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Physics-based hydrologic-response simulation: foundation for hydroecology and hydrogeomorphology

Keith Loague[1]*
Christopher S. Heppner[1]
Benjamin B. Mirus[1]
Brian A. Ebel[1]
Qihua Ran[1]
Adrianne E. Carr[1]
Susan H. BeVille[1] and
Joel E. VanderKwaak[2]

[1] *Department of Geological and Environmental Sciences, Stanford University, Stanford, CA, USA*
[2] *3DGeo Development Inc., Santa Clara, CA, USA*

*Correspondence to:
Dr Keith Loague, Department of Geological & Environmental Sciences, Stanford University, Bldg 320, Rm 118, Stanford, CA 94305-2115, USA. E-mail: keith@pangea.stanford.edu

Concept-Development Simulation

Two emerging and important disciplines within the large science of hydrology are *hydroecology* (Eagleson, 2002; Rodriguez-Iturbe and Porporato, 2004) and *hydrogeomorphology* (Sidle and Onda, 2004), each requiring an integrated understanding of hydrologic response at the surface and within the variably saturated subsurface. Obviously, the most useful tool for understanding ecological or geomorphic processes within a given hydrologically driven system is careful observation via detailed field measurements/experiments (e.g. Montgomery *et al*., 2002; Loheide and Gorelick, 2005). However, simulation of hydrologic response with comprehensive physics-based models can provide a strong foundation for concept development in both hydroecology and hydrogeomorphology.

The simulation of hydrologic response has received considerable attention in the last half century (see Beven (2000, 2002) and Singh and Woolhiser (2002)). In an often cited paper, Freeze and Harlan (1969) proposed a blueprint for a distributed physically based hydrologic model, based upon numerical solution to the coupled partial differential equations that describe water movement on the surface and within the variably saturated subsurface. At least three hydrologic-response models have been developed in the true spirit of the Freeze and Harlan blueprint: (i) *InHM* (VanderKwaak, 1999), (ii) *MODHMS* (Panday and Huyakorn, 2004), and (iii) *HydroGeoSphere* (Sudicky *et al*., 2005). The *Integrated Hydrology Model* (InHM) was designed to estimate quantitatively, in a fully coupled first-order approach, three-dimensional (3D) variably saturated flow and solute transport in porous media, 3D variably saturated flow and solute transport in macropores, and two-dimensional (2D) flow and solute transport over the land surface and in open channels. Successful applications of InHM include those of VanderKwaak and Loague (2001) and Loague *et al*. (2005).

Obviously, not all hydrologic-response simulations can (or should) be conducted with comprehensive physics-based models. Potentially the most effective use of physics-based simulation, related to hydroecology and hydrogeomorphology, is in the design of data collection strategies and identifying the next hypothesis-testing field experiment.

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Non-Trivial Problems

Having a physics-based mathematical model of hydrologic response is only part of the quest. The real problems are related to characterizing the other components of a given boundary-value problem (BVP) effectively (e.g. boundary conditions, initial conditions, and parameterization of soil hydraulic and hydrogeologic parameters). Two questions that are typically addressed in the formulation of a hydrologic-response BVP are whether the system leaks out the bottom and whether no-flow divides at the surface also hold for the subsurface.

It is well known that deterministic–conceptual simulation in hydrology requires a tremendous amount of information (see Bredehoeft (2005)). One may question, relative to physics-based hydrologic-response simulation if, as Philip (1980) asked:

> Can it be that the vast labor of characterizing these systems, combined with the vast labor of analyzing them, once they are adequately characterized, is wholly disproportionate to the benefits that could conceivably follow?

From our perspective, the answer to Philip's question is no. The details and characteristics resulting from the different hydrologic-response processes in realistic systems cannot be gleaned from simple modelling approaches. If one gets the hydrology wrong through oversimplification then it is unlikely that applications related to either hydroecology or hydrogeomorphology will be fully informative. In the following sections we investigate, for a specific case, the impact of two BVP simplification issues, i.e. dimensionality and transient versus steady-state simulation, that are common to the application of physics-based (as well as other) hydrologic-response models. We also investigate, for a second case, the impact of errors in the observed data relative to the assessment of model performance. The dimensionality, transient versus steady state, and model performance topics addressed herein are just the tip of the proverbial iceberg relative to substantive concept-development contributions, through the use of physics-based simulation, in either hydroecology or hydrogeomorphology.

Three-Dimensional versus Two-Dimensional Simulation

Despite the fact that the systems focused on are all 3D, most near-surface hydrologic-response simulations in hydroecology and hydrogeomorphology are one-dimensional or 2D. Mirus *et al.* (2006) demonstrate the difference between 3D and 2D (vertical slice) hydrologic-response simulation (using InHM) for a small upland catchment (C3) located within the H.J. Andrews Experimental Forest. The relatively small C3 catchment, with a forest road at the down-gradient boundary, is shown in Figure 1. The 3-month simulation period for the 3D C3 simulations is shown in Figure 2. Inspection of Figure 2 shows that both the timing and magnitude of the simulated and observed discharges match fairly well, considering the sparse information used to develop the BVP. Inspection of the flow path results in Figure 1, from the 3D simulation at the soil–bedrock interface, clearly shows the importance of convergent subsurface flow for the C3 system, which cannot be captured with 2D vertical slice simulation. The convergent subsurface flow at C3 results in higher pore water pressures within the axis of the hollow.

Mirus *et al.* (2006) further illustrate how getting the near-surface hydrology wrong, based upon simplifying the dimensionality of the hydrologic-response simulation, can propagate into hydrogeomorphology by using the 3D and 2D InHM simulated pore water pressures (at the 10 simulated measurement points in Figure 1) as input to a relatively simple (infinite) slope stability model, where the failure plane is assumed to be at the soil–bedrock interface along the axis of the hollow. *Factor of safety* (FS) results from the C3 slope stability estimates are illustrated in Figure 3 (note, slope failure at FS ≤ 1). Inspection of Figure 3 clearly shows the impact of the different pore water pressures, from the 3D and 2D hydrologic-response simulations, at a specific time (i.e. time H in Figure 2). Specifically, the FS values at all of the simulated measurement points resulting from the 2D hydrologic-response simulation are higher (more stable) than the FS values resulting from the 3D hydrologic-response simulation, which has a value of 1·01 at the culvert. The drop in the FS values for both cases at simulated measurement

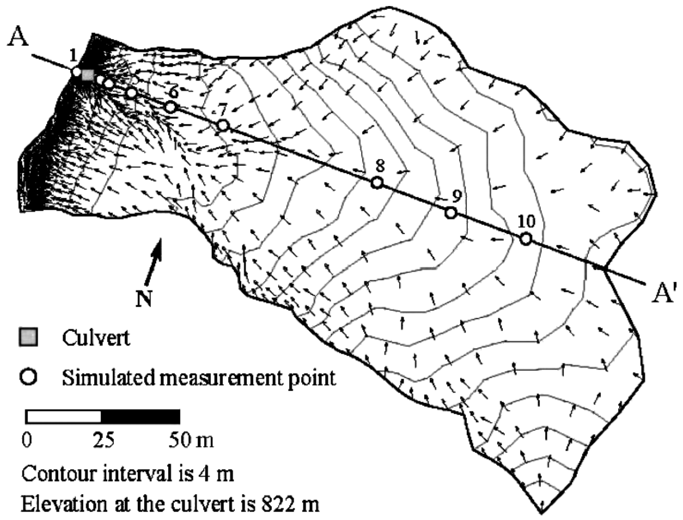

Figure 1. Catchment C3, located in the H.J. Andrews Experimental Forest (Oregon). Shown are the topography, 10 simulated measurement points (located at the soil–bedrock interface), location of the 2D vertical slice InHM simulation (A–A′), and a plan view snapshot of the subsurface flow directions taken from the 3D InHM hydrologic-response simulation at the soil–bedrock interface for the time identified by point H in Figure 2 (after Mirus *et al.* (2006))

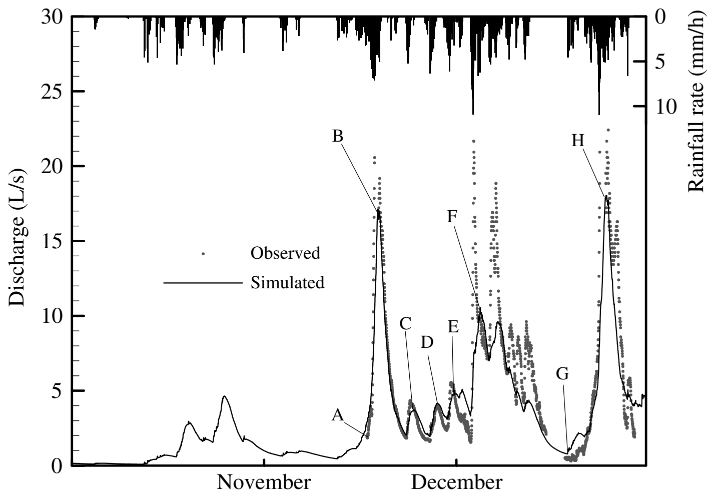

Figure 2. Observed versus InHM simulated C3 discharges for a 2-month period in 1996 that includes six runoff events (after Mirus *et al.* (2006)). The InHM warm-up period ends (runoff event 1 starts) at the time identified by point A. Points B, C, D, E, F, and H identify the times of simulated peak discharge for runoff events 1–6 respectively. The time at the end of the break in rainfall between runoff events 5 and 6 is identified by point G. The location of the culvert is shown in Figure 1

point 7 can be attributed to the slight topographic depression directly up-gradient. Obviously, from a risk-averse perspective, the FS results based on the 2D hydrologic-response simulations are not conservative. It is worth pointing out that, despite the failure of many Oregon hillslopes during the storm period identified in Figure 2, C3 did not fail.

Transient versus Steady-State Simulation

A fair amount of the hydrologic-response simulation that is conducted for applications in hydroecology and hydrogeomorphology is carried out in a steady-state mode. Although steady-state assumptions may be useful for large-scale annual water-

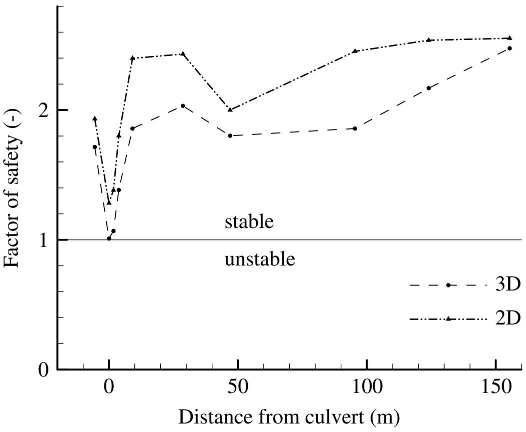

Figure 3. FS results for C3 at time H (see Figure 2) for the 10 simulated measurement points (see Figure 1) based upon pore water pressures estimated at the soil–bedrock interface from 3D and 2D InHM simulations (after Mirus *et al.* (2006)). The culvert is located at simulation measurement point 2

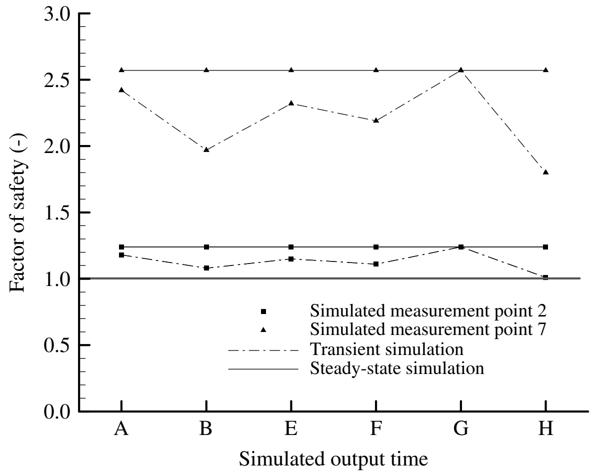

Figure 4. FS results for C3 at times A–H (see Figure 2) for simulated measurement points 2 and 7 (see Figure 1) based upon pore water pressures estimated at the soil–bedrock interface from 3D transient and steady-state InHM simulations. The culvert is located at simulation measurement point 2

balance estimates, they are generally unreliable for developing process-based relationships that are not time invariant.

A 3D steady-state simulation was conducted for C3 with InHM to illustrate the difference between transient and steady-state simulation. The steady-state simulation was based upon a long-term average rainfall of 0·26 mm h^{-1} (Waichler *et al.*, 2005). The simulated steady-state discharge for the long-term average rainfall rate is 1·03 l s^{-1}. The simulated steady-state discharge is poor in comparison with the observed values and the results from the transient simulation (see Figure 2).

As in the 3D versus 2D comparison described above, the pore water pressures from the steady-state C3 simulation were used to estimate (at six of the times identified in Figure 2) slope stability for simulated measurement points 2 and 7. Figure 4 facilitates a direct comparison between the FS values that are based on the transient (Mirus *et al.*, 2006) and steady-state hydrologic-response simulations. Inspection of the slope stability estimates in Figure 4 shows that the transient simulation leads to FS values that reflect the changes in the highly variable rainfall intensity, whereas the steady-state simulation leads to FS values that are constant. Figure 4 also shows that the steady-state simulation leads to FS values that overestimate the values from the transient simulation (e.g. 1·24 versus 1·01 at measurement point 2 at time H). Finally, Figure 4 shows that the FS values are lower (less stable) for measurement point 2 (where the water table is closer to the surface) than for measurement point 7 for both the transient and steady-state simulations.

Model Performance

The rigorous evaluation of model performance has received considerable attention in the last few years (e.g. Anderson and Bates, 2001; Iverson, 2003; Pebesma *et al.*, 2005; Wealands *et al.*, 2005). However, to the best of our knowledge, there are no established standards (e.g. specific statistical thresholds) for classifying model performance for models like InHM for different applications in hydrology. One major source of poor model performance is less-than-perfect observed data.

To investigate the impact of less-than-perfect observed data we take the Phase III (see Loague *et al.* (2005)) InHM simulation for R-5 rainfall-runoff event 68 (identified hereafter as the base case) as an *observed* data set. The 3D simulated response for the relatively small R-5, a *hypothetical reality* based (arguably) on the correct physics, is more complete than any real data set. Comparison of the R-5 base case with results from

Table I. Data error impacts on model performance evaluation. The observed data set (base case) is taken as an InHM simulation of rainfall-runoff event 68 for the R-5 catchment (Loague *et al.*, 2005)

Comparison	EF[a]	RRMSE[b] (%)	Q_{PK}[c] (l s^{-1})	ΔQ_{PK} (%)	Q_D[d] (mm)	ΔQ_D[e] (%)	Impact[f]
Base case versus base case[g]	1·00	0·0	138	—	22	—	—
Base case versus scenario A[h]	0·81	37	192	39	26	18	H
Base case versus scenario B[i]	0·89	28	101	−26	19	−14	H
Base case versus scenario C[j]	1·00	4	134	−3	22	0	L
Base case versus scenario D[k]	0·99	7	147	7	22	0	L
Base case versus scenario E[l]	0·93	22	166	20	26	18	M/H
Base case versus scenario F[m]	0·85	33	110	−20	18	−18	H

[a] Modelling efficiency $\text{EF} = [\sum_{i=1}^{n}(O_i - \overline{O})^2 - \sum_{i=1}^{n}(S_i - O_i)^2]/\sum_{i=1}^{n}(O_i - \overline{O})^2$, where S_i are the simulated values, O_i are the observed values, n is the number of samples, and $\overline{O}$ is the mean of the observed data. Note: when $S_i = O_i$, EF = 1·0.
[b] Relative root mean square error, $\text{RRMSE} = [\sum_{i=1}^{n}(S_i - O_i)^2/n]^{0\cdot5} \times 100/\overline{O}$. Note: when $S_i = O_i$, RRMSE = 0·0.
[c] Q_{PK}: peak stormflow.
[d] Q_D: average (across the catchment) stormflow depth.
[e] Δ is the difference between the base case value and the value for a given scenario, $\Delta = [(S - O)/O] \times 100$; where S is the simulated Q_{PK} (or Q_D) and O is the observed Q_{PK} (or Q_D).
[f] H: high; M: medium; L: low.
[g] Phase III simulation (Loague *et al.*, 2005).
[h] Base case with a 20% increase in rainfall.
[i] Base case with a 20% decrease in rainfall.
[j] Base case with a 20% increase in permeability.
[k] Base case with a 20% decrease in permeability.
[l] 20% increase in the base case stormflow discharge.
[m] 20% decrease in the base case stormflow discharge.

alternative InHM simulation scenarios facilitates, in a sensitivity-analysis mode, rigorous evaluation of data-error impacts that could conceivably be used to misjudge model performance. The six scenarios (A–F) considered in this example are for 20% increases/decreases in rainfall (A and B), near-surface permeability (C and D), and stormflow discharge (E and F). The errors considered for rainfall and stormflow discharge are both reasonable, whereas the errors for permeability are on the low side.

Table I summarizes the comparisons between the base case and scenarios A–F. Obviously, the EF and RRMSE values in Table I for the base case compared against itself are perfect. Inspection of Table I shows that changes in both the rainfall (e.g. EF values of 0·81 and 0·89 for scenarios A and B respectively) and the stormflow discharge (e.g. EF values of 0·93 and 0·85 for scenarios E and F respectively) had significant impacts, whereas changes in the permeability had little effect (e.g. EF values of 1·00 and 0·99 for scenarios C and D respectively). Impacts of the type seen in Table I for a real observed data set could easily be interpreted as a model performance problem (i.e. the data are correct, so the model must be wrong), which, as illustrated here, would be a mischaracterization. It is worth pointing out that the EF value for the 3D InHM simulation of C3 (see Figure 2) was 0·89 (Mirus *et al.*, 2006), which is well within the model performance ranges shown in Table I. Based on the simple food-for-thought example presented here, it is unfair to judge the performance of a physics-based model without some consideration for the possibility of errors in the field measurements/observations that are subsequently used in an observed versus simulated evaluation.

A Good Foundation

This article, to some degree, is a follow up to the commentary by Loague and VanderKwaak (2004). It is our contention that physics-based hydrologic-response simulation should not be viewed with fear and loathing based upon, for example, data shortcomings. Hopefully, better data, of the type needed to excite models like InHM effectively, are on the way (e.g. Hopmans and Pasternack, 2006).

It is our opinion that physics-based hydrologic-response simulation can provide a firm foundation for both hydroecology and hydrogeomorphology. A model like InHM, which can simulate both the *Horton* and *Dunne* mechanisms (processes that are not mutually exclusive), can, in a heuristic concept-development mode, reveal unknown nuances associated with, for example, spatio-temporal variability in near-surface soil hydraulic properties and flux boundaries and lead to the identification of new processes and/or quantitative delimiters for known processes. An example of building upon physics-based hydrologic-response simulation is the 2D multiple-species sediment transport algorithm that was recently added to InHM (Heppner *et al.*, 2006; Ran *et al.*, 2006). Obviously, the ability to investigate (via simulation) hydrologically driven erosion from surface-water generation processes other than Horton overland flow is important.

There are many open and challenging problems in hydrology related to surface–subsurface water interactions that have implications for hydroecology and hydrogeomorphology (e.g. preferential flow, multiple wetting fronts, new/old water, dynamics of partial/variable source areas, and multiple seepage faces). A better understanding of surface–subsurface water interactions (even in a generic mode) through comprehensive physics-based simulation could promote the effective employment of models simpler than InHM for specific problems.

Epilogue

When Jim Buttle invited the first author to prepare this commentary, the task serendipitously presented itself as a wonderful opportunity for our research group to collaborate on a single paper focused on some of the nuances associated with physics-based hydrologic-response simulation. The authors are currently engaged in InHM applications focused on, for example, cumulative watershed effects, sediment transport related to both the dam problem and regional-scale landscape evolution, slope stability, and where runoff begins and ends.

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