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ScienceDirect

Procedia Earth and Planetary Science 10 (2014) 7 – 15

Procedia
Earth and Planetary Science

Geochemistry of the Earth's Surface meeting, GES-10

Designing a Suite of Models to Explore Critical Zone Function

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Abstract

The Critical Zone (CZ) incorporates all aspects of the earth's environment from the vegetation canopy to the bottom of groundwater. CZ researchers target processes that cross timescales from that of water fluxes (milliseconds to decades) to that of the evolution of landforms (thousands to tens of millions of years). Conceptual and numerical models are used to investigate the important fluxes: water, energy, solutes, carbon, nitrogen, and sediments. Depending upon the questions addressed, these models must calculate the distribution of landforms, regolith structure and chemistry, biota, and the chemistry of water, solutes, sediments, and soil atmospheres. No single model can accomplish all these objectives. We are designing a group of models or model capabilities to explore the CZ and testing them at the Susquehanna Shale Hills CZ Observatory. To examine processes over different timescales, we establish the core hydrologic fluxes using the Penn State Integrated Hydrologic Model (PIHM) – and then augment PIHM with simulation modules. For example, most land-atmosphere models currently do not incorporate an accurate representation of the geologic subsurface. We are exploring what aspects of subsurface structure must be accurately modelled to simulate water, carbon, energy, and sediment fluxes accurately. Only with a suite of modeling tools will we learn to forecast – earthcast -- the future CZ.

Peer-review under responsibility of the Scientific Committee of GES-10

Keywords: Critical Zone; weathering; hydrology; ecology; watersheds

Peer-review under responsibility of the Scientific Committee of GES-10
doi:10.1016/j.proeps.2014.08.003

1. Critical Zone Science

A thin layer of the earth, located between the vegetation canopy and the lower depths of groundwater, supports terrestrial life. Since about 2006, this zone has been referred to as the *Critical Zone* (CZ) to indicate its importance to humans. In this zone, the high-temperature mineral assemblages in rocks re-equilibrate with surficial fluids to create regolith. Across the CZ, human life is largely supported by gradients in environmental variables that drive fluxes of water, energy, solutes, carbon, nitrogen, and sediments. Disturbingly, we are changing these fluxes at unprecedented rates. For example, if we extrapolate today's annual erosion rate of ~12 million metric tons forward into the next 40 years, we calculate that only 20% of the arable land needed for adequate nutrition will be available to support the 9 billion humans expected to live on the planet [1].

To understand evolution of the CZ and how we are perturbing it requires numerical models that can explore the tight coupling of physical, chemical, and biological – including human -- processes. Such models must target the important processes in response to tectonic, climatic, and anthropogenic forcings to "*earthcast*" the changing CZ. No single model can cross all the relevant timescales of CZ evolution. Since the evolution of the physical CZ is largely driven by the biota-catalyzed response of rocks to circulation of surficial fluids, the team of scientists at the Susquehanna Shale Hills Critical Zone Observatory (SSHCZO) in Pennsylvania (U.S.A.) is developing a suite of models that is based on the Penn State Integrated Hydrologic Model (PIHM). By developing simulation modules using PIHM as the core, we are promoting greater understanding of the evolution of the CZ at all timescales (Table 1, Figure 1). We are testing these models at the 8-hectare catchment known as Shale Hills and we will soon be upscaling to the larger Shavers Creek watershed (165 km^2) which contains it. This larger watershed now comprises the full SSHCZO.

Table 1. Models in use at the Susquehanna Shale Hills CZ Observatory.

Model name	Purpose	Responsible party	Timescale of simulations
PIHM[1]	Modelling hydrologic fluxes	C. Duffy	Minutes to decades
Flux-PIHM	Modelling water and energy fluxes	Y. Shi	Minutes to decades
Flux-PIHM-BGC	Modelling carbon and nitrogen fluxes	Y. Shi	Hours to decades
PIHM-SED	Modelling sediment transport	C. Duffy	Minutes to decades
RT-Flux-PIHM	Modelling reactive transport	L. Li	Minutes to decades
Regolith-RT-PIHM	Modelling reactive transport	L. Li	Minutes to millions of years
LE-PIHM	Modelling landscape evolution	R. Slingerland	Minutes to millions of years

[1]Penn State Integrated Hydrologic Model

2. Models

2.1. PIHM: Modelling hydrologic fluxes

The Penn State Integrated Hydrologic Model (PIHM) is a multi-scale, open-source hydrologic model where the major hydrological processes are fully coupled using the semi-discrete finite volume method [2]. PIHM represents our strategy for simulating distributed hydrologic processes at the catchment scale. Our interest focusses on devising a concise representation of watershed and/or river basin hydrodynamics that can simultaneously simulate the interactions among major physical processes. At the same time, our goal is to maintain the flexibility needed to add or eliminate states/processes/constitutive relations depending on the objective of the numerical experiment or

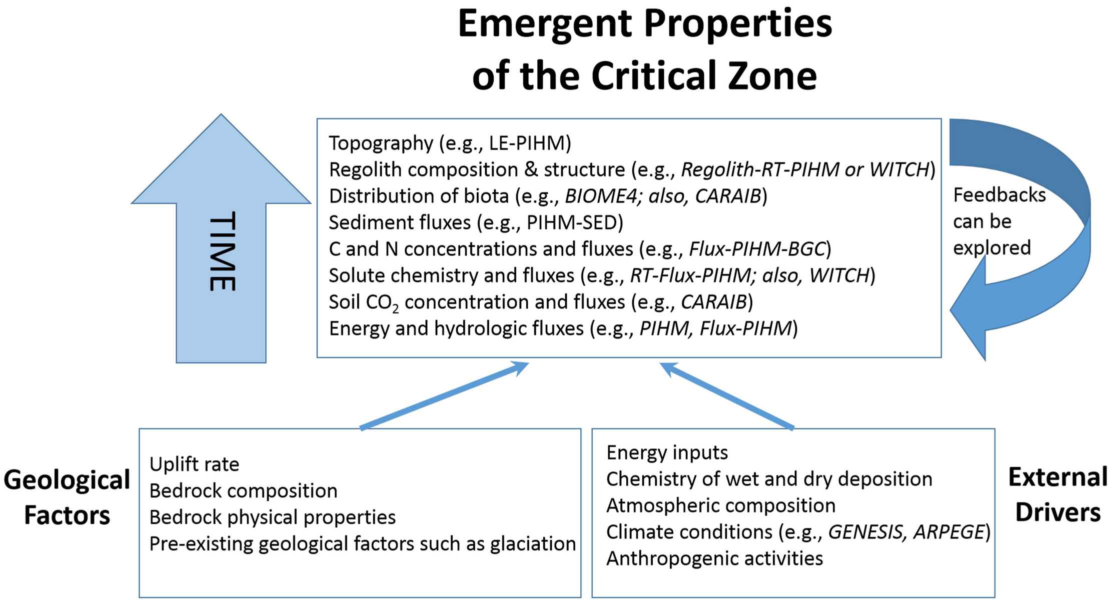


Figure 1. To quantify the evolution of the CZ requires multiple models and datasets to simulate processes at different timescales. The longest timescale models, landscape evolution models (i.e. LE-PIHM), can simulate changing topography, relief, drainage density, and the spatial distribution of regolith for $10^6 – 10^7$ years. At a slightly shorter timescale, reactive transport models (Regolith-RT-PIHM) can simulate changes in composition and porosity of regolith as it forms on bedrock over timescales up to 10^6 y; at the same time these models calculate stream and soil porewater chemistry averaged over years. Reactive transport models can also be used for shorter timescales to simulate stream or soil porewater chemistries (RT-Flux-PIHM). None of the PIHM family of models now can be used to calculate the distribution of biota: dynamic vegetation models such as BIOME4 and CARAIB can do this. Likewise, CARAIB can be used to simulate the carbon allocation and plant growth, heterotrophic respiration, and soil carbon content of the subsurface. The distribution of energy and hydrologic fluxes can be simulated with atmosphere – land surface models (Flux-PIHM) or hydrologic models (PIHM) over timescales up to 10^2 y.

purpose of the scientific application. The approach is based on the semi-discrete finite-volume method (FVM) which represents a system of coupled partial differential equations (e.g. groundwater, surface water, soil water, etc.), as a spatially-discrete fully coupled system. A closely linked GIS tool, PIHMgis, was developed [3, 4] to import catchment data for topography, soils, climate, land cover and geologic data; with support to construct the numerical mesh and assign parameters to each triangular mesh element [5]. With this tool, for example, the stream network and watershed boundaries, soil zones, ecological regions, hydraulic properties, climate zones, etc. are delineated. River elements have trapezoidal or rectangular cross-sections, with edges shared with triangular mesh for the catchment. Each local control volume contains all equations to be solved and this is referred to as the model kernel. The global system is solved by a state-of-the-art solver known as CVODE developed at the Lawrence-Livermore National Laboratory. The model code, descriptions and tutorials are available at: http://cataract.cee.psu.edu/PIHM/index.

The basic PIHM model couples equations for channel routing, surface overland flow, and subsurface flow together with interception, snow melt and evapotranspiration. For channel routing and overland flow governed by St. Venant equations, both kinematic wave and diffusion wave approximations are included. For saturated groundwater flow, the 2-D Dupuit approximation is applied. The unsaturated flow is incorporated using the 1-D vertically integrated form of Richards' equation. A simplified strategy for matrix-macropore flow is implemented based on a published method [6]. Recently, a new module for estimating the age of environmental tracers was tested at Shale Hills [4]. PIHM simulations have been conducted for time scales ranging from minutes to decades and spatial scales that range from the plot scale (1-10 m) to hillslopes (10-100 m) to river basins ($>10^4$ m).

2.2. Flux –PIHM: Modelling water and energy fluxes

Weather and climate models rely on land surface models (LSMs) to represent land-surface processes. Subsurface waters, however, are not well described in most LSMs. Hydrologic models, on the other hand, usually have simplified representations of evapotranspiration even though the accurate forecasting of peak discharge events depends on the forecasting of evapotranspiration, especially after extended dry periods. A coupled land surface hydrologic model, Flux-PIHM [7, 8], has been developed to combine the strengths of physically-based hydrologic modeling and land surface modeling. Flux-PIHM incorporates a land surface scheme, which is mainly adapted from the Noah LSM [9], and adds to PIHM the ability to simulate the surface energy balance (SEB) and the soil moisture profile. The newest version of Flux-PIHM adds an optional topographic solar radiation module, which enables the quantitative investigation of the effects of aspect on land surface and hydrologic processes in small watersheds. This addition to Flux-PIHM was developed because aspect has an important effect on some fluxes. Flux-PIHM thus provides high resolution prediction and reanalysis (i.e., model retrospective analysis driven by the meteorological forcing produced from atmospheric data assimilation systems) of watershed hydrologic and land surface states on time scales from minutes to decades. Because PIHM is capable of simulating lateral water flow as well as the saturated zone when it is within meters of the land surface, Flux-PIHM is able to represent some of the land surface heterogeneity caused by topography, including the spatial structure of the coupling between groundwater and SEB. Flux-PIHM has been calibrated at the Shale Hills watershed with both hydrologic predictions and SEB predictions. An evaluation of the model shows good agreement with observations. Flux-PIHM has also been used for parameter sensitivity analysis [8] and data assimilation experiments [10]. Unlike PIHM which only requires net radiation as the radiation forcing, Flux-PIHM requires downward solar radiation (separated direct and diffuse radiation if topographic solar radiation is turned on) and downward longwave radiation forcing for full SEB simulation. Because of the added land surface component, Flux-PIHM also requires more land surface parameters, e.g., the land surface emissivity, the water vapor exchange coefficient, and the Zilitinkevich parameter [7, 8].

2.3. Flux-PIHM BGC: Modelling carbon and nitrogen cycling

The terrestrial carbon and nitrogen cycles are now commonly incorporated into the LSMs used in earth systems models. These earth systems models facilitate study of the interactions between changing climate, atmospheric composition and terrestrial ecosystems. As noted above, however, most LSMs do not carefully describe subsurface waters. Thus the interactions of watershed topography with the structure of ecosystems and their biogeochemical cycles cannot readily be simulated for all systems. An ecosystem biogeochemical module such as the core of Biome-BGC will be incorporated into Flux-PIHM to explore this topic at time scales ranging from hours to decades. CZ data for Shale Hills and the larger Shavers creek watershed will be used to explore the capability of the coupled modelling system to simulate ecosystem carbon and nitrogen fluxes and stocks across the CZ landscape, focusing particularly on the interactions of ecosystem biogeochemistry with subsurface hydrology. Measurements of biomass, biomass increment, litterfall, leaf area, leaf and soil carbon and nitrogen content, root density distribution and ecosystem-atmosphere net carbon flux, in addition to the hydrologic measurements noted above, will be used to parameterize and/or evaluate the coupled model.

2.4. PIHM-SED: Modelling sediment transport

PIHM-SED is a physically-based, non-equilibrium, non-uniform, land-surface sediment transport model built on PIHM for simulations at the watershed scale. It predicts sediment transport on hillslopes and in channels, including the effects of surface/subsurface hydrological processes on sediment yield and the spatial distribution of erosion/deposition. PIHM-SED simulates erosion and transport by rain splash and overland flow, and bed material transport by flow through a network of rivers and channels using a diffusion wave approximation to St Venant's Equation. Sediment transport is approximated by a 2-D advection equation with a source term representing the balance between entrainment and deposition. An algorithm for bed armoring is included in the channel component. Bed evolution is predicted by the Exner Equation. All hydrological and sediment transport processes are defined on discretized unit elements as a fully coupled system of ordinary differential equations (ODEs) using a semi-discrete

FVM. In addition to the datasets required for PIHM, PIHM-SED requires spatial fields of sediment (soil) grain sizes and densities, critical shear stresses for sediment entrainment, sediment porosities, and Manning's roughness coefficient.

2.5. RT-Flux-PIHM: Modelling solute fluxes and mineral-water reactions

To simulate water-mineral-gas interactions, we are developing reactive transport modules (RTM) [11] coupled with PIHM. Using these modules allows integration of land surface hydrologic processes with subsurface solute transport and biogeochemical reactions. The module currently includes mineral dissolution and precipitation, ion exchange, sorption and desorption, and will have the capability to simulate abiotic and biotic redox reactions. Two modules will be developed focusing on two different temporal scales. The first module is RT-Flux-PIHM, which couples an RTM directly with Flux-PIHM [12], and targets processes over time scales of months to years. The second RT model is described in the next section, and is targeted at longer simulations.

RT-Flux-PIHM allows mechanistic understanding and prediction of meteorological, hydrologic, and ecological controls on stream water chemistry and chemical weathering at the watershed scale with high-resolution temporal climatic and hydrologic conditions. The model represents the vertical direction in three coarse layers: the unsaturated zone, saturated zone, and bedrock. To date, the model has been calibrated with tracer data (Cl(-I)) in stream water at SSHCZO for solute transport process. Model-data comparison for the reactive species Mg(II), a key cation that is released during clay weathering [13], indicates that ion exchange processes in the soil play a key role in determining Mg(II) concentrations in stream and soil porewaters.

2.6. Regolith-RT-PIHM: Modelling regolith formation

The second RT model, Regolith-RT-PIHM, will be developed to understand chemical weathering over geological time (10^4 – 10^6 years) [14]. The model will incorporate a high-resolution representation of layers of regolith and bedrock in the vertical direction; however, it will use a relatively coarse representation of climatic and hydrologic conditions averaged over periods of geological time. If climate variation is important during regolith formation, we may use a global climate model to simulate climate conditions for different time periods, and then use output from that model to drive a dynamic vegetation model to determine the distribution of biota and associated water fluxes, including drainage. The calculated drainage can be used as an average input to in turn drive Regolith-RT-PIHM to simulate regolith formation. This "cascade of models" approach is necessary because computational limitations do not allow full coupling of climate, biota, and regolith formation models. For example, a model cascade approach was recently used to simulate weathering of loess profiles for the last 10ky along a climosequence along the Mississippi river [15]. In that case, a weathering model, WITCH [16], was used to simulate weathering of the loess using output from the GENESIS v. 2 global climate model [17] for three time slices (10ky, 6 ky, 0 ky). In that model cascade, output from GENESIS was also used as input for the BIOME4 vegetation model [18] to calculate effects of vegetation. The vegetation model required mean monthly or daily climate variables (temperature, precipitation, hours of sunlight). Soil texture was another important input that affects the partitioning of water between infiltration and runoff and thus controls water for growth of vegetation as well as the extent of weathering.

Such a cascade of models will be useful in modelling ridgetop (1-D) profiles. With incorporation of an erosion module based on SED-PIHM, such a model cascade could also enable understanding of weathering along hillslopes. To constrain these models, data describing the current soil profile (mineralogical composition) and physical properties of rock and regolith (e.g., permeability) in the vertical direction, as well as parameters describing erosion such as shown in Figure 2 and discussed in the next section will be required.

2.7. LE-PIHM: Modelling landscape evolution

Over geologic time, processes not simulated by PIHM-SED become important, such as downslope creep of regolith due to freeze-thaw, tree-throw, landslides, and mudflows, and bedrock incision. Current landscape evolution models simulate these processes but do not include interactions among groundwater and overland flows, bedrock weathering, and the evolving landscape. To incorporate these processes, we developed LE-PIHM, a 3-D hydrologic-morphodynamic model for regolith formation and landscape evolution. Given that this module has

Governing equations for rock and regolith

1. Evolution of ground surface

$$\frac{\partial z}{\partial t}=\left(\frac{\sigma_{ro}}{\sigma_{re}}-1\right)\sec\theta P_0 e^{-\alpha H}-\frac{\partial q_x}{\partial x}+U-\frac{\partial E}{\partial x}$$

2. Evolution of bedrock

$$\frac{\partial e}{\partial t}=-\sec\theta P_0 e^{-\alpha H}+U$$

3. Evolution of regolith

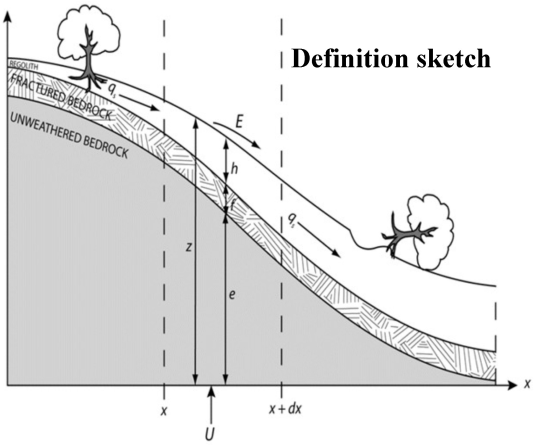
$$\frac{\partial h}{\partial t}=\frac{\partial z}{\partial t}-\frac{\partial e}{\partial t}=\frac{\sigma_{ro}}{\sigma_{re}}\sec\theta P_0 e^{-\alpha H}-\frac{\partial q_x}{\partial x}-\frac{\partial E}{\partial x}$$

4. General equation for downslope regolith flux

$$q_x=K_1\tan\theta+K_2\sin\theta\cos\theta+K_3\sin\theta$$

5. Downslope sediment transport

$$E=4(\tau_0^*-\tau_c^*)^{\frac{3}{2}}\sqrt{RgDD}$$



Governing equations for hydrology

1. Overland flow

$$\frac{dQ_w}{dt}=A\frac{1}{n}\left(\frac{A}{P}\right)^{\frac{2}{3}}S^{\frac{1}{2}}$$

2. Unsaturated Flow

$$C(\Psi)\frac{\partial\psi}{\partial t}=\nabla\cdot(K_w(\Psi)\nabla(\Psi+z))$$

3. Groundwater Flow

$$C(\Psi)\frac{\partial\psi}{\partial t}=\nabla\cdot(K_w(\Psi)\nabla(\Psi+z))$$

Parameters	Description	Unit
P_0	Bare bedrock weathering rate	m/yr
τ^*_c	Sediment critical Shields stress	dimension
τ^*_0	Overland flow Shields stress	dimension
D	Grain diameter	m
P	Channel wetted perimeter	m
S	Ground surface slope	dimensionless
ψ	Pressure head	m
σ_{ro}	Rock density	kg/m^3
σ_{re}	Regolith bulk density	kg/m^3
θ	Slope angle	Degree
R	Submerged specific gravity	dimensionless
C	Specific moisture capacity	1/m

Figure 2. Governing equations for PIHM-SED. Here, z is the elevation of the ground surface (m), α is an empirical factor in the soil production equation (1/m), H is regolith thickness (m), q_x is the volumetric flux of regolith in the positive x direction (m^2/y), U is uplift rate (m/y), E is the rate of regolith transported via overland flow (m^2/y), e is the elevation of the bedrock-regolith interface (m), h is regolith thickness (m), K_w is the hydraulic conductivity (m/y), K_1 is the viscous creep transport efficiency(m^2/y), K_2 is the transport efficiency attributed to tree root growth and decay(m^2/y), K_3 is the transport efficiency associated with tree-throw (m^2/y), g is the acceleration due to gravity (m/s^2), Q_w is volumetric water discharge (m^3/s), and A is the contributing drainage area (m^2).

been most recently developed, we summarize the governing equations and important variables in Figure 2. It fully couples the hydrologic processes in PIHM with hillslope and channel sediment transport processes.

LE-PIHM computes the feedbacks among infiltration, recharge, groundwater and surface water runoff, creation of regolith and regolith erosion by streams, and downslope movement by tree throw using the same semi-discrete finite volume strategy as PIHM. The model includes temporally and spatially variable bedrock uplift, regolith production as an exponentially decaying function of regolith thickness, and downslope regolith transport by linear or depth-dependent creep. Sediment transport for overland and channelized flow is predicted by the Meyer-Peter and

Müller excess shear stress transport equation using the updated coefficients of Parker. Bedrock channels incise at a rate proportional to the local flux of bedload and inversely proportional to the proportion of bed covered by alluvium. The bedrock and ground surfaces evolve to produce streams and hillslopes as an emergent property of the interacting hydrologic and sedimentary processes.

Three non-dimensional parameters govern the behavior of the system as defined by the following equations:

$$W^*=P_o/U \quad (1)$$
$$K^*=K/UL \quad (2)$$
$$S^*=D/UL \quad (3)$$

Here, P_o = the weathering rate of bare bedrock (m s^{-1}), U = the bedrock uplift rate (m s^{-1}), K = the hillslope diffusivity (m^2 s^{-1}), L = a system length scale (m), and D = the overland sediment transport diffusivity (m^2 s^{-1}). The latter parameter is a strong function of the local unit water discharge. In addition to the datasets required for PIHM, LE-PIHM requires spatial fields of sediment (soil) grain sizes and densities, critical shear stresses for sediment entrainment, sediment porosities, Manning's roughness coefficient, and estimates for P_o, U, and K.

3. Using Models to Explore Critical Zone Function

3.1. Exploring coupling and feedbacks

One of the main reasons to develop this suite of models is to explore tightly coupled processes and the nature of positive or negative feedbacks. For example, a comparison of simulations with and without full hydrologic-morphologic coupling illustrates the value of LE-PIHM (Figure 3). When landscape evolution is simulated without including groundwater processes, all precipitation on the land surface moves to the outlet by overland flow, thereby creating a lower relief and smoother landscape (Figure 3). Including groundwater hydrology allows water to travel through the regolith and exit lower in the catchment as a spring, thereby creating higher relief at steady-state, steeper valley walls, and box canyons. These features are consistent with groundwater-dominated landscapes in Florida and the Canyonlands of southern Utah. Therefore, during simulations of watersheds, steady-state landforms will emerge that possess convex and smooth channel profiles if K^* is relatively large and S^* small, whereas S^*-dominant landscapes possess concave and sharp channel and mountain profiles. Earlier landscape evolution models did not couple hydrologic processes with bedrock and soil weathering and transport processes and thus could not accurately simulate groundwater-dominated landscapes. PIHM-SED and LE-PIHM allow us to map the relationships between hydrologic parameters and landscape form (Figure 3).

4. Conclusion: Earthcasting

With a suite of models such as those described here, scientists will explore the tight coupling and feedbacks inherent to the complex CZ system. As models improve, it should also become possible to project -- earthcast -- the CZ into the future for different scenarios of human activity. An array of modules will be needed to project different processes. Here we have described one method of achieving this goal by using PIHM as the hydrologic backbone of many advanced and developing modules. This approach allows the CZ scientist a flexible and evolving modelling strategy for including new processes and for exploring other model codes and inter-comparisons.

One example of how an earthcast might be completed is related to the study of rates of soil formation on loess along the Mississippi valley that has already been mentioned [19]. To earthcast solute fluxes and soil changes, a general circulation model (ARPEGE [20]) was run for 100 y from the 1960s into the future for three soil locations along the Mississippi under the assumption that the atmospheric CO_2 increased according to IPCC scenario A1B [21]. The ARPEGE outputs were input into a dynamic vegetation model (CARAIB [22]) to calculate water fluxes through the soils [23]. With these forcings, a weathering model (WITCH [16]) was used to earthcast future solute fluxes. Using this cascade approach, it was observed that the projected increase in atmospheric CO_2 caused elevated temperatures that decelerated the rates of carbonate depletion in the soils but increased the rates of silicate depletion. However, changes in drainage were even more important in controlling weathering than temperature: weathering increased wherever drainage increased along the north-south transect. Somewhat counterintuitively, changes in soil atmospheric CO_2 were unimportant because, although higher temperature caused higher subsurface CO_2 production rates, higher diffusive loss rates due to the elevated temperatures kept soil CO_2 relatively constant into the future. The cascade of models led to identification of a new concept, the terrestrial lysocline – the layer of the soil where carbonate mineral saturation changes rapidly with depth and which, like the oceanic lysocline, moves up or down in response to environmental change.

We will similarly explore cascades of models including ARPEGE -CARAIB → RT- Flux – PIHM or ARPEGE - CARAIB → LE – PIHM to simulate soil formation or landscape evolution respectively at the SSHCZO and then to make earthcasts into the future. By utilizing modules to quantify important processes within a flexible and reusable framework we will unravel the important feedbacks and couplings that make it difficult to understand evolution of the CZ.

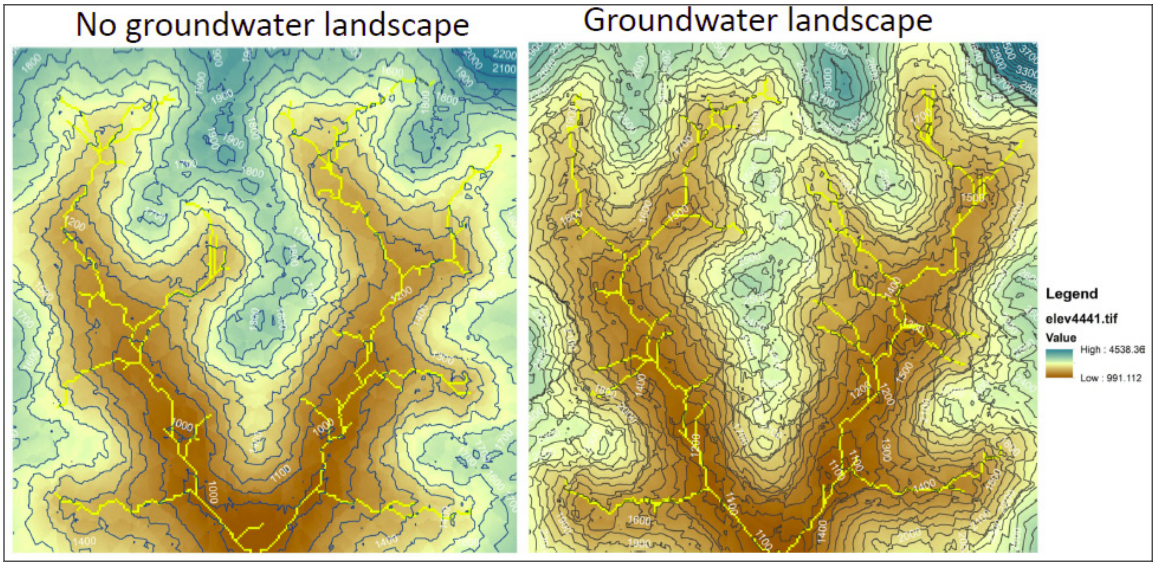


Figure 3. Landform elevation maps (color coded from brown for low to blue for high) for two steady-state landforms developed under conditions of identical uplift rate and other relevant parameters. At steady state, the erosion rate must balance the uplift rate. Left: Without infiltration, all precipitation moves to the outlet by overland flow, thereby creating a lower relief and smoother landscape; Right: By including groundwater hydrology, water moves through the regolith to exit lower in the catchment, thereby creating a higher relief at steady-state, steeper valley walls, and box canyons. These latter features are consistent with groundwater-dominated landscapes in Florida and the Canyonlands of southern Utah.

Acknowledgements

This work was funded by NSF Critical Zone Observatory program grants to CJD (EAR 07-25019) and SLB (EAR 12-39285, EAR 13-31726).

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