Some recent studies (successes and challenges)

Extensions and evolution of the model
CATHY (CATchment HYdrology) model description

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

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

\[ \sigma = S_w S_s + \phi(dS_w/d\psi) \]

water saturation = \( \theta/\theta_s \) [\( \ell \)]

volumetric moisture content [\( \ell^3/\ell^3 \)]

saturated moisture content [\( \ell^3/\ell^3 \)]

specific storage [1/L]

porosity (= \( \theta_s \) if no swelling/shrinking)

pressure head [L]

time [T]

saturated conductivity tensor [L/T]

relative hydraulic conductivity [\( \ell \)]

zero in x and y and 1 in z direction

vertical coordinate +ve upward [L]

subsurface equation coupling term (more generally, source/sink term) [\( \ell^3/\ell^3 T \)]

ponding head (depth of water on surface of each cell) [L]

hillslope/channel link coordinate [L]

discharge along s [\( \ell^3/T \)]

kinematic wave celerity [L/T]

hydraulic diffusivity [\( \ell^2/T \)]

surface equation coupling term (overland flow rate) [\( \ell^3/LT \)]

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**Main features of the model**

Path-based description of surface flow across the drainage basin; several options for identifying flow directions, for separating channel cells from hillslope cells (same governing equation), and for representing stream channel hydraulic geometry.

The coupling term for the model is computed as the balance between atmospheric forcing (rainfall and potential evaporation) and the amount of water that can actually infiltrate or exfiltrate the soil. This threshold-based boundary condition switching partitions potential fluxes into actual fluxes and changes in surface storage.
Various functional forms for $S_w(\psi)$ and $K_{rw}(\psi)$

Heterogeneities ($K_{sx}$, $K_{sy}$, $K_{sz}$, $S_s$, $\phi$) by "zone" and by layer

DEM-based (uniform) grid or user-defined (nonuniform) surface grid input

3D grid automatically generated with variable layer thicknesses and different base ("bedrock") shapes

Finite element spatial integrator (Galerkin scheme, tetrahedral elements, linear basis functions)

Weighted finite difference discretization in time

Time-varying boundary conditions: Neumann, Dirichlet, source/sink terms, seepage faces, and atmospheric fluxes

Adaptive time stepping; Newton and Picard linearization; selection of CG-type linear solvers; etc
Overland (hillslope rills) and channel flow along s

DEM pre-analysis for definition of cell drainage directions, catchment drainage network and outlet, etc

"Constant critical support area": overland flow \( \forall \) cells with upstream drainage area \( A < A^* \); else channel flow (2 other threshold-based options also implemented)

Leopold & Maddock scaling relationships; Muskingum-Cunge solution scheme (explicit and sequential); etc

"Lake boundary-following" procedure to pre-treat lakes

Storage and attenuation effects of lakes and other topographic depressions are accounted for by transferring with infinite celerity all the water drained by the "buffer" cells to the "reservoir" cell; level pool routing calculates the outflow from this cell:

\[
\frac{\partial V}{\partial t} = I(t) - O(h^*)
\]
Surface flow module (drainage network flow characteristics)

Surface runoff propagated through a network of rivulets and channels automatically extracted from the DEM.

Spatial (term I) and temporal (term II) variations of flow characteristics of the drainage network (stream channel geometry $W$ and conductance coefficient $k_s$) derived from application of downstream (according to upstream drainage area) and at-a-station (according to flow discharge) fluvial relationships:

\[
W(A, Q) = W(A_s, Q_f) Q_f (A_s)^{-b'}(A/A_s)^{w(b''-b')} Q^{b''}
\]

\[
k_s(A, Q) = k_s(A_s, Q_f) Q_f (A_s)^{-y'}(A/A_s)^{w(y''-y')} Q^{y'}
\]

"Pond_head_min" threshold parameter accounts for microtopography

Coupled system solved sequentially*: surface first, for $Q^{k+1}$ and $h^{k+1}$; then subsurface, for $\psi^{k+1}$; finally overland flow rates $q_{L}^{k+1}$ are back-calculated from subsurface solution

[*sequential solution procedure but with iterative BC switching during subsurface resolution to resolve the coupling]

Nested time stepping: one or more surface solver time steps for each subsurface time step (based on Courant and Peclet criteria for the explicit surface routing scheme; also reflects typically faster surface dynamics compared to subsurface)

Interaction between cell-based surface grid and node-based subsurface grid includes input option for coarsening of latter grid. Allows us to exploit slower subsurface dynamics and looser grid constraints (implicit scheme), and can lower CPU and storage costs of 3D module
Boundary condition-based coupling (surface BC switching procedure)

Case I: Ponded surface
- No runoff; Surface no longer ponded but stays saturated.
- Surface run-off from excess rainfall; Surface stays ponded (increase from x to 2x).
- Actual infiltration is 2x not 3x as calculated and not x as given by rainfall rate.
- Surface run-off/ponding decreases from 3x to x, stays ponded; Typical atmospheric BC just switched from rainfall to evaporation (this + next 3 cases).

Case II: Saturated but not ponded
- No runoff; Switch to Neumann BC; Actual infiltration is x as calculated; Actual evaporation is x not 2x as given by potential rate.

Case III: Unsaturated
- No runoff; Switch to Neumann BC; Actual infiltration is x not 2x as calculated; Actual evaporation is 0 not x as given by potential rate.

Case IV: Dry (stage-two drying)
- No runoff; Surface no longer ponded but stays saturated;
- All return flow and ponding contribute to satisfy evaporation demand (2x not 3x).

Analogous, but more straightforward (as treated in subsurface-only mode)
Some recent studies (successes and challenges)

- Recharge estimation, impact of heterogeneity
- Hydrograph separation, model coupling approaches
- Bedrock leakage
- Predicting near-surface soil moisture state
- Hysteresis in storage–discharge dynamics
- Rill flow vs sheet flow
- Simulation of multiple response variables
- Problem of grid scale invariance
Loose coupling (simplified model) vs CATHY: is hydrograph separation really so straightforward?

<table>
<thead>
<tr>
<th>Water budget component (mm/y)</th>
<th>HELP + FEFLOW</th>
<th>CATHY</th>
</tr>
</thead>
<tbody>
<tr>
<td>Precipitation</td>
<td>1038</td>
<td>1038</td>
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<tr>
<td>Evapotranspiration</td>
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<td>556</td>
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<tr>
<td>Recharge</td>
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<td>233</td>
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<tr>
<td>Total Discharge</td>
<td>456</td>
<td>500</td>
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<tr>
<td>Surface runoff</td>
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<td>/</td>
</tr>
<tr>
<td>Subsurface runoff</td>
<td>36</td>
<td>/</td>
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<tr>
<td>Baseflow</td>
<td>189</td>
<td>/</td>
</tr>
<tr>
<td>Exchange with regional fractured aquifer</td>
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<td></td>
</tr>
<tr>
<td>+ve (reg.aq. to hillslope)</td>
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<td>77</td>
</tr>
<tr>
<td>-ve (hillslope to reg.aq.)</td>
<td>17</td>
<td>4</td>
</tr>
<tr>
<td>Storage change</td>
<td>14</td>
<td>55</td>
</tr>
</tbody>
</table>

Bedrock leakage (idealized hillslopes / sloping unconfined aquifers)

Spatially distributed leakage rates calculated after Darcy’s law - 5% inclination, $k_{\text{soil}} = 1 \times 10^{-5}$ m/s, $k_{\text{aquifard}} = 1 \times 10^{-8}$ m/s

Water table profiles calculated by hsB at $t = 50$ days as function of constant leakage rates

Questioning a fundamental paradigm in hillslope hydrology.

Highly dependent on downslope BC treatment – not just a numerical issue.
Predicting near-surface soil moisture state (des Anglais river basin, southwestern Quebec)

CLASS (red) and CATHY (black) results for monthly soil water content at different depths (shallow to deep from top to bottom) and for past (left) and future (right) climate projections.

Is there a bias in the model? Possible causes:
- surface BC handling (eg, need seepage faces along stream banks?);
- too-coarse temporal rainfall resolution (peak rain rates get smoothed out → more infiltration, less surface runoff);
- missing transpiration;
- too-coarse grid around steep terrain (eg, Covey Hill) misses important dynamics;
- missing agricultural (eg, tile) drainage;
- …

Simulated (top) and observed (bottom) responses in shallow, deep, and intermediate observation wells for 7-8 August 2009 (left) and 16-18 August 2009 (right) rainfall events.

CATHY can reproduce hysteresis and thresholding behavior observed in the relationship between the subsurface storage and discharge responses of a small catchment. No ad hoc parameterization is needed.

Is there any link to or contribution from unsaturated zone hysteresis?

Nature and role of nonlinear phenomena in atmosphere–land surface–soil–aquifer interactions and feedbacks are poorly understood.
Rill flow vs sheet flow (benchmark tests for model intercomparison)

Evolution of the point of intersection between the water table and the land surface for the sloping plane test case. The outlet face is at x = 400 m. ParFlow: solid line; CATHY: dashed-dotted (sheet flow) and dashed (rill flow).

Benchmarking is a complicated business even for synthetic test cases ... Why and how do different models (even based on the same equations) perform differently? And what to do about it??
Simulation of multiple response variables (Biosphere 2 Landscape Evolution Observatory)

All three variables are integrated measures of the hillslope response. How does the model perform when we examine distributed responses? And what happens when we include solute transport?

Issue of equifinality: does the mechanism we invoke imply (sole) causation?

“Perfect knowledge” of the bottom BC … how much does this help?

Comparison of simulation results at 3 different DEM resolutions: average monthly streamflow discharge, catchment-averaged daily water table depth, and cumulative frequency distribution of surface soil saturation after a 10-day rain period.

There are many reasons (causes) for grid scale invariance (and not limited to just the CATHY model). One of the most serious challenges in catchment-based hydrological / ecological modeling …

Extensions and evolution of the model (flow and transport; other processes)

Flow (water quantity and distribution)

Surface

\[ \frac{\partial Q}{\partial t} + c_k \frac{\partial Q}{\partial s} = D_h \frac{\partial^2 Q}{\partial s^2} + c_k q_s \]

Subsurface

\[ \sigma(S_w) \frac{\partial \psi}{\partial t} = \nabla \cdot [K_s K_r(S_w)(\nabla \psi + \eta_z)] + q_s \]

Transport (water quality and interactions with other substances)

Surface

\[ \frac{\partial Q^m}{\partial t} + c_t \frac{\partial Q^m}{\partial s} = D_c \frac{\partial^2 Q^m}{\partial s^2} + c_t q_{ts} \]

Subsurface

\[ \frac{\partial \theta c}{\partial t} = \nabla \cdot [-q c + D \nabla c] + q_{tss} \]

Evolution of the model

Catchment/DEM-based subsurface flow modeling

Variable density transport (an early coupled model)

Surface/subsurface flow coupling

Improved grid-based DEM analysis

Advanced numerics

Data assimilation

Surf/subsurf & flow/ transport coupling

Ecohydrological modeling (LSM coupling, vegetation, energy balance, CO2, nutrient cycles)

Detailed experiments, geophysical inversion, parameter estimation, sensitivity & uncertainty analysis, model intercomparison, biogeochemistry & soil weathering, sediment transport & erosion, soil freezing & snowmelt, preferential flow, unstructured grids, …
Collaborators

Mario Putti, Annamaria Mazzia, Matteo Camporese, Gabriele Manoli, Sara Bonetti – University of Padua, Italy
Stefano Orlandini, Giovanni Moretti – University of Modena and Reggio Emilia, Italy
Mauro Sulis – now at University of Bonn, Germany
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