Preview of Award 1331726 - Annual Project Report

Cover

Federal Agency and Organization Element to Which Report is Submitted:	4900
Federal Grant or Other Identifying Number Assigned by Agency:	1331726
Project Title:	Using the Susquehanna - Shale Hills CZO to Project from the Geological Past to the Anthropocene Future
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Recipient Organization:	Pennsylvania State Univ University Park
Project/Grant Period:	10/01/2013 - 09/30/2018
Reporting Period:	10/01/2013 - 09/30/2014
Submitting Official (if other than PD\PI):	N/A
Submission Date:	N/A
Signature of Submitting Official (signature shall be submitted in accordance with agency specific instructions)	N/A

Accomplishments

*** What are the major goals of the project?**

Here, we organize our answer in terms of our hypothesis teams. Our goals for each hypothesis include mentoring of postdocs, undergraduate students, and graduate students. The science focus for each hypothesis is discussed below, along with the goals of the Infrastructure, Data, and Outreach teams.

Hypothesis 1: (Kirby, Bierman, Brantley, Singha, Lin)
The major goals of hypothesis 1 are to i) characterize the distribution of fractures in the shallow subsurface of the Observatory; ii) evaluate the degree to which variations in fracture distributions reflect climatic (or paleo-climatic) conditions at the site; and iii) assess the impact of climatic variations on the rates and processes of regolith production and erosion.
Hypothesis 2: (Kaye, Brantley, Eissenstat, Li)
The major goal of the hypothesis is to discover whether the distribution of weathering reactions across a landscape can be described as a function of biotic and abiotic production and consumption of acids (CO_2, DOC) and O_2. We will compare CO_2 and O_2 depth profiles to mineralogy and pore water chemistry to link production and consumption of acids and O_2 with weathering reactions. As time allows, our goal is to amplify this work by measurements of soil N_2O and N cycling.

Hypothesis 3: (Eissenstat, Davis, Kaye, Brantley)

The major goals of hypothesis 3 are to examine the functions of deep roots and their potential effects of deep roots on regolith formation.

Hypothesis 4: (Lin, Duffy, Eissenstat, Davis)

The major goals of hypothesis 4 are to investigate the effects of macropores in controlling fluid flow and chemistry in soils derived from various lithologies.

Hypothesis 5: (Li, Brantley, Kaye, Russo)

Understanding regolith formation and its response to natural and anthropogenic perturbations are critical for addressing societal and climatic challenges. Although regolith covers the majority of Earth's continents, its formation has not been well understood and quantified. The Susquehanna Shale Hills Critical Zone Observatory (SSHCZO) provides a natural laboratory for understanding regolith formation and for earthcasting across temporal and spatial scales. In particular, field studies have revealed that the depletion in regolith on the northern slope is less severe than on the south side in Shale Hill watershed. This hypothesis addresses whether water flux exerts the strongest control on elemental depletion and regolith formation. Our goal here is to understand the topological, hydrological, and climatic controls of regolith formation through process-based models across scales with constraints from soil profile data, and stream water and pore water chemistry.

Hypothesis 6: (Brantley, Li, Kaye, Davis, Shi)

Predicting stream water chemistry as a function of discharge in any given watershed has remained an elusive goal. The Susquehanna Shale Hill Critical Zone Observatory acts as a *natural laboratory* where we are investigating how the hydrologic connectivity, water residence time, distribution of organic matter, ability of soils to exchange cations control solute behavior under varying lithology (shale vs. sandstone) and land-use (agriculture vs. forested). Here we will utilize a field-modeling evolutionary approach, where we will utilize field data to inform a coupled reactive transport hydrologic model (RT-Flux-PIHM; see Hyp 5) to examine the complex processes that control stream water solute concentrations, which will help to inform our future field sampling efforts (both spatially and temporally). The eventual goal is to create a model capable of predicting the stream solute chemistry from all three sub-catchments (forested shale, forested sandstone, agriculture shale) and potentially Shavers Creek.

Hypothesis 7: (Davis, Eissenstat, Shi, Lin, Kaye)

In this hypothesis we focus on the importance of topography, watershed lithology and land use on the interaction between the carbon and water cycles.

Hypothesis 8: (Shi, Davis, Eissenstat, Lin)

Here we expand on what we have learned at the Shale Hills watershed by extrapolating to the Shavers Creek watershed, and combine the strength of a high-fidelity model, i.e., Flux-PIHM, and a "minimum" observing system, i.e., a re-locatable multi-sensor measurement array, to provide realistic land surface and hydrologic reanalysis and projections of the Shavers Creek watershed.

Hypothesis 9: (Brantley, Godderis, Li, Sullivan)

In this hypothesis we plan to quantify the effects of increasing atmospheric CO2 and variable climatic conditions (temperature, precipitation and evapotranspiration) on silicate and carbonate mineral weathering rates. We want to be able to forecast – earthcast – weathering into the future for different scenarios of human impact. Following a cascade modeling approach developed by personnel in our team – Brantley, Godderis (Goddéris et al. (2013), we are exploring how increasing atmospheric CO2 will impact climatic conditions and biota and how this will in turn affect shale weathering and solute fluxes. We are linking together an atmospheric global circulation model (ARPEGE), dynamic vegetation model (CARAIB) and geochemical model (WITCH). This modeling approach is currently being developed at Shale Hills given the substantial hydrogeochemical database available and will then – time permitting -- be tested on a shale climosequence transect that spans Wales to Puerto Rico.

Infrastructure Team:

Goals of the infrastructure team are to provide and maintain necessary physical resources to support research at

SSHCZO. This includes maintenance of electrical power to instrumentation, sensor installation, calibration, and troubleshooting, development of personnel to perform field research, and collaboration with Hypothesis teams and Data Management staff to ensure data and physical samples are stored according to mutually agreeable standards. The Infrastructure team also provides support to the Hypothesis teams with regard to site selection and development.

Data Team:

The goals of the data team are to parse, organize, and post new data files submitted by investigators to the local web data portal.

Outreach Team:

The goals of the outreach team are to promote the information that has been learned at SShczo to other scientists, to students, and to the public.

*** What was accomplished under these goals (you must provide information for at least one of the 4 categories below)?**

Major Activities:

H1:

Major activities include i) characterization of fracture distribution in a series of boreholes via direct (televiewer) and indirect (wireline geophysical logs) methods; ii) collection of a series of shallow seismic surveys to assess geotechnical properties of the regolith and underlying bedrock; and iii) collection and analysis of a suite of isotope measurements (meteoric 10Be) across a range of topographic gradient and aspect.

H2:

Over the past year we continued to monitor soil CO_2 at multiple depths at ridgetop, midslope and valley floor locations along one planar slope and one swale slope at Shale Hills. In addition, this year we added new measurements of N_2O from these soil gas samplers. To increase our understanding of aspect effects on the critical zone we installed new gas sampling tubes on the north slope and monitored soil CO_2 over the growing season. We moved six Apogee oxygen sensors previously located at the south swale and south planar valley floor at shale hills to new midslope positions and completed new calibration tests of these sensors. Using a different sensor (a hand held O_2 monitor) we initiated new measurements of O_2 concentrations from the soil gas access tubes so that O_2 concentrations are now collected whenever soil CO_2 and N_2O are measured.

We completed two manuscripts related to this hypothesis and they are still in revision or review. The first documents patterns of soil CO_2 throughout the shale hills catchment. The second uses stable isotopes of C and S to determine the source of acids for weathering of ankerite and pyrite from shale. We also began the work to identify soil gas sampling sites in the new sandstone subcatchment as part of our scaling up to Shavers creek watershed.

H3:

Major activities include assessing root length density by depth using both soil coring and profile wall mapping of roots on pits. Mycorrhizal colonization and root morphology in relation to rooting depth are also being examined.

H4:

Major activities included the enhancement of GPR protocol for investigating soil macropores and the testing of EMI for detecting soil moisture patterns. We also continue the monitoring and maintenance of real-time soil moisture monitoring at the Shale Hills.

H5:

We developed and coupled a generalized reactive transport (RT) module to an existing land surface watershed model, Flux-PIHM, which has been carefully calibrated to enable the reproduction of water data at SSHCZO. The new model, RT-Flux-PIHM, can simulate solute transport together with geochemical processes, including aqueous complexation, mineral dissolution and precipitation, surface complexation, and ion exchange. With this model, direct comparison of kinetic weathering rate between north and south slopes of the watershed become possible. This new model is one of the first attempts to incorporate geochemical reactions with meteorological and hydrology processes at the watershed scale.

Existing data for the model include the stream water chemistry, pore water chemistry, and soil profile in Shale Hills. These data will also be collected in the other 3 sites in the larger Shavers Creek watershed. Please refer to activities in Hyp 6 for details.

H6:

Three stream water sites (SCAL, SCBL, SCO) were established along the main stem of Shavers Creek in September 2013. Over this period field instrumentation was tested and stream water samples have been collected (bi-monthly to monthly) and analyzed for anions, cations, DOC, and alkalinity. At two locations (SCAL, SCBL) stage discharge relationships are being developed by relating synoptic stream water discharge measurements (hand-held Acoustic Doppler Profiler) with stage measurements collected at rates of 30-min (Hobo water level logger; September through present). At Shavers Creek Outlet (SCO), preliminary discharge measurements have been accomplished using an Acoustic Doppler Channel Profiler (ADCP). At all three locations, conductivity and temperature sensors (Hobo; collection rate of 30-min) have been tested and now provide a continuous downstream comparison of parameters from the Shale Hills catchment to the Shavers Creek outlet. In addition, calibration of the dissolved organic carbon (DOC) component of the *s::can* stream water chemistry sensor was commenced and is expected to be complete by Fall 2014. Finally, initial analysis of the contributing area of varying land-use, soil type and lithology have been completed for all three sites along the main stem of Shavers Creek.

H7:

Yu et al. (2014) and Graduate student Yuting He compared Flux-PIHM and Biome-BGC predictions of discharge, soil water content, soil temperature, and evapotranspiration with observations at Shale Hills. The comparison between Flux-PIHM and Biome-BGC reveals the strength and weaknesses of both models and paves the way towards coupling the models.

Yu (2014) tested linking PIHM with Biome-BGC at Shale Hills watershed.

A solar position algorithm (SPA) has been added to Flux-PIHM, adding the ability to calculate solar radiation taking into account slope, aspect, shading of nearby terrain, and the ratio between incoming direct and diffuse solar radiation. Postdoc Shi has been working with graduate student Katie Gaines in the Ecology team to incorporate root distribution into Flux-PIHM to improve the root water uptake modeling.

With the new infrared gas analyzer (IRGA) installed on the flux tower, we have collected the eddy covariance data using the new IRGA and have processed the data and calculated the surface heat fluxes and carbon fluxes. Those data will be used to calibrate and evaluate the coupled hydrologic-carbon-nitrogen model.

H8:

Shi et al. (2014 JHM) evaluated the parameter sensitivity of Flux-PIHM at the Shale Hills watershed. Shi et al. performed both synthetic (Shi et al. 2014 WRR) and real (Shi et al., in review) data assimilation experiments to evaluate the ability of the ensemble Kalman filter (EnKF) in Flux-PIHM parameter estimation. The experiments found the "minimum requirement" of observations for proper parameter estimation, and will provide guidelines for observational system design.

H9:

We developed a baseline shale weathering and solute flux model by linking the physically-based land surface hydrologic model, Flux-PIHM (Penn State Integrated Hydrologic Model) to the numerical chemical weathering model WITCH. We built in a new module in Flux-PIHM to calculate the effect of aspect on solar radiation on hillslopes. We tested the control of aspect on shale weathering using this new topographic solar radiation component in Flux-PIHM. We utilized soil water Mg2+ measured on samples to first compare WITCH model output to today's observations. In particular, we are examining the sensitivity of our model output to assumptions about the effective reactive surface area and clay mineral thermodynamic data. Finally, in collaboration with SSHO team member Sullivan, Yves Godderis added an elemental nutrient cycling module to WITCH to investigate the control of vegetation cycling on soil solution concentrations of Ca2+, K+ and Si.

Infrastructure Team:

We refurbished the weir at the Shale Hills site (cleaning weir box and replacing the v-notch plate); repaired and reinstalled a LI-7500A gas analyzer for the flux tower at Shale Hills; installed pressure transducers in groundwater wells along the watershed divide and near the stream outlet; relocated of soil O2 sensors; relocated sapflow sensors; repaired the snow scale; tested a spectrometer planned for use at Shale Hills and other sites; and expanded the wireless sensor network to support soil moisture monitoring.

Data Team:

We set up a Microsoft SQL Server database for sensor-based CZO data for automated batch download of sensor data, and have begun setting up web pages for controlled community access to those data. We created Google MapsTM-based GIS instrument and sampling site map of Shale Hills field site.

Specific Objectives:

Hypothesis 1: (Kirby, Bierman, Brantley, Singha, Lin)

Specific objectives included i) evaluating whether fracture density and depth distribution vary with hillslope position or topographic aspect; ii) evaluating whether transport rates of regolith downslope vary with position or aspect; and iii) quantifying rate laws for regolith transport.

Hypothesis 2: (Kaye, Brantley, Eissenstat, Li)

Our objective for the duration of the 5 year project is to instrument catenas within the target sub-catchments (shale, forested sandstone, agricultural calc. shale) of Shaver's Creek with co-located lysimeters for pore water chemistry (ions, DOC) and gas-sampling tubes or sensors (CO2 and O2). We will place lysimeters, soil gas sampling tubes (point measurements), buried soil CO2 continuous sensors, and Apogee soil O2 sensors at depths in the B horizon (matrix flow) and at the high-flow AB and BC horizon interfaces. Our work at Shale Hills taught us that analysis of weathering processes is best accomplished using carefully located catena transects of ridgetop, midslope and valley floor locations along planar slopes and swales. Measurements will be analyzed to assess effects of lithology (sandstone, shale, calcareous shale) and land use (forested versus agricultural). Our proposed plan was to instrument one ridgetop, two midslope, and one valley floor site to define our catena investigation. We may or may not have enough funding to complete that entire deployment now that we have started working in the sandstone site. We will likely maintain that level of activity in Shale Hills, but we may have to limit ourselves to fewer sites in the sandstone site.

For the current reporting year, our objective was to continue monitoring soil CO2 at shale hills, add O2 measurements at shale hills, add soil N2O measurements at shale hills, and select transects for research at the new sandstone site.

Hypothesis 3: (Eissenstat, Davis, Kaye, Brantley)

Specific objectives included examining root length density as a function of hill slope position using multiple methods and assess mycorrhizal colonization, root diameter and respiration of these roots. Work is being extended from forested shale to forested sandstone.

Hypothesis 4: (Lin, Duffy, Eissenstat, Davis)

Specific objectives included 1) developing noninvasive geophysical surveys to detect and quantify macropores and related preferential flow, and 2) real-time and high-frequency soil moisture monitoring and the enhancement of The Hydropedograph Toolbox for analysis of time series soil moisture profiles.

Hypothesis 5: (Li, Brantley, Kaye, Russo)

We are developing an RT module, including the data structures and algorithms that constitute RT-Flux-PIHM as a major objective during this period. The new model is designed to use Flux-PIHM as its driver so that carefully calibrated hydrological parameters can be directly used to reproduce the hydrological processes. This could possibly exert dominant control on the regolith formation at SSHCZO. With the incorporation of meteorological processes in Flux-PIHM, the role of climatic conditions in controlling regolith formation can also be directly evaluated.

Hypothesis 6: (Brantley, Li, Kaye, Davis, Shi)

We are measuring discharge temperature and EC at all three stream water locations along Shavers Creek. We are also now completing monthly to bi-monthly sampling of stream water chemistry. We will begin stream sampling in the sandstone subcatchment.

Hypothesis 7: (Davis, Eissenstat, Shi, Lin, Kaye)
We are comparing Flux-PIHM and Biome-BGC predictions with field observations to study the strength and weaknesses of both models and the breadth and quality of the available observational records.
We are coupling Flux-PIHM and Biome-BGC to produce a high-resolution carbon-hydrology modeling system for the study of water-carbon interaction.
We are testing the hypothesis that Flux-PIHM hydrology will create significant spatial patterns in watershed carbon cycling that bear resemblance to the spatial structures found in the observational record.
Hypothesis 8: (Shi, Davis, Eissenstat, Lin)
We are identifying the minimum requirement of observations for realistic hydrologic and land surface prediction.
We are testing hydrologic parameter transferability and generalizability at 1) new catchments to be instrumented, next the sandstone site, and 2) eventually across the entire Shavers Creek watershed.
We are testing the hypothesis that knowledge of the soil origins and bedrock will strengthen our ability to upscale the hydrologic model across the Shavers Creek watershed.
Hypothesis 9: (Brantley, Godderis, Li, Sullivan)
Objective 1: We are incorporating the effect of aspect into Flux-PIHM.
Objective 2: We are incorporating nutrient cycling in vegetation in WITCH.
Objective 3: We are developing a cascade of models that can earthcast weathering. Objective 4: We are simulating water chemistry and soil chemistry using WITCH, driven by Flux-PIHM.
Infrastructure Team:
Objectives for the infrastructure team included returning the eddy covariance system to full operation, supporting research activities at Shale Hills, and expanding the wireless sensor network to the intensive soil moisture observation sites ("supersites") at Shale Hills. A big objective is to instrument the main stem of Shavers creek and the new sandstone subcatchment.
Data Team:
Objectives included ensuring CZO data are available on local and national CZO data repositories and are locatable via CZO Geoportal and CUAHSI HIS, including creating or modifying datasets and/or metadata file formats as required. Objectives also include coordinating equipment and content and operated equipment for local CZO seminars and web conferences. We are also working with MFA student on audio sonification project using local CZO data. We are also learning GIS concepts and software in order to support such data and we are creating a Microsoft SQL Server database for local archiving of and access to sensor-based data.
Outreach Team:
Objectives: 1) An MFA student is learning to sonify our data for the public. 2) We are working with local high school students to measure stream chemistry in areas related to shale gas development. 3) We are running a seed grant competition. 4) We are publishing papers. 5) We ran a special session at AGU on CZ Tope. 6) We continue to teach and train people to use PIHM.

Significant Results:

H1:

We have made a significant advance in our understanding of topographic asymmetry in watersheds. Despite variations in hillslope gradient of approximately 10°, mass fluxes do not depend on the facing direction of hillslopes in the Observatory. That is, our data reveal spatially uniform lowering rates of ~20-30 meters per million years. This observation requires that regolith transport is more vigorous on hillslopes that receive greater insolation.

H2:

We found that chemical weathering in shallow soils is dominated by clay transformation, and DIC concentrations in soil pore waters are low (<200 micromoles/L). Groundwater chemistry therefore shows different saturation indices with respect to ankerite. The 13C of DIC in these groundwaters documents mixing between the ankerite and soil CO2 end members.

Pyrite oxidation in bedrock likely released sulfuric acid and played a minor role in the ankerite dissolution, shifting the 13C of groundwater DIC slightly above the expected mixing values. At the catchment scale, the stream SO4 is dominantly derived from wet deposition, as the isotopic ratios of S in stream SO4 are around 3 per mil, well within the range of acid deposition.

We also report significant results from our first measurements of N2O through soil profiles of the shale hills catchment. We collected samples from multiple depths along swale and planar catenas. Substantial amounts of N2O accumulated within the soil profile. The peak in soil N2O concentrations generally lagged peak soil CO2 concentrations by several weeks.

H3:

Despite trees being much taller on the valley floor, they do not have deeper roots than much shorter trees on the midslope and ridgetop. There is also little evidence they are getting deeper water. At least for limited samples, mycorrhizal colonization did not decrease dramatically with rooting depth.

H4:

Subsurface lateral flow networks can be non-invasively mapped by time-lapse ground-penetrating radar. After radargram standardization, reflection differences between pre-wetting radargrams and radargrams collected after infiltrations could pinpoint the occurrence of subsurface lateral flow.

H5:

RT-Flux-PIHM has been written in the past year with more than 184,000 lines of C code. Currently the code can simulate geochemical processes including mineral dissolution and precipitation, surface complexation, aqueous complexation, and ion exchange. A general reactive transport framework has been implemented so the code can also incorporate additional types of reactions, including abiotic and biotic redox reaction, microbial activities, and nutrient uptake by roots.

Validation of the reactive species and chemical weathering is ongoing. We found that we cannot reproduce the Mg(II) pore water and stream water concentrations at the same time, potentially due to the ignorance of lateral flow in the undersaturated zone in PIHM.

H6:

We observed that Shavers Creek stream water conductivity and its variability increases downstream (SCAL<SCBL<SCO) with the biggest differences

observed during the summer. Ion analysis suggests stream water Cl- and Na+ concentrations consistently decreased downstream, while SO42-, Ca2+ and Mg2+ and Sr2+ increased in concentrations downstream. The increase in concentrations of elements released by weathering (Ca2+ and Mg2+ and Sr2) is concurrent with an increase in contributing area underlain by limestone and siltstone lithology. The elevated SO42-, especially at the SCO site is likely attributed to the increase in agriculture land-use.

H7:

Flux-PHIM and Biome-BGC comparison: Flux-PHIM did a better job in simulating stream discharge, soil temperature, and ET. Biome-BGC, surprisingly, appears to capture seasonal variability in watershed (Shale Hills) soil moisture better than Flux-PIHM.

Linking PIHM with Biome-BGC: Yu (2014) showed that the using Biome-BGC simulated LAI improved PIHM prediction of discharge, compared with the model run that used default NLCD climatological LAI.

Flux-PIHM improvement: Flux-PIHM successfully resolves the observed hill-slope scale (101 m) spatial soil moisture pattern at the Shale Hills watershed with reasonable predictions of soil moisture.

Watershed micrometeorology: We found that on clear, calm nights, the rapid, spatially divergent cooling pattern characteristic of the early evening transitions exists within the watershed. This cooling pattern was absent on windier, cloudier nights. Down valley flow appears to develop on the nights that experience the early evening transition.

H8:

Observation system design: Shi et al. (2014 JHM) revealed the six most important parameters in Flux-PIHM and found the likely efficiency of different observations in parameter estimation. Shi et al. (2014 JHM) showed that only *in situ* outlet discharge, soil water content at one point, and the land surface temperature averaged over the whole watershed, the EnKF can provide unique and accurate estimates of the key parameter values, i.e., an accurate representation of watershed hydrology at the Shale Hills watershed. The estimated parameter values are very close to the control case in which discharge, water table depth, soil moisture, land surface temperature, surface heat fluxes, and transpiration rate are all assimilated.

Implementation of PIHM at Shaver's Creek: Xuan Yu implemented PIHM at Shave's Creek watershed and performed calibration using groundwater level data.

Development of parallel Flux-PIHM EnKF code: The development of parallel Flux-PIHM EnKF code significantly reduced the time requirement of running the data assimilation system.

H9:

We progressively tested the controls of aspect, mineral reactive surface area, clay thermodynamic constants, and vegetation cycling (uptake and decomposition) on soil water solute fluxes by linking meteorological forcings (the Phase—2 North American Land Data Assimilation System; NLADS-2) and hydrologic (Flux-PIHM) model to the weathering box-model WITCH.

To test the potential control of vegetation cycling on soil water solute concentrations, we developed a basic nutrient cycling module for WITCH.

Based on this module, elemental release (Ca^{2+}, K^+, Si) from vegetation back into the soil was several orders of magnitude greater than fluxes estimated from shale weathering. With this moduel, WITCH was able to simulate the range in of Ca^{2+}, K^+, and Si in soil water solutes that had been observed in the field for both the sun-facing and shaded hillslopes. In addition, Mg^{2+} concentrations in solution were only minimally influenced by the vegetation cycling.

Infrastructure Team:

Returning the eddy covariance tower at Shale Hills to operational status and maintaining the weir are critical to ongoing research activities at SSHCZO. Under the new proposal, preliminary work in the new sandstone forested site is crucial to understanding how we can meet our research goals at that site and produce comparable results to work at Shale Hills. The infrastructure team has dug four soil pits at the catena/transect locations outlined in the proposal (ridge top, 2 mid-slope, and valley floor) and begun installation of sensor systems at the pits.

Details of infrastructure developments for each hypothesis are given in Table 1 (see attachment)

Data Team:

Began learning CUAHSI HydroDesktop in order to verify CZO data cataloging by CUAHSI HIS. Imported pre-existing sensor-based data into Microsoft SQL Server database. Created and tested web pages designed to access SQL Server database. Began expanding GIS instrument map web page to include geospatial data for instruments and sampling sites from new SSHCZO field sites.

Key outcomes or Other achievements:

Hypothesis 1: (Kirby, Bierman, Brantley, Singha, Lin)

Nicole West completed and successfully defended her PhD.

Hypothesis 2: (Kaye, Brantley, Eissenstat, Li)

None to report at this time

Hypothesis 3: (Eissenstat, Davis, Kaye, Brantley)

None to report.

Hypothesis 4: (Lin, Duffy, Eissenstat, Davis)

Two publications.

Hypothesis 5: (Li, Brantley, Kaye, Russo)

Although the development of reactive transport module is based on well-documented methodologies and algorithms, new numerical techniques have been used during the code development. The RT module currently utilizes an operator splitting scheme that described in Zysset et al.4 to solve for the advection diffusion reaction equation (ADR). This scheme is an Implicit-Explicit (IMEX) method where the linear part of ADR equation (transport, diffusion) is solved explicitly and the strongly non-linear part (reaction) is solved implicitly. The stability of explicit methods strongly depends on the selection of time step, which is in turn governed by the ratio of velocity to length of control volume in a finite volume discretization. Very often, a handful of control volumes with the largest flow velocity will enforce the simulator to take infinitesimal time steps and significantly slow down the simulation. To avoid this, we applied a technique called local time stepping (LTS)4, which allows the simulated domain to march in time with non-uniform time steps. This technique reduced the simulation time for RT-Flux-PIHM by a factor of 25.

Hypothesis 6: (Brantley, Li, Kaye, Davis, Shi)

In Spring of 2014, the 71-acre reservoir located between the SCAL and SCBL stream monitoring locations was restored and is currently being refilled. To explore the hydrologic effects of dam restoration on geochemical behavior of streams and tributaries, we are evaluating the hydrogeochemical response of the dam restoration on sections of Shavers Creek and the neighboring Shale Hills tributary. Baseline information before the completed restoration was collected by the PSU fall 2013 GEOSC 413W, Techniques in Geochemistry. The class had 11 students (6 undergraduates, 5 graduate students). Groundwater levels at 19 well within the lake and 8 well at Shale Hills will be utilized to examine the hydrologic response to dam restoration. Next fall, GEOSC 413W students (we anticipate 10-15 students) will follow up on this project once the dam has been restored.

Hypothesis 7: (Davis, Eissenstat, Shi, Lin, Kaye)

Four papers and three theses were products of this team.

Hypothesis 8: (Shi, Davis, Eissenstat, Lin)

Vegetation is being mapped at the Sandstone site including tree species distribution and trunk diameter in belt transects parallel with the contour at various hillslope positions (midslope, ridge, valley floor) through collaboration with Margot Kaye.

Hypothesis 9: (Brantley, Godderis, Li, Sullivan)

1)We developed an aspect module for Flux-PIHM. 2) We developed a biotic cycling model for WITCH. 3) We produced two publications.

Infrastructure Team:

The infrastructure team continues to learn more about the complications surrounding wireless network deployment in a steep, densely forested site. Ongoing work will enhance the wireless network to reduce downtime and improve network stability. Newly developed contacts with PA Bureau of Forestry staff and private landowners in the Shavers Creek region will be crucial to provide access and facilitate research in new parts of the watershed.

Data Team:

We produced an update of data on our website and an updated map of Shale Hills that shows all deployed instrumentation.

*** What opportunities for training and professional development has the project provided?**

Hypothesis 1: (Kirby, Bierman, Brantley, Singha, Lin)

Two PhD students and one postdoctoral researcher worked on this project. Nicole West successfully defended her PhD, "*Topographic Fingerprints of Hillslope Erosion in the Central Appalachians Revealed by Meteoric Beryllium-10*" in May, 2014 in the Department of Geosciences. Ashlee Dere successfully defended her PhD, “Rates and Mecanisms of Shale Weathering across a Latitudinal Climosequence” in June 2014 also in Geosciences. Brian Clarke worked as a postdoctoral researcher until March, 2013.

Hypothesis 2: (Kaye, Brantley, Eissenstat, Li)

We placed one postdoc (Elizabeth Hasenmueller) in a tenure track faculty position. Her advisors contributed to her professional development by supporting presentations at national meetings, critiquing her application materials, and coaching her in several practice job interview seminars. We recruited a new graduate (Lillian Hill) student to the project and are enabling her to start work this summer prior to her official matriculation in to the graduate program. We recruited two REUs to the project (Christine Kim and Jessica Fisher (Brown University)). We mentored additional graduate students (Ashlee Dere, Tiffany Yesavage, Julie Weitzman), including development graduate fellowship proposals, coaching in mock comprehensive exams, and support for presentations at regional and national meetings. One PSU student (Bret Turner) has begun work on their senior honors thesis to measure soil diffusivity, and that student has participated in lab writing workshops (in J. Kaye's lab) and had the opportunity to present and discuss their research proposal with the lab group.

Hypothesis 3: (Eissenstat, Davis, Kaye, Brantley)

Two PhD students worked partially on the project. Katie Gaines is in her 4th year of her PhD program in Ecology and Annie Klodd is finishing her first year of her PhD program in Plant Biology.

Hypothesis 4: (Lin, Duffy, Eissenstat, Davis)

One Master student (Isaac Hopkins) has been collecting, maintaining, and analyzing soil moisture data collected from the Shale Hills. Three visiting scholars from China have been given the opportunity to work in Lin's Lab related to the Shale Hills research.

Hypothesis 5: (Li, Brantley, Kaye, Russo)

During this period, a Ph.D. student, Chen Bao, has been trained to develop, test, optimize, and validate RT-Flux-PIHM. Two undergrads are working on the project: Jessica Fisher (Brown Univ), Reese Davis (Penn State).

Hypothesis 6: (Brantley, Li, Kaye, Davis, Shi)

A total of fourundergraduates (Molly Cain, Jessica Fisher, Nina Bingham, and Brianna McClure) were trained to collect and analyze groundwater and surface water chemistry. Baseline information before the completed restoration was collected by the PSU fall 2013 GEOSC 413W, Techniques in Geochemistry. The class had 11 students (6 undergraduates, 5 graduate students). Groundwater levels at 19 wells within the lake and 8 wells at Shale Hills will be utilized to examine the hydrologic response to dam restoration. Next fall, GEOSC 413W students (we anticipate 10-15 students) will follow-up on this project once the dam has been restored. One postdoctoral student Pamela Sullivan was trained in field and lab and theoretical work, and taught 413W.

Hypothesis 7: (Davis, Eissenstat, Shi, Lin, Kaye)

Yuting He, Ph.D student.

Yuning Shi, PostDoc researcher.

Burkely Twiest, M.S., Graduated May 2014.

Lauren Smith, M.S., Graduated 2013.

Hypothesis 8: (Shi, Davis, Eissenstat, Lin)

Two undergraduates are helping with the vegetation mapping and being trained in forest ecology.

Yuning Shi, PostDoc researcher.

Xuan Yu, PhD, Graduated May 2014.

Hypothesis 9: (Brantley, Godderis, Li, Sullivan)

Yves Goddéris and Yuning Shi trained postdoctoral research Pamela Sullivan in hydrologic and geochemical modeling techniques. Postdoc Pam Sullivan worked closely with graduate students Ashlee Dere and Elizabeth Herndon to understand controls on solute chemistry in Shale Hills. Elizabeth Herndon, a student funded on Shale Hills CZO prior to 2014, is now a faculty member at Kent State.

Infrastructure Team:

The infrastructure team worked with two undergraduate student and three graduate students directly on infrastructure projects during the reporting period. Training includes installation and maintenance of sensor and data logger systems, field data collection methods, and sample collection and archiving. Other students are trained on an ad-hoc basis as required by their research needs.

Data Team:

The data team consists of Dan Arthur, who works closely with J. Williams and A. Neal. Arthur attended introductory Drupal web content management system course, completed a 3-volume self-paced ESRI ArcGIS Tutorial training course, studied various book and web resources to update knowledge in PHP web scripting language for web maintenance and development, and learned Python scripting language for data file processing tools, as well as Microsoft SQL Server 2008 management for database development and maintenance. He also began learning CUAHSI HydroDesktop.

*** How have the results been disseminated to communities of interest?**

Hypothesis 1: (Kirby, Bierman, Brantley, Singha, Lin)
Ashlee Dere taught elementary school as part of the associated Carbon Earth project. Her projects focused on soils.

Hypothesis 3: (Eissenstat, Davis, Kaye, Brantley)
Katie Gaines worked with 6th graders to improve science education. Part of her teaching modules included aspects of her research supported by the CZO. The students recently presented the results of their class projects at a school event open to the public. They also were able to visit the catchment to learn more about the research in progress there during an end of the year field trip.
Hypothesis 4: (Lin, Duffy, Eissenstat, Davis)

The International Workshop on "*Hydropedology and Integrated Natural Resources Management,*" was presented June 29-30, 2013, in Beijing, China. (Organizers: Xiaoyan Li and H. Lin)

A symposium, "Interdisciplinary Studies across the Critical Zone," was presented at the annual meetings of Geological Society of America, Oct. 27-30, 2013, Denver, CO. (Organizers: J. Holloway, J. Morrison, M. Goldhaber, and H. Lin)
Hypothesis 5: (Li, Brantley, Kaye, Russo)
A manuscript on the development of RT-Flux-PIHM and its validation for SSHCZO is in progress, with a tentative title "Development of a hydrological-meteorological reactive transport model RT-Flux-PIHM."
Hypothesis 6: (Brantley, Li, Kaye, Davis, Shi)
Matthew Kenney, a Master of Fine Arts student at PSU, has developed a musical composition to related how incoming rainfall transmits through Shale Hills watershed. He accomplished this piece by sonifying water isotope data that had been collect from different sources (rain, stream, groundwater) overtime (2009-2011). He has presented the work at a national art meeting, a local high school and on campus. Matthew's continued effort in 2014 to synthesize CZO sensor data through sonfinication will help to make CZO science accessible to the community.
Ongoing research investigating the potential hydrologic influence of dam restoration on Shavers Creek and surrounding ecosystem was disseminated to the community through the local Center County new paper (http://www.centredaily.com; Nov 2013, B. Milazzo) as well as through a national environmental magazine (Environmental Monitor, http://www.fondriest.com/news/, Jan 27 2014, A. Card). Molly Cain, an undergraduate student at PSU, also present baseline results from the investigation 2014 Pennsylvania Groundwater Symposium.
Hypothesis 7: (Davis, Eissenstat, Shi, Lin, Kaye)
A Flux-PIHM wiki web page has been added to the web (http://cataract.cee.psu.edu/PIHM/index.php/Land_Surface_Scheme:_Flux-PIHM). The Flux-PIHM code now is also available for download at a GitHub page (https://github.com/shiyuning/Flux-PIHM-2.0) for the community to use.
Eddy covariance flux data are available on the CZO web site.
Hypothesis 8: (Shi, Davis, Eissenstat, Lin)
The Flux-PIHM EnKF system code now is available for download at a GitHub page (https://github.com/shiyuning/Flux-PIHM-EnKF-2.0) for the community to use.
Hypothesis 9: (Brantley, Godderis, Li, Sullivan)

Through both poster and oral presentations, postdoctoral researcher Pamela Sullivan presented work on approaches to Earthcasting shale weathering and solute transport at regional (GSA-Appalachian, 2014), national (AGU Annual Meeting, 2013) and international (Goldschmidt, 2013; EGU, 2014) meetings. Recently Susan Brantley, Christopher Duffy and others presented a conceptual system of models that utilizes the Penn State Integrated Hydrologic Model (PIHM) for the core hydrologic fluxes needed to *Earthcast* different biotic, geomorphic and geochemical processes through the additional of flexible modules.

Infrastructure Team:

Infrastructure developments have been reported to the SSHCZO community through presentations at local (PSU) seminars. As infrastructure developments at new sites become permanent, information will be accessible via criticalzone.org. As appropriate, publications may be developed to describe the infrastructure systems at SSHCZO and how they may apply to the wider research community.

Data Team:

The cyberspecialist worked with investigators and other members of local CZO Data Team to make data available online via local and national repositories, including CZO Geoportal and CUAHSI HIS. He also answered inquiries from investigators both internal and external to the SSHCZO concerning data access, and provided such information and access as appropriate.

Outreach Team:

The outreach team is working with a local highschool (State College Area High School) to deploy sensors on Moshannon creek upstream and downstream of shale gas development activity. The highschool students who were involved have collected data and analyzed it and presented it a workshop in State College (Shale Network Workshop).

*** What do you plan to do during the next reporting period to accomplish the goals?**

Hypothesis 1: (Kirby, Bierman, Brantley, Singha, Lin)

Although Brian Clarke collected a wonderful data set of shallow seismic velocities, he was unable to complete the analysis and interpretation of these data. Nicole West is continuing to work on this as a postdoctoral researcher, and we anticipate having initial results in the next period.

Hypothesis 2: (Kaye, Brantley, Eissenstat, Li)

We will test, purchase, and install soil CO2 sensors at two depths in midslope positions on north and south slopes in the shale hills catchment and at the new sandstone site. Purchase and install soil O2 sensors and lysimeters at the same locations. We will collect soil samples for elemental analysis at these locations.

We will build and install new soil gas access tubes on north slopes at the shale and sandstone catchments. Manually sample these tubes on a monthly basis for CO2 and O2. These manually sampled tubes will complement the continuously measured sensors described above.

We will continue monitoring soil N2O and O2 on the south planar and swale slopes in the shale hills catchment.

Hypothesis 3: (Eissenstat, Davis, Kaye, Brantley)

We will continue investigation of rooting density, mycorrhizal colonization and fungal species composition in relation to hillslope position at the shale hills and sandstone sties.

Hypothesis 4: (Lin, Duffy, Eissenstat, Davis)

We will continue to use geophysical tools to investigate macropores and related preferential flow, and to use real-time soil moisture monitoring to quantify the frequency of preferential flow occurrence. The work will be expanded to the forested sandstone site.

Hypothesis 5: (Li, Brantley, Kaye, Russo)

We plan to continue simulating the shale-weathering scenario using RT-Flux-PIHM model in the coming year to understand key controls of regolith formation processes at the the watershed scale. We also plan to backward and forward cast the formation of regolith over geological time under relevant hydrological conditions at different locations of Shale Hills (ridge top, mid slope, and valley floor) using 2D reactive transport model along a catena. Vertical soil depletion profiles of various elements will be used as constraints for the model. The combination of understanding processes in the short-term, watershed scale and long-term, small scale processes will elucidate the mechanisms and controls of chemical weathering across temporal and spatial scales. It will also help understand process coupling at the larger Shaver's Creek watershed.

Hypothesis 6: (Brantley, Li, Kaye, Davis, Shi)

We plan to analyze the changes related to the dam restoration and to begin to use a reactive transport model to analyze the data. We will be collecting data in the new sandstone site and more data for the main stem of Shavers creek

Hypothesis 7: (Davis, Eissenstat, Shi, Lin, Kaye)

We will compare and evaluate Flux-PIHM and Biome-BGC using more observations, and test Biome-BGC's sensitivities to soil moisture, soil temperature, and LAI.

We will couple Flux-PIHM with Biome-BGC and perform preliminary calibration and evaluation.

We will compute fluxes via eddy covariance at the Shale Hills and Sandstone sites, and compile other carbon cycle observations to be used in joint constraint of the merged carbon and water cycle modeling system, focusing on Shale Hills for the model-data synthesis.

Hypothesis 8: (Shi, Davis, Eissenstat, Lin)

We will continue mapping vegetation at the sandstone site. We will implement Flux-PIHM at the sandstone site and perform synthetic data assimilation experiments to identify the "minimum requirement" of observations at the sandstone site, and compare with the requirement at Shale Hills.

Hypothesis 9: (Brantley, Godderis, Li, Sullivan)

Climatic forcing from A1B IPCC carbon emissions scenario (APREGE), and the biotic, hydrologic and CO2 forcing from a dynamic global vegetation model (CARAIB) will be linked to a weathering model (WITCH) to earthcast the future weathering at Shale Hills in the next 100 years.

Infrastructure Team:

The infrastructure team plans to excavate soil pits and deploy soil moisture and soil gas (O2, CO2) at the new sandstone forested site. Sapflow sensors and a stream gauge are planned as well. As of writing (2014-06-09) soil pits have been excavated and soil samples collected for analysis.

The infrastructure team is also planning to install an eddy covariance system near the sandstone site. The tower is owned and operated by Crown Castle, Inc. and negotiations are underway to install the sensors and determine permitting and fees. The eddy covariance system is planned for a ~1 year deployment.

Specific objectives for the infrastructure team going forward include completion of the stream monitoring site at the outlet of Shavers Creek, including cellular modem telemetry, installation of soil moisture and soil gas sensors at the sandstone site, and training students to collect and process data from these sites.

Data Team:

The cyberspecialist will continue managing and maintaining access to data via local and national repositories, working with investigators and local CZO Data Team to provide access to new data as they become available. He will continue working with national CZO Data Manager and CZOData team to improve organization and access via Geoportal and CUAHSI HIS. Joined subcommittees of CZOData Information Management Committee in order to assist with national CZO data networking, development, and visualization efforts. He will complete web page access to local Microsoft SQL Server database for sensor-based data, including providing visualization of posted data. He will work with investigators to assume responsibility for processing raw sensor-based datasets into forms of data that can be shared with the community.

Outreach Team:

The outreach team will continue to work with the highschool students to collect and analyze data on Moshannon creek. The MFA student will continue to sonify data. We will be planning our Tree Workshop for next summer. We will fund 2 to 3 seed grant activities. We will continue to disseminate PIHM.

Supporting Files

Filename	Description	Uploaded By	Uploaded On
Table1.pdf	Table 1 provides details regarding infrastructure deployment.	Susan Brantley	06/16/2014
CZO Budget_YEAR 2_Final.pdf	Year 2 Budget and Justification	Susan Brantley	06/16/2014

Products

Books

Book Chapters

Yu, X., C. J. Duffy, J. Kaye, W. T. Crow, G. Bhatt, and Y. Shi (2014). Reanalysis of water and carbon cycle models at a critical zone observatory. *Remote Sensing of the Terrestrial Water Cycle* Venkat Lakshmi. American Geophysical Union. Washington, D.C.. . Status = AWAITING_PUBLICATION; Acknowledgement of Federal Support = Yes ; Peer Reviewed = No

Conference Papers and Presentations

Hasenmueller, E.A., Jin, L., Smith, L.A., Kaye, M.W., Lin, H., Brantley, S.L., Kaye, J.P. (2013). *Depth and topographic controls on soil gas concentrations and fluxes in a small temperate watershed*. American Geophysical Union Annual Conference. San Francisco, CA. Status = PUBLISHED; Acknowledgement of Federal Support = Yes

Brantley, S., H. Lin, P. Sullivan, X. Gu, E. Hasenmueller, J. Kaye (2014). *Exploring how rock turns to regolith at the Susquehanna Shale Hills Critical Zone Observatory, Central Pennsylvania*. Geological Society of America Northeastern Section. Lancaster, PA. Status = PUBLISHED; Acknowledgement of Federal Support = Yes

Ma, L., Teng, F-Z., Ke, S., Yang, W., Jin, L., Brantley, S. L (2014). *Mg isotope fractionation during shale weathering in the Shale Hills Critical Zone Observatory: Accumulation of light Mg isotopes in soils by clay mineral transformation*. Goldschmidt Conference. Sacramento, CA. Status = PUBLISHED; Acknowledgement of Federal Support = Yes

Holleran, M., Jin, L., Bazilevskaya, K., White, T. and Brantley, S.L. (2014). *Pyrite oxidation initiates weathering reactions in shale at depth*. Goldschmidt Conference. Sacramento, CA. Status = PUBLISHED; Acknowledgement of Federal Support = Yes

Ma, L., Guo, J., Herndon, E., Jin, L., Sanchez, D., and Brantley, S.L. (2014). *Quantifying the signature of the industrial revolution from Pb, Cd and Zn isotopes in the Susquehanna Shale Hills Critical Zone Observatory*. Goldschmidt Conference. Sacramento, CA. Status = PUBLISHED; Acknowledgement of Federal Support = Yes

Chen Bao, Li Li, Yuning Shi, Changhe Qiao, Pamela L. Sullivan, Susan L. Brantley, and Christopher Duffy (2013). *Understanding the Hydrological Controls on the Water Chemistry at the Watershed Scale Using an Integrated Hydro-Meteo -Geochemical Model PIHM-RT (poster)*. American Geophysical Union (AGU) Fall meeting. San Francisco, CA. Status = PUBLISHED; Acknowledgement of Federal Support = Yes

Heidari, P., Li, L., Jin, L., and Brantley, S. L. (2014). *Unravelling controls on Marcellus Shale weathering*. Goldschmidt Conference. Sacramento, CA. Status = PUBLISHED; Acknowledgement of Federal Support = Yes

Jin, L., Ogrinc, N., Yesavage, T., Hasenmueller, E., Ma, L., Kaye, J. and Brantley, S.L. (2013). *Using C and S isotopes to elucidate carbonic versus sulfuric acid reaction pathways during shale weathering in the Susquehanna Shale Hills Critical Zone Observatory*. American Geophysical Union annual conference. San Francisco, CA. Status = PUBLISHED; Acknowledgement of Federal Support = Yes

Brantley, S.L., Gu, X., Jin, L., Rother, G., Cole, D., and Balashov, V. (2013). *Water-Organic-Rock Reactions Recorded in*

Pores in Shales from the Marcellus and Rose Hill Formations. American Geophysical Union Annual Conference. San Francisco, CA. Status = PUBLISHED; Acknowledgement of Federal Support = Yes

Inventions

Journals

Duffy, C., et al (2014). Designing a system of models to understand the critical zone. *Procedia Earth and Planetary Science*. . Status = AWAITING_PUBLICATION; Acknowledgment of Federal Support = Yes ; Peer Reviewed = Yes

Godderis, Y. and S. L. Brantley (2013). Earthcasting the future Critical Zone. *Elementa*. 1 . Status = PUBLISHED; Acknowledgment of Federal Support = Yes ; Peer Reviewed = Yes ; DOI: 10.12952/journal.elementa.000019

Herndon, E.M., C.E. Martínez, S.L. Brantley (2014). Spectroscopic (XANES/XRF) characterization of contaminant manganese cycling in a temperate watershed. *Biogeochemistry*. . Status = UNDER_REVIEW; Acknowledgment of Federal Support = Yes ; Peer Reviewed = Yes

Herndon, E.M., L. Jin, D.M. Andrews, D.M. Eissenstat, S.L. Brantley (2014). Vegetation acts as a capacitor for manganese contamination at the Susquehanna/Shale Hills Critical Zone Observatory. *Global Biogeochemical Cycles*. . Status = UNDER_REVIEW; Acknowledgment of Federal Support = Yes ; Peer Reviewed = Yes

Nicole West, Eric Kirby, Paul Bierman, and Brian A. Clarke (2014). Aspect-dependent variations in regolith creep revealed by meteoric 10Be. *Geology*. 42 (6), 507. Status = PUBLISHED; Acknowledgment of Federal Support = Yes ; Peer Reviewed = Yes ; DOI: 10.1130/G35357.1

Shi, Y., K. J. Davis, F. Zhang and C. J. Duffy, and X. Yu (2014). Parameter estimation of a physically-based land surface hydrologic model using an ensemble Kalman filter: A multivariate real-data experiment. *Geophysical Review Letters*. . Status = SUBMITTED; Acknowledgment of Federal Support = Yes ; Peer Reviewed = Yes

Shi, Y., K. J. Davis, F. Zhang, and C. J. Duffy (2014). Evaluation of the parameter sensitivity of a coupled land surface hydrologic model. *Journal of Hydrometeorology*. 15 279. Status = PUBLISHED; Acknowledgment of Federal Support = Yes ; Peer Reviewed = Yes ; DOI: 10.1175/JHM-D-12-0177.1

Shi, Y., K. J. Davis, F. Zhang, C. J. Duffy, and X. Yu (2014). Parameter estimation of a physically-based land surface hydrologic model using the ensemble Kalman Filter: A synthetic experiment. *Water Resources Research*. 50 706. Status = PUBLISHED; Acknowledgment of Federal Support = Yes ; Peer Reviewed = Yes ; DOI: 10.1002/2013WR014070

West, N., Kirby, E., Bierman, P., Slingerland, R., Ma, L., Rood, D., and Brantley, S. L. (2013). Regolith production and transport at the Susquehanna Shale Hills Critical Zone Observatory: Part 2 - Insights from meteoric 10Be. *Journal of Geophysical Research, Earth Surface*. 118 1. Status = PUBLISHED; Acknowledgment of Federal Support = Yes ; Peer Reviewed = Yes ; DOI: 10.1002/jgrf.20121

Yu, X., C. Duffy, D. Baldwin, and H.S. Lin (2014). The role of macropores and multi-resolution soil survey datasets for distributed surface-subsurface flow modeling. *Journal of Hydrology*. . Status = AWAITING_PUBLICATION; Acknowledgment of Federal Support = Yes ; Peer Reviewed = Yes ; DOI: 10.1016/j.jhydrol.2014.02.055

Zhang, J., H.S. Lin, and J. Doolittle (2014). Soil layering and preferential flow impacts on seasonal changes of GPR signals in two contrasting soils. *Geoderma*. 213 560. Status = PUBLISHED; Acknowledgment of Federal Support = Yes ; Peer Reviewed = Yes

Licenses

Other Products

Other Publications

Patents

Technologies or Techniques

Thesis/Dissertations

Smith, Lauren A. *Above ground Carbon Distribution across a temperate watershed (Master of Science Thesis)*. (2013). The Pennsylvania State University. Acknowledgement of Federal Support = Yes

Yu, Xuan. *Modeling, parameter optimization, and ecohydrologic assessment of watershed systems (Ph.D. Dissertation)*. (2014). The Pennsylvania State University. Acknowledgement of Federal Support = Yes

Twiest, Burkely L.. *Spatial and temporal evolution of the nocturnal surface layer in a small, steep watershed*. (2014). The Pennsylvania State University. Acknowledgement of Federal Support = Yes

West, Nicole. *Topographic Fingerprints of Hillslope Erosion in the Central Appalachians Revealed by Meteoric Beryllium-10 (PhD Dissertation)*. (2014). The Pennsylvania State University. Acknowledgement of Federal Support = Yes

Websites

Participants/Organizations

What individuals have worked on the project?

Name	Most Senior Project Role	Nearest Person Month Worked
Brantley, Susan	PD/PI	2
Davis, Kenneth	Co PD/PI	1
Duffy, Christopher	Co PD/PI	1
Eissenstat, David	Co PD/PI	1
Li, Li	Co PD/PI	1
Bierman, Paul	Co-Investigator	1
Kaye, Jason	Co-Investigator	1
Kirby, Eric	Co-Investigator	1
Lin, Henry	Co-Investigator	1
Singha, Kamini	Co-Investigator	1
Clarke, Brian	Postdoctoral (scholar, fellow or other postdoctoral position)	3
Hasenmueller, Elizabeth	Postdoctoral (scholar, fellow or other postdoctoral position)	6
Karwan, Diana	Postdoctoral (scholar, fellow or other postdoctoral position)	1
Shi, Yuning	Postdoctoral (scholar, fellow or other postdoctoral position)	12

Name	Most Senior Project Role	Nearest Person Month Worked
Sullivan, Pamela	Postdoctoral (scholar, fellow or other postdoctoral position)	12
West, Nicole	Postdoctoral (scholar, fellow or other postdoctoral position)	6
Neal, Andrew	Staff Scientist (doctoral level)	12
Bao, Chen	Graduate Student (research assistant)	6
Dere, Ashlee	Graduate Student (research assistant)	6
Gaines, Katie	Graduate Student (research assistant)	6
He, Yuting	Graduate Student (research assistant)	6
Hopkins, Isaac	Graduate Student (research assistant)	6
Twiest, Burkely	Graduate Student (research assistant)	6
Weitzman, Julie	Graduate Student (research assistant)	6
Yu, Xuan	Graduate Student (research assistant)	6
Zhang, Yu	Graduate Student (research assistant)	6
Arthur, Dan	Non-Student Research Assistant	12
Williams, Jennifer	Non-Student Research Assistant	12

Full details of individuals who have worked on the project:

Susan L Brantley
Email: brantley@essc.psu.edu
Most Senior Project Role: PD/PI
Nearest Person Month Worked: 2

Contribution to the Project: Principal Investigator; Lead PI on Hypothesis 9

Funding Support: n/a

International Collaboration: Yes, France
International Travel: Yes, France - 0 years, 0 months, 5 days

Kenneth J Davis
Email: kjd10@psu.edu
Most Senior Project Role: Co PD/PI
Nearest Person Month Worked: 1

Contribution to the Project: co-principal investigator; lead PI on hypothesis 7

Funding Support: n/a

International Collaboration: No
International Travel: No

Christopher J Duffy
Email: cxd11@psu.edu
Most Senior Project Role: Co PD/PI
Nearest Person Month Worked: 1

Contribution to the Project: Co-investigator

Funding Support: n/a

International Collaboration: No
International Travel: No

David M Eissenstat
Email: dme9@psu.edu
Most Senior Project Role: Co PD/PI
Nearest Person Month Worked: 1

Contribution to the Project: Co-Prinicipal Investigator; lead PI on Hypothesis 3

Funding Support: n/a

International Collaboration: No
International Travel: No

Li Li
Email: lili@eme.psu.edu
Most Senior Project Role: Co PD/PI
Nearest Person Month Worked: 1

Contribution to the Project: co-investigator; lead PI on Hypothesis 5

Funding Support: n/a

International Collaboration: No
International Travel: No

Paul Bierman
Email: pbierman@uvm.edu
Most Senior Project Role: Co-Investigator
Nearest Person Month Worked: 1

Contribution to the Project: Geomorphologist/Geochemist - works on Hypothesis 1

Funding Support: CZO

International Collaboration: No

International Travel: No

Jason Kaye
Email: jpk12@psu.edu
Most Senior Project Role: Co-Investigator
Nearest Person Month Worked: 1

Contribution to the Project: Soil Biogeochemist - works on Hypotheses 2, 3, 5, and 6

Funding Support: CZO

International Collaboration: No
International Travel: No

Eric Kirby
Email: eric.kirby@geo.oregonstate.edu
Most Senior Project Role: Co-Investigator
Nearest Person Month Worked: 1

Contribution to the Project: Geomorphologist - works on Hypothesis 1

Funding Support: CZO

International Collaboration: No
International Travel: No

Henry Lin
Email: hul3@psu.edu
Most Senior Project Role: Co-Investigator
Nearest Person Month Worked: 1

Contribution to the Project: Hydorpedologist - works on Hypotheses 1, 4, 7, and 8

Funding Support: CZO

International Collaboration: No
International Travel: No

Kamini Singha
Email: ksingha@mines.edu
Most Senior Project Role: Co-Investigator
Nearest Person Month Worked: 1

Contribution to the Project: Hydrogeologist - works on Hypothesis 1

Funding Support: CZO

International Collaboration: No
International Travel: No

Brian Clarke
Email: bac43@psu.edu

Most Senior Project Role: Postdoctoral (scholar, fellow or other postdoctoral position)
Nearest Person Month Worked: 3

Contribution to the Project: Geomorphologist - worked on Hypothesis 1

Funding Support: CZO

International Collaboration: No
International Travel: No

Elizabeth Hasenmueller
Email: hasenmuellerea@slu.edu
Most Senior Project Role: Postdoctoral (scholar, fellow or other postdoctoral position)
Nearest Person Month Worked: 6

Contribution to the Project: Hydrochemist - works on Hypothesis 2

Funding Support: CZO

International Collaboration: No
International Travel: No

Diana Karwan
Email: dlkarwan@umn.edu
Most Senior Project Role: Postdoctoral (scholar, fellow or other postdoctoral position)
Nearest Person Month Worked: 1

Contribution to the Project: Cross-CZO Post-doctoral Fellow

Funding Support: NSF

International Collaboration: No
International Travel: No

Yuning Shi
Email: yshi@psu.edu
Most Senior Project Role: Postdoctoral (scholar, fellow or other postdoctoral position)
Nearest Person Month Worked: 12

Contribution to the Project: Hydrologist - works on Hypothesis 7 and 8

Funding Support: CZO

International Collaboration: No
International Travel: No

Pamela Sullivan
Email: pls21@psu.edu
Most Senior Project Role: Postdoctoral (scholar, fellow or other postdoctoral position)
Nearest Person Month Worked: 12

Contribution to the Project: Hydrochemist - works on Hypotheses 6 and 9

Funding Support: CZO

International Collaboration: No
International Travel: No

Nicole West
Email: nxw157@psu.edu
Most Senior Project Role: Postdoctoral (scholar, fellow or other postdoctoral position)
Nearest Person Month Worked: 6

Contribution to the Project: geomorphologist - works on Hypothesis 1

Funding Support: CZO

International Collaboration: No
International Travel: No

Andrew Neal
Email: aln16@psu.edu
Most Senior Project Role: Staff Scientist (doctoral level)
Nearest Person Month Worked: 12

Contribution to the Project: Watershed Specialist

Funding Support: CZO

International Collaboration: No
International Travel: No

Chen Bao
Email: cub200@psu.edu
Most Senior Project Role: Graduate Student (research assistant)
Nearest Person Month Worked: 6

Contribution to the Project: works on Hypothesis 5

Funding Support: CZO

International Collaboration: No
International Travel: No

Ashlee Dere
Email: ald271@psu.edu
Most Senior Project Role: Graduate Student (research assistant)
Nearest Person Month Worked: 6

Contribution to the Project: shale weathering along transect sites

Funding Support: CZO

International Collaboration: No
International Travel: No

Katie Gaines
Email: kpgaines@psu.edu
Most Senior Project Role: Graduate Student (research assistant)
Nearest Person Month Worked: 6

Contribution to the Project: works on tree physiology

Funding Support: CZO

International Collaboration: No
International Travel: No

Yuting He
Email: yzh120@psu.edu
Most Senior Project Role: Graduate Student (research assistant)
Nearest Person Month Worked: 6

Contribution to the Project: works on PIHM and Biome-BGC

Funding Support: CZO

International Collaboration: No
International Travel: No

Isaac Hopkins
Email: ieh105@psu.edu
Most Senior Project Role: Graduate Student (research assistant)
Nearest Person Month Worked: 6

Contribution to the Project: works on Hypothesis 4

Funding Support: CZO

International Collaboration: No
International Travel: No

Burkely Twiest
Email: blt5086@psu.edu
Most Senior Project Role: Graduate Student (research assistant)
Nearest Person Month Worked: 6

Contribution to the Project: micro-meteorology

Funding Support: CZO

International Collaboration: No
International Travel: No

Julie Weitzman
Email: jnw142@psu.edu
Most Senior Project Role: Graduate Student (research assistant)
Nearest Person Month Worked: 6

Contribution to the Project: works on Hypothesis 2

Funding Support: CZO

International Collaboration: No
International Travel: No

Xuan Yu
Email: xxy113@psu.edu
Most Senior Project Role: Graduate Student (research assistant)
Nearest Person Month Worked: 6

Contribution to the Project: works on PIHM and flux-PIHM

Funding Support: CZO

International Collaboration: No
International Travel: No

Yu Zhang
Email: yzz130@psu.edu
Most Senior Project Role: Graduate Student (research assistant)
Nearest Person Month Worked: 6

Contribution to the Project: works on PIHM-sed

Funding Support: CZO

International Collaboration: No
International Travel: No

Dan Arthur
Email: dka12@psu.edu
Most Senior Project Role: Non-Student Research Assistant
Nearest Person Month Worked: 12

Contribution to the Project: Data Manager / Cyberspecialist

Funding Support: CZO

International Collaboration: No
International Travel: No

Jennifer Williams
Email: jzw126@psu.edu
Most Senior Project Role: Non-Student Research Assistant
Nearest Person Month Worked: 12

Contribution to the Project: Program and Sample Coordinator

Funding Support: CZO

International Collaboration: No

International Travel: No

What other organizations have been involved as partners?
Nothing to report.

Have other collaborators or contacts been involved? Yes

Impacts

What is the impact on the development of the principal discipline(s) of the project?

Hypothesis 1: (Kirby, Bierman, Brantley, Singha, Lin)
We are the first team to simultaneously measure soil production rate and erosion rate in one catchment on the same samples. Our papers are highly regarded on this topic. We have extended this work to include treatment of curvature of ridgetops, and we have related denudation rate measurements to curvature.
Hypothesis 2: (Kaye, Brantley, Eissenstat, Li)
We have completed papers documenting the relationship between weathering advance and landscape position, as well as CO2 flux and landscape position. The distribution of soil gas and its effects on weathering as a function of landscape position is an important aspect of weathering and carbon cycling that has largely been neglected.
Hypothesis 3: (Eissenstat, Davis, Kaye, Brantley)
We have highlighted the importance of trees in the water balance, and the depth from which tree water is extracted.
Hypothesis 4: (Lin, Duffy, Eissenstat, Davis)
We have developed one of the pre-eminent datasets of soil moisture in a small catchment.
Hypothesis 5: (Li, Brantley, Kaye, Russo)
We are:

1. Gaining fundamental understanding and knowledge on chemical weathering and their hydrological and climatic controls.
2. Providing a modeling tool to integrate and decouple the processes of interests in multiple earth system disciplines, including geochemistry, hydrology, and meteorology. This essentially enables closer interaction and the conversation among these disciplines. This tool will be a significant asset for the geochemistry community, the CZO community, and the general earth system sciences.

Hypothesis 6: (Brantley, Li, Kaye, Davis, Shi)
We are developing new infrastructure on the main stem of Shavers creek and in the new sandstone subcatchment.
Hypothesis 7: (Davis, Eissenstat, Shi, Lin, Kaye)
We are establishing Flux-PIHM as a land surface – hydrologic model that can incorporate aspects of the landscape.
Hypothesis 8: (Davis, Shi, Eissenstat, Lin)
We are developing new infrastructure on the main stem of Shavers creek and in the new sandstone subcatchment.
Hypothesis 9: (Brantley, Godderis, Li, Sullivan)
We have published the first paper on earthcasting weathering into the next century in the face of climate change.
Infrastructure Team:
We are developing new infrastructure on the main stem of Shavers creek and in the new sandstone subcatchment.

What is the impact on other disciplines?

Hypothesis 1: (Kirby, Bierman, Brantley, Singha, Lin)
We are the first team to simultaneously measure soil production rate and erosion rate in one catchment on the same samples. Our papers are highly regarded on this topic. We have extended this work to include treatment of curvature of ridgetops, and we have related denudation rate measurements to curvature. These efforts are important in that they are bringing the geomorph and geochem disciplines closer.
Hypothesis 2: (Kaye, Brantley, Eissenstat, Li)
We were able to use DOE money to analyze neutron scattering of shale chips from Shale Hills and from the Marcellus shale weathering project to determine porosity. This led us to better understanding how porosity is distributed in the Marcellus and led us to a submitted paper on Marcellus shale porosity – of interest to hydrocarbon companies.
Hypothesis 3: (Eissenstat, Davis, Kaye, Brantley)
We have mapped root depth in Shale Hills and are relating that to weathering depths and CO2 dynamics. This led to a funded (DOE) project on carbon cycling.
Hypothesis 4: (Lin, Duffy, Eissenstat, Davis)
We have developed the use of GPR for shale lithologies.
Hypothesis 5: (Li, Brantley, Kaye, Russo)

1. We provided insights on how geochemistry / chemical weathering influence water and elemental cycles.

2. We are providing a modeling tool to integrate and decouple the processes of interests in multiple earth system disciplines, including geochemistry, hydrology, and meteorology. This essentially enables closer interaction and the conversation among these disciplines. This tool will be a significant asset to the CZO community and the general earth system sciences.

3. We succeeded in developing RT-Flux-PIHM also yielded insights and numerical techniques that will be useful to other disciplines. The adoption of local time stepping (LTS) techniques significantly increased the efficiency of reactive transport algorithms by significantly reducing the number of call to the implicit solvers. This technique is very useful when the simulation domain has highly heterogeneous field where orders of magnitude difference in time scales exist for different processes. Examples include however not limited to rivers and watershed, wells and reservoir, fracture and matrix.

Hypothesis 6: (Brantley, Li, Kaye, Davis, Shi)
We are starting to deploy a sc::ann instrument to measure chemistry of stream waters. This sensor will possibly change how geochemists do their work (ie using a sensor instead of grab sampling). We also used the sensor to investigate brine discharge from oil/gas wells in PA and have used that deployment to submit a paper about how many sensors might be needed in PA to detect issues in areas of shale gas development.
Hypothesis 7: (Davis, Eissenstat, Shi, Lin, Kaye)
We have developed a model, Flux-PIHM, that can allow hydrologists and meteorologists to investigate the importance of the land surface in water and energy cycling.
Hypothesis 8: (Davis, Shi, Eissenstat, Lin)
We are developing a deployable set of instrumentation to measure the most important aspects of water, energy, and carbon budgets in a large catchment to enable hydrologic modelling: we are moving from "measure everything everywhere" to "measure only what you need".
Hypothesis 9: (Brantley, Godderis, Li, Sullivan)
The CZO team worked with Yves Godderis to develop a cascade of models that can enable earthcasting (future projection) of weathering. This model cascade is an exemplar of other types of cascades that could be used for earthcasting other processes.
Infrastructure and Data Teams:

As a support structure in the SSHCZO organization, the infrastructure and data teams ensure the success of field operations for the various hypothesis teams and ensure that data can be used by those outside of the CZO.

What is the impact on the development of human resources?

Hypothesis 1: (Kirby, Bierman, Brantley, Singha, Lin)
Mentored postdocs, undergraduates and graduate students.
Hypothesis 2: (Kaye, Brantley, Eissenstat, Li)
Mentored postdocs, undergraduates and graduate students.
Hypothesis 3: (Eissenstat, Davis, Kaye, Brantley)
Mentored postdocs, undergraduates and graduate students.
Hypothesis 4: (Lin, Duffy, Eissenstat, Davis)
Mentored postdocs, undergraduates and graduate students.
Hypothesis 5: (Li, Brantley, Kaye, Russo)
A Ph.D. student, Chen Bao, has been trained to develop, test, optimize and validate Flux-PIHM-RT and to understand critical zone sciences. Two undergrads are working on the project: Jessica Fisher (Brown Univ), Reese Davis (Penn State)
Hypothesis 6: (Brantley, Li, Kaye, Davis, Shi)
Mentored postdocs, undergraduates and graduate students.
Hypothesis 7: (Davis, Eissenstat, Shi, Lin, Kaye)
Mentored postdocs, undergraduates and graduate students.
Hypothesis 8: (Davis, Shi, Eissenstat, Lin)
Mentored postdocs, undergraduates and graduate students.
Hypothesis 9: (Brantley, Godderis, Li, Sullivan)
Mentored postdocs, undergraduates and graduate students.
Infrastructure Team:
The infrastructure team collaborates with hypothesis teams to provide training to students in field methods and technical skills related to their research. This includes sample collection, sensor operation and installation, data logger programming, data management and processing, and measurement theory.

What is the impact on physical resources that form infrastructure?

Hypothesis 1: (Kirby, Bierman, Brantley, Singha, Lin)
This team completed a borehole in Shale Hills.
Hypothesis 2: (Kaye, Brantley, Eissenstat, Li)
This team dug and investigated three soil pits in Shale Hills.
Hypothesis 3: (Eissenstat, Davis, Kaye, Brantley)
This team measured root density versus depth in the soil pits.
Hypothesis 4: (Lin, Duffy, Eissenstat, Davis)
This team purchased instrumentation to map soil series.
Hypothesis 5: (Li, Brantley, Kaye, Russo)
The H5 team is working to establish soil pits along catenas in the new sandstone catchment. These pits will be analyzed for chemistry and mineralogy and will have sensors for measurement of soil gases and collection of soil waters. Three of five pits have been dug, but we will deepen them.
Hypothesis 6: (Brantley, Li, Kaye, Davis, Shi)
This team completed baseline measurements to set the stage for an investigation of before and after the Shavers creek dam
Hypothesis 7: (Davis, Eissenstat, Shi, Lin, Kaye)
This team is developing sensor approaches for the new catchments.

Hypothesis 8: (Davis, Shi, Eissenstat, Lin)
This team is developing new sensor approaches for the new catchments.
Hypothesis 9: (Brantley, Godderis, Li, Sullivan)
No infrastructure work
Infrastructure Team:
The infrastructure team is directly responsible for the maintenance of physical resources of SSHCZO research. Existing infrastructure at Shale Hills and new installations at the proposed sites in Shavers Creek are overseen by the infrastructure team. These responsibilities include programming, physical installation, troubleshooting, maintenance, and decommissioning.

What is the impact on institutional resources that form infrastructure?

The infrastructure team is the core institutional resource for physical equipment, technical expertise and personnel support for research at SSHCZO.

What is the impact on information resources that form infrastructure?

Hypothesis 1: (Kirby, Bierman, Brantley, Singha, Lin)
All data are being published online
Hypothesis 2: (Kaye, Brantley, Eissenstat, Li)
All data are being published online
Hypothesis 3: (Eissenstat, Davis, Kaye, Brantley)
All data are being published online
Hypothesis 4: (Lin, Duffy, Eissenstat, Davis)
All data are being published online
Hypothesis 5: (Li, Brantley, Kaye, Russo)
The reactive transport module developed for Flux-PIHM or PIHM is a highly versatile, portable code that requires minimum data interface with the driver model. Furthermore, the model utilized a connection-based approach, which makes it very convenient to couple with other driver model. The developed model will be shared with the community to understand CZO science.
Hypothesis 6: (Brantley, Li, Kaye, Davis, Shi)
All data are being published online
Hypothesis 7: (Davis, Eissenstat, Shi, Lin, Kaye)
All data are being published online
Hypothesis 8: (Davis, Shi, Eissenstat, Lin)
All data are being published online
Hypothesis 9: (Brantley, Godderis, Li, Sullivan)
All data are being published online
Infrastructure Team:
The infrastructure team works in close collaboration with the data team to ensure that data collected from field sites are incorporated into data management systems. Data collected at Shale Hills are entered into a database which will provide SSHCZO and other researchers access to near-real-time data. New spatial data are also compiled into a geodatabase which is revised approximately once per year to reflect new measurement sites and new geospatial data available from external sources.

What is the impact on technology transfer?

The infrastructure team has worked closely with staff at Stroud Water Research Center/Christina River Basin CZO regarding the deployment of wireless networking technologies as well as in situ spectrometers for water quality monitoring. The training function of the infrastructure team promotes the dissemination of technical skills for the operation, maintenance of sensor systems and data processing in support of research at SSHCZO. The infrastructure team is also working closely with the manufacturer of the sc::ann sensor to understand and perhaps improve algorithms for interpreting sc::ann data.

What is the impact on society beyond science and technology?

The largest impact on society beyond science and technology is the new generation of scientists who are being trained to cross disciplinary boundaries.

Changes/Problems

Changes in approach and reason for change

Hypothesis 1: (Kirby, Bierman, Brantley, Singha, Lin)
Brian Clarke, our postdoc, is no longer working for us because he has not been successful in writing up his results.
Hypothesis 2: (Kaye, Brantley, Eissenstat, Li)
We may not have enough money to instrument our full catena design. We may only instrument two mid slope soil sites in the sandstone catchment.
Hypothesis 3: (Eissenstat, Davis, Kaye, Brantley)
No problems to report.
Hypothesis 4: (Lin, Duffy, Eissenstat, Davis)
No problems to report.
Hypothesis 5: (Li, Brantley, Kaye, Russo)
Nothing to report
Hypothesis 6, 7, 8, 9
Nothing to report.
Infrastructure Team:
The infrastructure team has experienced delays regarding the deployment of eddy covariance at a third-party tower near the sandstone site. Ongoing communications with the tower owners have been slower than anticipated but progress is occurring.
Deployment of wireless data systems remains a logistical concern for the SSHCZO infrastructure team. The steep, terrain and dense forest at Shale Hills and the new sandstone forested site make wireless network deployment a complex and costly undertaking. Many systems still require manual data downloads on a provisional basis until wireless radios and a consistent transmission network can be deployed.
Details regarding infrastructure deployment can be found in Table 1.

Actual or Anticipated problems or delays and actions or plans to resolve them
Nothing to report.

Changes that have a significant impact on expenditures
Nothing to report.

Significant changes in use or care of human subjects
Nothing to report.

Significant changes in use or care of vertebrate animals
Nothing to report.

Significant changes in use or care of biohazards
Nothing to report.