Annual Report for Period: 11/2010 - 10/2011 Principal Investigator: Duffy, Christopher J. Organization: PA St U University Park Submitted By: Duffy, Christopher - Principal Investigator Title: CZO: Susquehanna/Shale Hills Critical Zone Observatory Submitted on: 07/30/2011 Award ID: 0725019

# **Project Participants**

Senior Personnel			
	Name: Duffy, Christopher		
	Worked for more than 160 Hours:	Yes	
	<b>Contribution to Project:</b>		
	Stable Isotope and Computational Hydrology		
	Name: Slingerland, Rudy		
	Worked for more than 160 Hours:	Yes	
	Contribution to Project:		
	Geomorphology		
	Name: Brantley, Susan		
	Worked for more than 160 Hours:	Yes	
	Contribution to Project:		
	Geochemistry		
	Name: Singha, Kamini		
	Worked for more than 160 Hours:	Yes	
	Contribution to Project:		
	Hydrogeophysics		
	Name: Nyquist, Jonathan		
	Worked for more than 160 Hours:	Yes	
	Contribution to Project:		
	Name: Davis, Kenneth		
	Worked for more than 160 Hours:	Yes	
	<b>Contribution to Project:</b>		
	Meteorology		
	Name: Eissenstat, David		
	Worked for more than 160 Hours:	Yes	
	<b>Contribution to Project:</b>		
	Plant Ecology		
	Name: Kaye, Jason		
	Worked for more than 160 Hours:	No	
	Contribution to Project:		
	Soil Science		
	Name: Kirby, Eric		
	Worked for more than 160 Hours:	Yes	
	Contribution to Project:		
	Geomorphology		

Name: Lin, Henry Worked for more than 160 Hours: Yes **Contribution to Project:** Soil Science Name: Miller, Douglas Worked for more than 160 Hours: Yes **Contribution to Project:** Informatics Name: Reed, Patrick Worked for more than 160 Hours: Yes **Contribution to Project:** Computational Hydrology, Cyberinfrastructure Name: Salvage, Karen Worked for more than 160 Hours: Yes **Contribution to Project:** Groundwater Geochemical Modeling Name: Dressler, Kevin Worked for more than 160 Hours: Yes **Contribution to Project:** Snow Hydrology, Hydrologic Modeling, Site and Project Management Name: Fletcher, Raymond Worked for more than 160 Hours: Yes **Contribution to Project:** Geochemistry Name: White, Timothy Worked for more than 160 Hours: Yes **Contribution to Project:** Geology, Liaison to Transect Participants, Project Management Name: April, Richard Worked for more than 160 Hours: Yes **Contribution to Project:** Transect Participant Name: Harbor, David Worked for more than 160 Hours: Yes **Contribution to Project:** Transect Participant Name: Mathur, Ryan Worked for more than 160 Hours: Yes **Contribution to Project: Transect Participant** Name: Teferi, Tsegaye Worked for more than 160 Hours: Yes **Contribution to Project: Transect Participant** Name: Santos, Hernan Worked for more than 160 Hours: Yes

Contribution to Project:	
Transect Participant	
Name: Boyer, Elizabeth	
Worked for more than 160 Hours:	Yes
<b>Contribution to Project:</b>	
Name: Tuttle, Michelle Worked for more than 160 Hours:	No
Contribution to Project:	INO
USGS Scientist	
Name: Lichtner, Peter	
Worked for more than 160 Hours:	No
Contribution to Project:	110
Los Alamos National Lab Scientist	
Name: Goldhaber, Marty	
Worked for more than 160 Hours:	No
Contribution to Project:	
Geochemistry	
Name: Steefel, Carl	
Worked for more than 160 Hours:	No
<b>Contribution to Project:</b>	
USGS scientist	
Name: Lehnert, Kirsten	
Worked for more than 160 Hours:	No
Contribution to Project:	
Geochemistry Informatics	
Name: Miller, Tom	
Worked for more than 160 Hours:	Yes
Contribution to Project:	
Name: Fedo, Chris	
Worked for more than 160 Hours:	Yes
Contribution to Project:	
- <b>y</b>	

# Post-doc

Name: Jin, Lixin		
Worked for more than 160 Hours:		
Contribution to Project:		
Leads geochemistry field experiment		
Name: Graham, Chris		
Worked for more than 160 Hours:		
Contribution to Project:		
Leads Hydropedology field experiment		

# **Graduate Student**

#### **Undergraduate Student**

#### **Technician**, **Programmer**

#### **Other Participant**

Name: Cherrey, Kelly Worked for more than 160 Hours: Yes Contribution to Project: In charge of installing sensors and communications

Name: Williams, Jennifer Worked for more than 160 Hours: Yes Contribution to Project:

Name: Duffy, Colin Worked for more than 160 Hours: Yes Contribution to Project:

**Research Experience for Undergraduates** 

#### **Organizational Partners**

**CZEN: The Critical Zone Environmental Ne** 

CUAHSI: The CUAHSI Hydrologic Informati

GfG Geoinformatics for Geochemistry pro

#### **Crossbow Technologies Inc.**

Crossbow Technologies Inc. (http://www.xbow.com/eKo/) has been instrumental in helping us plan for a new direction at the Shale Hills CZO allows 2-way communication and control for all sensors in a high resolution adaptive sensor array. Seed money has also been made available to test the Crossbow system by the Penn State Institute for CyberScience (ICS) and Penn State Institutes for Energy & the Environment.

#### **Other Collaborators or Contacts**

Crossbow Technologies Inc. (http://www.xbow.com/Eko/) has been instrumental in helping us plan for a new direction at the Shale Hills CZO that will ultimately allow 2-way communication and control for all sensors in a high resolution adaptive sensor array. More information on this will be presented next year but seed money has been made available to test the design by the Penn State Institute for CyberScience (ICS) and Penn State Institutes for Energy & the Environment.

#### **Activities and Findings**

**Research and Education Activities: (See PDF version submitted by PI at the end of the report)** see attached file

#### **Findings:**

see attached file under activities

#### **Training and Development:**

Opportunities for Training, Development, and Mentoring

Graduate Students: CZO-funded or from contributing research\* (completion date)

Name: Andrews, Danielle, (2011) PhD Soil Science Name: Baldwin, Doug, (2011) MS Soil Science Name: Bhatt, Gopal, PhD (2010) Civil and Environmental Engineering Name: Bhattacharyya, Amrita, PhD Soil Science Name: Dere, Ashlee, PhD Geosciences Name: Fuller, Robert, PhD Geosciences Name: Gaines, Katie, PhD Ecology Name: Graham, Chris, Post-Doc, Soil Science Name: Herndon, Beth, PhD Geoscience Name: Holmes, George, (2011) MS Civil and Environmental Engineering Name: Johnson, Mitch, MS Geoscience Name: Kumar, Mukesh\*, PhD (2009) Civil and Environmental Engineering Name: Kuntz, Brad, MS (2010) Geosciences Name: Li, Wenfang, MS (2009) Civil and Environmental Engineering Name: Li, Shuangcai\*, PhD (2008) Civil and Environmental Engineering Name: Naithani, Kusum, Post-Doc Ecology Name: Shi, Yuning, PhD Meteorology Name: Takagi, Ken, MS (2009) Soil science Name: West, Nicole, PhD Geosciences Name: Wubbles, Jane, MS (2010)Horticulture Name: Williams, Jennifer PhD Geosciences Name: Yesavage, Tiffany, PhD Geosciences Name: Yu, Xuan, PhD Civil & Environmental Engineering Name: Zhang, Jun, PhD (2011) soil science

Lin Ma (Geoscience, Penn State) measured U disequilibrium isotopes on Shale Hills samples at the Univ of Strasbourg with Francois Chabaux. Beth Herndon (Penn State) learned to run mesocosm experiments at Univ of Sheffield. Jennifer Williams and Ashlee Dere (Penn State) visited Plynlimon, Wales, a shale site that will become part of our satellite sites.

George Holmes (MS CEE Dept. Penn State) participated in the International CZO Experience. The experience started in Vienna, Austria with two weeks visiting scientists at the IAEA (International Atomic Energy Agency). The first week was spent at a short course demonstrating how to operate a Los Gatos Research Liquid Water Stable Isotope Analyzer. The second week was spent working with Brent Newman on the GNIR (Global Network of Isotopes in Rivers) database. The database was made public this year and Brent is encouraging publishing papers using the data. He also spent time with Tomas Vitvar and Luis Araguas concerning the Shale Hills CZO. The next spent three weeks were in Zurich, Switzerland working with Manfred Staehli at WSL (Swiss Federal Institute for Forest, Snow and Landscape Research). Where he was able to talk with many scientists about the Shale Hills CZO, and I also was able to discuss related projects like the BigLink Damma Glacial Forefield and the Cottbus Watershed in Germany. At WSL he gave a presentation that outlined all three CZO projects with focus on Shale Hills. He was able to visit the Damma Glacier Forefield and see the set up of the instrumentation, and I was also part of a trip to the Rietholzbach research catchment. The final week was spent in Davos, Switzerland at the Goldschmidt Conference with many talks related to the Shale Hills CZO.

Undergraduate Students working on the Shale Hills CZO:

Nick Kaiser, Geosciences PSU Jose Morales, Geosciences, Univ of Puerto Rico Kristen Jurinko, Soil Science Dept.PSU Shaquandra Wilson, Geoscience Univ of W Alabama Terryl Daniels, Geosciences, PSU Valentina Prado Geosciences, PSU Mitchell Johnson, Geosciences, PSU Tamika Shannon, Geosciences, PSU Maurice Dukes, Geosciences, PSU Nate Wysocki, Geosciences, PSU Nathan Barber, Geosciences, PSU Ahmad Yusof, Geosciences, PSU Erica Folio, Geosciences, PSU

Example Research Experience for Undergraduates:

Name: Jurinko, Kristen Contribution to Project: REU at Penn State University Soil Science Dept, Summer 09. See Hydropedology findings for a description of this research.

Name: Nick Kaiser REU at Penn State University Soil Science Dept, Summer 09

Nick Kaiser's summer REU project focused on the measurement of soil respiration in the Shale Hills catchment. He was mentored by Dr. Jason Kaye, Dr. Lixin Jin (postdoc), and Danielle Andrews (graduate student). Over the summer, Nick tested hypotheses regarding relationships among soil CO2 concentrations, soil respiration, and soil microclimate. He made weekly trips to the field site where he used soil access tubes to sample soil gas from multiple depths. At the same locations he measured soil moisture using at TDR probe, and surface soil respiration using a portable infrared gas analyzer and soil cover (a chamber used to capture CO2 diffusing out of the soil). Using Fick's law of diffusion he predicted soil CO2 flux throughout the profile and compared these values to soil moisture, soil temperature, and surface soil flux measured with the soil cover. His work has led to important insights on the role of soil water in controlling gas diffusion, and has inspired the possible use of simple gas access syringes for cheap, highly replicated measurements of soil respiration. At the end of the summer, Nick attended the Ecological Society of America meeting in Albuquerque where he was exposed to a wide array of carbon cycling talks that provide context for his work at Shale Hills. Nick is now a senior at Gannon University in northwestern PA where he is double-majoring in math and chemistry.

Name: Jose Morales Contribution to Project: Jose Morales (Univ of Puerto Rico, Hispanic American) measured metal contents of vegetation in leaves at Shale Hills.

Name: Shaquandra Wilson Contribution to Project: Shaquandra Wilson (Univ of W Alabama, African American) developed a new membrane for use in root boxes to image enzyme production around roots.

Name: Jose Valentina Prado Contribution to Project: (see Geophysics)

Name: Mitchell Johnson Contribution to Project: (see Geophysics)

Name: Tamika Shannon Contribution to Project: (see Geophysics)

Name: Maurice Dukes Contribution to Project: (see Geophysics)

Name: Nate Wysocki Contribution to Project: (see Geophysics)

Name: Maurice Dukes Contribution to Project: (see Geophysics)

Name: Nathan Barber

Name: Ahmad Yusof Contribution to Project: (see Geophysics)

Name: Erica Folio Contribution to Project: (see Geophysics)

Name: Dernier, Gabrielle, REU Hydrology. Rose Hulman College. Carried out hydraulic tests on 20 wells at Shale Hills and compiled a report showing the mean distribution of hydraulic conductivity with depth for the watershed. This critical to modeling study.

# **Outreach Activities:**

Outreach Activities for the Shale Hills CZO

1. STEM Field School: The State College Area School District,

SCASD, has formed a summer STEM Academy, a new initiative that uses field and experiential instructional techniques to engage our students in STEM areas. The goal of this Academy was to improve the middle school to high school transition by engaging students early in their high school career with academic experiences of the highest caliber. Incoming first year high school students along with pre-service and master teachers learned how to measure and monitor soil moisture, collect GPS data, install a weather station, and observe the hydrologic cycle through rain and groundwater

simulation systems. Data collected from school premises will be compared to data streaming from the catchment to develop STEM curriculum modules, thus engaging students in relevant,

project-based collaborative research.

2. PIHM Workshop: As part of our Critical Zone cross-site activities, the Shale Hills CZO helo a workshop August 2-4, 2010 titled: Multiscale Modeling Using the Penn State Integrated Hydrologic Modeling System (PIHM). PIHM is multi-process, multi-scale hydrologic modeling tool, where the physical processes are fully coupled using the semi-discrete finite volume method (http://www.pihm.psu.edu). This workshop provided hands-on experience in using PIHM for modeling watershed dynamics. Participants learned to use a customized GIS interface to PIHM (called PIHMgis) for i) automated ingestion of model parameters from national databases, ii)

conditional domain decomposition of the model domain, iii) performed multistate simulations and calibration and iv) visualized model results. A goal of the workshop was to stimulate crosssite

CZO modeling activities. The Departments of Anthropology and Civil and Environmental Engineering hosted Jaime J. Carrera-Hern?ndez, PhD, Professor of Applied Geosciences at Instituto Potosino de

Investigaci?n Cient?fica y Tecnol?gica (IPICyT) in San Luis Potos?, M?xico on August 4, 2010. Dr. Carrera's nterests are in the analysis of the impact that human activities have on the hydrological cycle and on the development of tools to analyze water management policies. He is also interested in the use of remotely sensed imagery for the development of physically-based, distributed hydrogeological modeling along with the use of Relational Databases for the efficient

development of these models, as exemplified in the Basin of Mexico Hydrogeological Database (BMHDB). Carrera has applied some of these tools to estimate potential aquifer recharge in the Basin of Mexico and to analyze the impact that urban growth has had on aquifer recharge.

3. CZO Field School: The Shale Hills CZO is a research and teaching platform open to the academic community that supports general environmental education especially as it relates to environmental information, modeling and earth systems infrastructure. The inaugural field school was offered May 31 - June 9 and attracted 16 participants

(undergraduate to post-doc) from 9 countries. During the two week school, the junior scientists experienced field techniques, instrumentation set-up and deployment, as well as modeling and

database utilization. The data and models generated at Shale Hills and the surrounding region are widely used in the classroom by CZO scientists and grad students as well as non-CZO researchers through the real-time capability. To date, several of the international participants have begun collaborative research projects initiated during the school.

CZO REU Summer Field School brought together 7 undergraduates from collaborating institutions. This summer, the CZO Field School adds a new dimension with two weeks of field work followed by one week of data analysis. Undergraduate participation includes two students from the University of Puerto Rico Mayaguez, one student from Alabama A&M Univ., one from University of Tennessee, one from Washington & Lee University, one from Juniata College and one from Penn State. Field work, organized by Dr. Tim White and Ashlee Dere (PhD Candidate), will complete research at the CZO Shale Transect sites in New York, Virginia, Tennessee and Alabama. Work will include sampling and digging soil pits on hillslopes, GPR transects, shale fracture density and tree throw measurements.

4. Shale Satellite Sites: Ashlee Dere (Geoscience, Penn State) and her advisors, Tim White and Sue Brantley, are working to understand the influence of climate on rates of shale weathering and rates of soil formation by investigating a series of soils on shale from Wales

to New York to Puerto Rico. Each of these 'satellite sites' is run with a partner institution and many of these are primarily

undergraduate-serving institutions. This work thus provides

opportunities for faculty and students at other institutions to

interact with scientists from Penn State. Students from each

satellite institution spent two weeks this past summer (2010) at

PSU learning about Shale Hills and the instrumentation used in

the catchment. Those students were taught how to set-up and collect data from a weather station as well as how to describe soils and collect samples. Ashlee and Nicole West (Geoscience, Penn State) have visited almost all the sites to date, working with students and faculty at the corresponding institutions.

5. This summer (2010), nine undergraduate students took a special class Geosc 497A: The Hydrogeophysics Field Experience with Dr. Kamini Singha from May 18 to June 5. Four students were from Penn State, and five came from Historically Black Universities: three students attended from Jackson State University in MS and one each from Fort Valley State University in GA and Elizabeth City State University in NC. These students combined field experimentation, data analysis, and numerical modeling with in-class instruction during the three-week program to develop hypotheses regarding the processes controlling solute transport. The Shale Hills Critical Zone Observatory was the 'home base' for this field camp. Environmental consultants, government employees, and small companies will be coming through the field camp to demonstrate hydrogeophysical field equipment and highlight jobs in environmental fields. Graduates from this program were be able to: (1) apply their knowledge of mathematics, science, and engineering to real field problems, (2) conduct experiments, and analyze and interpret data, (3) function in multidisciplinary teams, and (4) communicate their scientific data and analyses effectively.

The 3rd Annual Hydrogeophysics Field Camp hosted nine undergraduates this summer (2011). The 3rd annual hydrogeophysics field camp, offered by Dr. Kamini Singha, has come to completion. Nine undergraduate participants, from rising sophomores to rising seniors, spent three weeks collecting a wide range of data from the CZO and nearby Lake Perez. New data included images from the optical televiewer and gamma logs, GPR, pumping/slug tests and electrical resistivity measurements. Using COMSOL, a multiphysics software designed for analysis and visualization, the students built numerical models and learned the intricacies of field data interpretation.

6. Lehigh University Professor Frank Pazzaglia brought his class geology to visit the Shale Hills CZO on March 28th ,2009. Professor Daniel Bain also brought his Groundwater Geology Class Visit from the University of Pittsburgh on April 3rd, 2009. The field trips were lead by Kevin Dressler. The students received an overview of the

Critical Zone Observatory project and a field guide to accompany the day's activities. The group covered topics both in the water laboratory in the field. The following demonstrations were provided to the students in  $\sim$ 1 hr discussions:

1) O18 and H2 Isotopes using the Los Gatos Laser Isotope Analyzer (by George Holmes ?

MS Student in Engineering)

2)Geology of the region and Shale Hills specifically (by Timothy White ? Senior Research Associate)

3)Tour of Shale Hills Infrastructure including data retrieval, communications, wireless network and overall hydrological experimental design (by Kevin Dressler ? Research Associate Penn State Institutes of Energy and Environment)

4)Geophysical techniques and execution of a well log exercise (by Brad Kuntz ? MS Student in Geosciences)

5) Soil Pit and Soil Moisture experimental design and data collection techniques (by

Danielle Andrews ? PhD Student in Soil Sciences)

6) Geochemistry experimental design, current results and collection of Lysimeter and ISCO

Data (by Lixin Jin ? Postdoctoral Scholar in Geosciences)

7) Ecophysiology of Tree Species in the Shale Hills Catchment. Overview of speciation by landscape position and design of Sap Flow experiments (by Jane Wubbels ? Graduate student in Horticulture )

7. Penn State University Graduate Course in Surface Water Hydrology (CE561) ? April 21st ? April 30: As their final project, members of this graduate class were tasked with developing a method to develop water budgets. The Concept was as follows:

The Shale Hills Watershed has been a testbed for hydrologic studies since the 1970's. The State of Pennsylvania is interested in using Shale Hills as a prototype for developing water budgets across the state that will allow improved management of surface and groundwater supplies at other sites. That is they need a 'method' to develop water budgets that you would recommend. The 'water budget' generally be categorized as having 3 components:

1) data analysis (climate, soils, stream, vegetation, groundwater);

2) hydrologic conceptualization and characterization;

3) modeling-simulation-forecasting. In class we have discussed a range of issues and tools that can be applied to developing improved water budgets. The final product is a report that develops this prototype for the State.

Note that generally the State DEP is interested in 3 water issues: drought/flood/supply.

Kevin Dressler supervised 4 class periods regarding this project and led the group on a field trip to the site to illuminate both the current Critical Zone project and the previous studies done at the site in the 1970's.

8. International: Lin Ma (Penn State) measured U disequilibrium isotopes on Shale Hills samples at the Univ of Strasbourg with Francois Chabaux. Beth Herndon (Penn State) learned to run mesocosm experiments at Univ of Sheffield. Jennifer Williams and Ashlee Dere (Penn State) visited Plynlimon, Wales, a shale site that will become part of our satellite sites. S Riggins (Univ of CO, Boulder) visited the British Geological Survey. As a graduate student working on the Shale Hills Critical Zone Observatory I was able to travel to both Austria and Switzerland for a total of six weeks. While in both countries I was able to create a relationship with scientists working on projects similar to the Shale Hills CZO, and I was able to further my knowledge on many aspects of the critical zone.

George Holmes (MS CEE Dept. Penn State) participated in the International CZO Experience. The experience started in Vienna, Austria with two weeks visiting scientists at the IAEA (International Atomic Energy Agency). The first week was spent at a short course demonstrating how to operate a Los Gatos Research Liquid Water Stable Isotope Analyzer. The second week was spent working with Brent Newman on the GNIR (Global Network of Isotopes in Rivers) database. The database was made public this year and Brent is encouraging publishing papers using the data. He also spent time with Tomas Vitvar and Luis Araguas concerning the Shale Hills CZO. The next spent three weeks were in Zurich, Switzerland working with Manfred Staehli at WSL (Swiss Federal Institute for Forest, Snow and Landscape Research). Where he was able to talk with many scientists about the Shale Hills CZO, and I also was able to discuss related projects like the BigLink Damma Glacial Forefield and the Cottbus Watershed in Germany. At WSL he gave a presentation that outlined all three CZO projects with focus on Shale Hills. He was able to visit the Damma Glacier Forefield and see the set up of the instrumentation, and I was also part of a trip to the Rietholzbach research catchment. The final week was spent in Davos, Switzerland at the Goldschmidt Conference with many talks related to the Shale Hills CZO.

9. Craig Rasmussen (Arizona CZO) and Susan Brantley led six Webinars with three to 12 participants in each to discuss how to compare soil chemistry developed on granitic protolith as a function of climate variables. Rasmussen is developing this study into a publication to be submitted in 2009-2010 with co-authors from the CZEN and seminar group. Alex Blum (Boulder CZO) was involved. The approach being developed will be used for the shale satellite sites.

10. Sue Brantley teamed with international colleagues (Francois Chabaux, Yves Godderis, Mohammed Rafi Sayyed) to convene a special session entitled 'Rates and mechanisms on erosion and weathering processes: from experiments to models' at the Goldschmidt 2009 meeting in Davos, Switzerland. The session included 28 talks and 28 posters.

11. Heather Buss (USGS) and Lixin Jin have organized a special session entitled 'Water in the Critical Zone: Major Elements, Trace Elements, and Isotopes as Biogeochemical Tracers' for the AGU 2009 meeting in San Francisco, CA.

12. Data and technology are being shared with colleagues in research across Penn State colleges and universities associated with the project, as well as operational state and federal agencies (e.g. NOAA Mid-Atlantic River Forecast Center, Susquehanna River Basin Commission, USGS, USDA, EPA).

13. Collaboration is occurring with the Shaver's Creek Environmental Center to share ournew wireless communication system. The tower installed for this research project is now providing internet services to the entire Penn State Forest. The system is allowing the center to create a virtual classroom for K-12 education on their site, several hundred meters away from Shale Hills CZO.

14. Transect site CZO Partners: measurements, data management and integration

An all hands meeting was held for the transect participants last year and a 2nd meeting in Sept. of 2009. At the meeting all PIs for the transect

sites (see Fig 4) and for the main Penn State site were present to discuss plans for the first year including logistics, instrumentation, and site specific issues. The main result was a field plan for selecting sites for instrumentation and approval of both core activities and instrumentation to be placed at each site along transect.

It was determined that the transect site PIs would take and record data locally. Afterward a copy will be transferred to the core data set held at Penn State University and maintained.

From the meeting it was determined that the first year main focus should be development of the regional shale transect; and assessment of parent material heterogeneity as a control on soil type. Both are ongoing.

Shale transect development still remains in the early phase of site selection. Rich April, Colgate has visited numerous sites in the greater central New York region. His most recent foray led to the identification of the most suitable site visited thus far: close to Colgate with site access on Rose Hill equivalent shale, but with a surficial geology dominated by till. Timothy White will visit this site in the coming month or so.

Ryan Mathur, Juniata, has been very active over the past few summers in his pursuit of Marcellus Shale studies. Timothy White has visited a suitable site with Ryan, Lixin Jin, Jennifer Williams, and Ryan's undergraduate student, in May, which they subsequently cored and have been working on this summer. Another site may eventually be chosen for instrumentation to better mimic the slope and aspect of the Shale Hills drainage basin.

Teferi Tsegaye, Alabama A&M, has delegated the site selection activity to a geologist and soil scientist on his staff. Tim White has communicated with them several times. They have collected the requisite geologic and soil maps and are in the process of dentifying a site in northeastern Alabama.

Larry McKay is working on recruiting a PhD student, his desired strategy for moving his shale transect site forward. October will be the month in which his transect site will be selected. David Harbor, Washington and Lee, will work together with Timothy White this fall to locate a site. Timothy White has contacted two faculty members at University of Puerto Rico Mayaguez and a prospective graduate student there to determine interest/feasibility of their transect site. From previous visits and field work he has pinpointed a few sites to discuss with the group.

The assessment of Rose Hill Shale heterogeneity has progressed nicely as an offshoot of Poonam Giri's (recent BS Geosciences graduate, soon-to-be MS student, Geosciences) senior thesis overseen by Tim White. Her senior thesis involved a geochemical study of an excellent Rose Hill Shale outcrop near Allenport, PA. The total carbonate profile aided in delineation of four geochemical/lithologic facies in the formation and consequently guidance in sampling of soils developed on each facies. Soil cores were taken from ridgetop and slope locations in each of three facies. Distinct soil profiles were identified over each facies. This summer Poonam has sampled the fourth facies at Allenport. In addition, she sampled a bedrock section near Reedsville, PA, at the base of the Rose Hill Shale that overlaps with the Allenport section thus providing 100% coverage of the formation. She sampled ridgetop and slope soils at the Reedsville site. Furthermore, an ore bank and an undisturbed soil profile near Greenwood Furnace State Park were sampled. This focuses on determining whether recent pedogenesis on the ore bank can be differentiated from the nearby undisturbed soil, thus providing some insight into the rate of soil formation on the Rose Hill Shale. Analyses of the summer samples are ongoing.

#### Journal Publications

Anderson, S.A., R. C. Bales, and C. J. Duffy, "Critical Zone Observatories: Building a network to advance interdisciplinary study of Earth surface processes", Mineralogical Magazine, p. 7, vol. 72, (2008). Published,

Brantley, S.L., Goldhaber, M.B., and Ragnarsdottir, V, "Crossing disciplines and scales to understand the Critical Zone", Elements, p. 307, vol. 3, (2007). Published,

Qu Y., C. J. Duffy, "A semi-discrete finite volume formulation for multiprocess watershed simulation", Water Resour. Res., p., vol. 43, (2007). Published, doi:10.1029/2006WR005752

Lin, H.S., and X. Zhou, "Evidence of Subsurface Preferential Flow Using Soil Hydrologic Monitoring in the Shale Hills Catchment.", European J. of Soil Science, p. 34, vol. 59, (2008). Published,

Brantley, SL, "Geology - Understanding soil time", SCIENCE, p. 1454, vol. 321, (2008). Published, 10.1126/science.116113

Brantley, S.L. and White, A.F., "Approaches to Modeling Weathered Regolith", Reviews in Mineralogy and Geochemistry, p. 435, vol. 70, (2009). Published,

Kumar, M., G. Bhatt, and C.J. Duffy, "An efficient domain decomposition framework for accurate representation of geodata in distributed hydrologic models", Geographical Information Science, p., vol., (2009). Accepted,

Lin, H.S., and X. Zhou, "Evidence of Subsurface Preferential Flow Using Soil Hydrologic Monitoring in the Shale Hills Catchment", European J. of Soil Science, p. 34, vol. 59, (2008). Published,

Lin, H.S., and X. Zhou, "Comments on Energy-based Pedogenic Models by Field and Minasny (2008) and Rasmussen (2008)", Soil Science Society of America Journal, p., vol., (2009). Accepted,

Lin, H.S., and X. Zhou, "Earths Critical Zone and Hydropedology: Concepts, Characteristics, and Advances", Hydrology and Earth System Science Discussions, p. 3417, vol. 6, (2009). Published,

Lin, H.S., J. Zhang, D. Andrews, K. Takagi, and J. Doolittle, "Hydropedologic investigations in the Shale Hills catchment", GEOCHIMICA ET COSMOCHIMICA ACTA, p. A552, vol. 72, (2008). Published,

Jin, L.;Ravella, R.;Ketchum, B.;Bierman, P.R.;Heaney, P.;White, T.S.;Brantley, S.L.;, "Mineral weathering and elemental transport during hillslope evolution at the Susquehanna/Shale Hills Critical Zone Observatory", Geochimica et Cosmochimica Acta, p. 3669-3691, vol. 74, (2010). Published,

Ma, Lin; Chabaux, Francios; Pelt, Eric; Blaes, Estelle; Jin, Lixin; Brantley, Susan, "Regolith Production Rates Calculated with Uranium-series Isotopes at the Susquehanna/Shale Hills Critical Zone Observatory", Earth and Planetary Science Letters, p., vol., (2010). Accepted,

Kumar, M.;;Bhatt, G.;;Duffy, C.J.;, "An object-oriented shared data model for GIS and distributed hydrologic models", International Journal of Geographical Information Science, p. 1061-1079, vol. 24, (2010). Published,

Lin, H.S.;, "Comments on Energy-based Pedogenic Models by Field and Minasny (2008) and Rasmussen (2008)", Soil Science Society of America Journal, p. 337-339, vol. 74, (2010). Published,

Lin, H.S.;, "Earth's Critical Zone and hydropedology: Concepts, characteristics, and advances", Hydrology and Earth System Science, p. 25-45, vol. 14, (2010). Published,

Lin, H.S.;, "Linking principles of soil formation and flow regimes", Journal of Hydrology, p., vol., (2010). Published,

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## Web/Internet Site

#### URL(s):

http://www.czo.psu.edu/

#### **Description:**

Our new Shale Hills-Susquehanna Critical Zone Observatory website was implemented recently. We are still working on content but the site is up and running and fully linked to the National CZO page. The website will host all Shale Hills data and provides an overview of CZO science activities.

## **Other Specific Products**

Product Type: Software (or netware)

#### **Product Description:**

We are developing community models for integrated hydrologic modeling a data handling for modeling. These are known as the Penn State Integrated Hydrologic Model PIHM and PIHM\_GIS

#### **Sharing Information:**

The software is available as open source projects Source Forge

http://sourceforge.net/projects/pihmmodel/

http://sourceforge.net/projects/pihmgis/

#### **Product Type:**

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Software (or netware)
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#### **Product Description:**

During 2009 the Hydrology group completed a multi-platform watershed modeling software platform called PIHM\_GIS. The software allows the user to build a distributed watershed model from basic GIS layers for topography, soils, vegetation, geology, and climate inputs.

#### **Sharing Information:**

The Penn State modeling team has also posted its software PIHM and PIHM\_GIS, to the CSDMS website: http://csdms.colorado.edu/wiki/Models

#### **Product Type:**

Data or databases

#### **Product Description:**

RTH\_NET has been completely upgraded by Kelly Cherrey to provide real time hydrologic and weather data at Shale Hills for CZO scientists and is being utilized by the CUAHSI-WATERS community.

#### Sharing Information:

http://www.rthnet.psu.edu/

#### **Product Type:**

Data or databases

#### **Product Description:**

SAP\_NET is a new network established this year by Dave Eisenstat and a team of scientists from Oregon State University with support for networking and power by Kelly Cherrey to measure sapflow (transpiration) along a tree transect at Shale Hills.

eKo\_NET is a new network established this year by Colin Duffy and a team of Penn State researchers to measure groundwater level/temperature/electrical conductance, soil moisture/tension/temperature/electrical conductance, and snow depth. The Crossbow adaptive Sensor Net technology is used for this array.

LPM is a our new disdrometer or Laser Precipitation Monitor.

ISO\_NET is a network of stable isotope monitoring of precipitation events (up to 8, 4hourly integrated water samples) automatically collected. An ISCO auto-sampler for streamflow at the outlet collected daily, 2 ISCO auto-samplers for shallow groundwater collected daily, 6 soil moisture lysimeter sites sampled on a weekly basis, and 14 new observations wells drilled into the weathered shale sampled on a weekly basis.

#### **Sharing Information:**

RTH\_NET, SAP\_NET, and LPM are in ?flat-file? format while eKo\_net is a SGQL database. Basic meta-data and permissions is also provided. http://cataract01.cee.psu.edu/czo/ The ?flat file? site is meant to be a simple service for all users to access raw data from Shale eKo.net data is in a SQL database format http://cataract01.cee.psu.edu/czo/eko/

#### **Product Type:**

#### DVD

## **Product Description:**

A set of 3 DVD for The 1st International Conference on Hydropedology held July 28-31, at Penn State Univ. in University Park, PA.

# Sharing Information:

Available from Prof Henry Lin

#### **Product Type:**

#### Data or databases

#### **Product Description:**

A relational database, CZchemDB, which contains soil data collected at the SSHCZO as well as additional soil data, legacy and other CZO's. **Sharing Information:** 

The database is available on the SSHCZO website. We currently include 21 investigators from 11 institutions representing 46 different field locations, one of which is international (Plynlimon, Wales, UK). Two CZO's, Luquillo and Jemez River Basin - Santa Catalina Mountains CZO, have contributed data. Total contributions thus far represent 255 cores collected, 2237 samples analyzed which produced 33,142 data values. We have 10 additional template contributions to add to the database but are waiting on modifications for EarthChem compatibility.

#### Contributions

#### **Contributions within Discipline:**

The Shale Hills CZO provides a multi-disciplinary framework for the study of regolith development and function in the critical zone. The Geochemistry group has developed a model for shale weathering at SSHO. We have assessed the geochemical reactions that are occurring and we have used uranium disequilibrium isotopes to estimate the residence time of regolith. We have discovered that Mn atmospheric deposition to SSHO is significant and that this deposition may be common in industrialized countries. Ecology team has developed a model code to predict a spatial map of LAI. We selected regions of low (red), intermediate (orange) and high (yellow) LAI to study the inter- and intra-specific differences in maximum light use efficiency (REU Project: John) and leaf structure (REU Project: Shelly) of plants living in different light environments. We are in the

process of conducting a vegetation survey of the watershed to coincide with a LiDAR flight of the CZO which is scheduled to take place in mid to late July. We have selected 40 plots, of 15m radius each, in deciduous, conifer, and mixed forest areas, as well as wetland meadow and grassland sites. In each forest plot we counted the number of trees and measured tree height and diameter at breast height (DBH). For the wetland meadow and grassland sites we identified the predominant plant species. Within one week of the LiDAR flight (tentatively scheduled for 7/14/2010 and 7/15/2010), we will measure LAI and canopy closure at each plot and vegetation height at the grassland and meadow sites. The data we collect during the vegetation survey will allow us to ground truth the land cover

and LAI data collected during the LiDAR flight. From our sapflow study characteristics of stem hydraulic architecture in some genera (Pinus) was linked to soil moisture distribution in central Pennsylvania, but not in other genera (Carya and Quercus)

Hydrology Land Surface Modeling Team: The CZO data (time series, geospatial, open source modeling) are being provided to the community through SourceForge http://sourceforge.net/projects/pihmmodel/ and

http://sourceforge.net/projects/pihmgis/. During 2009 the Hydrology group completed a multi-platform watershed modeling software platform called PIHM\_GIS. The software allows the user to build a distributed watershed model from basic GIS layers for topography, soils, vegetation, geology, and climate inputs. Physically-based distributed models seek to simulate state variables in space and time while using heterogeneous input data for climate, land use, topography and hydrogeology. In the process of incorporating several physical data layers in a hydrologic model requires intensive effort in data gathering, development as well as topology definitions. Traditionally Geographic Information System (GIS) has been used for data management, data analysis and visualization. Joint use and development of sophisticated numerical models and commercial GIS systems poses challenges that result from proprietary data structures, platform dependence, inflexibility in their data models and non-dynamic data-interaction with pluggable software components. Alternatively this tool presents an open-source, platform independent, extensible and 'tightly-coupled' integrated GIS interface to Penn State Integrated Hydrologic Model (PIHM) called PIHMgis. The tight coupling between the GIS and the model is achieved by developing the PIHMgis data-model to promote minimum data redundancy and optimal retrievability. Minimum data redundancy and

optimal retrievability are facilitated through carefully designed data-model classes, relationships and integrity constraints. Two papers have been published (Kumar, Bhatt, and Duffy, 2009a,b) and a monograph is being written to describe the software for classroom, research, and operational watershed modeling. The first generation of PIHM and PIHM\_GIS focus on distributed hydrologic modeling. However, in years 3 and 4 solute, and sediment transport will be added. By year 5 we hope to have the geochemical model implemented. The figure below shows how PIHM\_GIS uses hypsometry to constrain the

unstructured numerical grid along lines of constant elevation for the Little Juniata watershed, and an example for the PIHM\_GIS interface.

An important flux that is not included in most other models is the negative recharge or upward flux from the water table. It appears to be at least 5% on an annual basis. This flux is basically the capillary rise from the water table that occurs as the soil moisture dries due to plant water usage. Yuning Shi working with Ken Davis has implemented a new land surface scheme in PIHM and at Shale Hills is comparing the model latent heat flux (net evapotranspiration or ET) to the eddy flux measurements for latent heat and sensible heat

flux. Yuning is finding that groundwater may have a significant affect on the land surface energy fluxes, especially for shallow water table settings. This is important since most land surface models do not include this effect.

Geomorphology Team have discovered that the valley bottom regolith/alluvium represents a polygenetic deposit that appears to contain relict post-glacial-maximum material. 10Be concentrations appear to increase downslope, consistent with soil transport. Lidar-imaged subtle pits and mounds are prevalent and exhibit an approximate spacing of 5 m and are interpreted to be a result of tree-throw. Using meteoric 10Be measurements at SSHO, we have estimated that the residence time of soils on the southern ridge top is ~10-11 ky, while soils further downslope have greater inventories consistent with slow rates of downslope creep. Sediment cores collected from the valley fill at SSHO suggest the presence of buried hillslope colluvium along the southern side of the valley floor. The combination of stratigraphic observations and 10Be residences suggest that regolith presently mantling ridgetops has formed over at least the Holocene, whereas colluvium and soils toward the valley floor are inferred to be older, perhaps even relict from glacial times in the Late Pleistocene.

Hydrogeophysics Team has carried out preliminary modeling of the soil cores at Shale Hills with simple dual-domain mass transfer models indicate that the fraction of immobile porosity in the aquifer is larger in the shale than in the soil derived from that shale, which has important implications to estimating age of water. Interestingly, it appears mass transfer rates only vary slightly throughout the geologic section, indicating that the diffusive length scale does not vary significantly. These results are only preliminary, however, and will be compared to results based on CTRW modeling.

Hydropedology Team: The time-lapse GPR radargrams revealed the general infiltration wetting front and preferential flow pattern that were significantly different between different types of soils and hillslopes within the CZO, which were then confirmed by simulation modeling results. Time-lapsed GPR is proved as a useful methodology for improved understanding of hydrologic connectivity in the subsurface, which facilitates the formulation and test of different conceptualizations of subsurface network modeling.

We have found that preferential flow occurs across the Shale Hills CZO. Ridge and hillslope sites are controlled by initial soil moisture (preferential flow occurs more often when the soil is dry) and during the late summer. Swale and valley sites, while more likely when the soil is dry, are more sensitive to the internal storm precipitation intensity dynamics. Preferential flow occurs at these sites when storms are long, with an extended prewetting, followed by a large spike in precipitation intensity. These findings will help in determining the locations and timing of preferential flow in steep, forested environments.

An important goal of watershed modeling effort at Shale Hills has been to evaluate all terms in the water budget, including the separation of transpiration by plants and evaporation, estimation of recharge to groundwater and the fraction of streamflow due to surface runoff and groundwater baseflow. The figure in FIndings illustrates the calculated water budget from PIHM using a simulation for 2009.

Shale Transect Team: Initial results show soil depth increases as a function of temperature, with shallow (~30 cm) profiles in Wales and Pennsylvania varying up to 630 cm deep in Puerto Rico. Depletion profiles of Na, a proxy for feldspar dissolution, are less than 20 % depleted at the surface in Wales and Pennsylvania, 50-60% depleted in Virginia and Tennessee, and 100% depleted at the surface in Puerto Rico. Using estimated soil residence times, apparent activation energies for Na depletion were calculated using different assumptions to range from 15-19 kcal mol-1, values that are slightly higher than those reported for Na plagioclase dissolution in the laboratory.

#### **Contributions to Other Disciplines:**

Collaboration with the Chesapeake Bay Research Consortium has fostered relationships with the ocean community. The Shale Hills CZO site was a recommended site in the Mid-Atlantic NEON RFI. The Chesapeake Community Modeling Program is also an important partner for our modeling effort and PI Duffy serves on the Steering Committee.

The Community Surface Dynamics Modeling System (CSDMS) deals with the ever-changing, dynamic interface between lithosphere, hydrosphere, cryosphere, and atmosphere. CSDMS is a diverse community of experts promoting the modeling of earth surface processes by developing, supporting, and disseminating integrated software modules that predict the erosion, transport, and deposition of sediment and solutes in landscapes and their sedimentary basins. CSDMS produces protocols for community-generated, continuously evolving, open

software, distributes software tools and models, and provides cyber-infrastructure to promote the quantitative modeling of earth surface processes. The Penn State modeling team has also posted its software PIHM and PIHM\_GIS, to the CSDMS website: http://csdms.colorado.edu/wiki/Models

We are developing a close relationship with the Delaware CZO team as they have adopted our model (PIHM) and we are actively sharing ideas and strategies that will move the watershed modeling science forward and more closely couple models to CZO data.

#### **Contributions to Human Resource Development:**

Cohorts in education levels of undergraduate, graduate, and post-doc are being trained in field, laboratory and modeling studies regarding hydrologic science. The CZO has engaged a variety of institutions in this regard including universities and undergraduate colleges directly associated with the project. The CZO has also provided many site visits to investigators from universities, the interested public, the National Science Foundation, the National Resource

Conservation Service (USDA), US Geological Survey, and various state agencies and non-profit groups.

Chris Duffy is interacting with the State College Area School District (SCASD), regional STEM Professional Development Center, coordinating filed trips for students (18-19 Aug) to the Shale Hills CZO. Colin Duffy is constructing a weather station for the high school and he and Chris Graham are providing field seminars on the use of environmental sensors as part of the STEM program.

An REU summer field school was conducted from June 5 ? June 25 in which seven undergraduates, representing Penn State, Juniata College, Washington and Lee University, University of Tennessee, Alabama A&M University and the University of Puerto Rico ? Mayaguez, participated in two weeks of field work followed by one week of laboratory work and data processing.

#### **Contributions to Resources for Research and Education:**

The Shale Hills CZO is a research and teaching platform open to the academic community that supports general environmental education especially as it relates to environmental information, modeling and earth systems infrastructure. The data and models generated at Shale Hills and the surrounding region are widely used in the classroom by CZO scientists and grad students as well as non-CZO researchers through the real-time capability.

A number of CZO investigators participated in CZO Summer School led by Tim White May 31-June 9. The Field school participants carried out a full range of CZO activities which is currently being written up by Tim.

#### **Contributions Beyond Science and Engineering:**

The Shale Hills-Susquehanna CZO is developing a new generation of models and experimental observations that will eventually be implemented in operational models to forecast drought, flood, water supply and water quality for a fully coupled approach to surface and groundwater systems. The contribution of our sediment and geochemical-

weathering research is fundamental to predicting how to manage land and water resources within the Chesapeake bay and watershed, as well as similar locations around the world.

#### **Conference Proceedings**

#### **Special Requirements**

Special reporting requirements: None Change in Objectives or Scope: None Animal, Human Subjects, Biohazards: None

#### Categories for which nothing is reported:

Any Conference





**Observatory Setting** The Susquehanna-Shale Hills Critical Zone Observatory (SSHO CZO) lies within the Valley and Ridge Physiographic Province of the central Appalachian Mountains in Huntingdon County, Pennsylvania (40°39'52. 39"N 77°54'24.23"W). It is a first order basin characterized by relatively steep slopes (25-35%) and narrow ridges. The stream is a tributary of Shavers Creek (185 km<sup>2</sup>) that eventually discharges into the Juniata River, a tributary of the Susquehanna River Basin. The SSHO basin is oriented in an east-west direction and the major side slopes have almost true north and south facing aspects. Elevation ranges from 256 meters at the outlet to 310 meters at the highest point in the watershed. The relatively uniform side slopes are periodically interrupted by seven distinct topographic depressions (swales).

The Shale Hills Critical Zone Observatory

Figure 1. The Shale Hills 8 hectare Watershed illustrating regolith development on steeply dipping shale bedrock. Image from NSF NCALM lidar survey.

**Climate:** SSHO has a humid continental climate. Temperatures average  $9.5^{\circ}$ C with large seasonal differences: January temperature is  $-5.4^{\circ}$ C, July is 19.0°C. The highest temperature recorded is 33.5°C (April 27, 2009) lowest  $-24.8^{\circ}$ C (January 17, 2009). Annual average relative humidity is 70.2%. Atmospheric deposition in PA is still characterized by acidic (pH~4) precipitation. 2009 water balance: Precipitation 1028 mm, Evapotranspiration 59.4 mm, Recharge 31.9 mm, Runoff 509 mm, with a runoff ratio of 49.6% and interception of 28.4 mm.

*Soils:* Shallow to moderately deep, gently dipping to steep, well drained residual shale soils exist on the ridge tops, while along slopes and in the valley bottom soils

have formed on a colluvial and alluvial mantle of shale chips. Typical surface soil textures are silt loam, with the percentage of channery shale increasing with depth. Effective rooting depth (depth to bedrock) ranges from 15 cm on ridge tops to 165 cm in some areas on the slopes. Soil structure is moderately developed throughout the basin. Soils are typically saturated along the stream and exhibit redoximorphic features as a result of seasonal soil saturation. A 3 - 5 cm organic layer that contains decaying leaf litter overlies all soils in the watershed. Figure 2 illustrates the bare-earth Digital Elevation Model from the NCALM Lidar survey.



*Ecosystem:* The SSHO forest ecosystem is dominated by oak (Quercus), hickory (Carya) and pine (Pinus) species. Hemlock (Tsuga canadensis), red maple (Acer rubrum), white oak (Quercus alba) and white pine (Pinus strobus) line the deep, moist soils of the stream banks, while on the drier, shallower north and southfacing slopes, red oak (Quercus rubra), chestnut oak (Quercus prinus), pignut hickory (Carva glabra) and mockernut hickory (Carya tomentosa) are dominant, with Virginia pine (*Pinus virginiana*) only appearing on the north-facing ridge tops. Understory woody species include plants in the Ericaceae family (including Vaccinium spp.), service berry (Amelanchier spp.), hawthorn (Crataegus spp.), raspberry/blackberry (Rubus spp.), sugar maple (*Acer saccharum*) saplings and witch hazel (Hamamelis virginiana).

*Land Use:* Historically, the region was logged for charcoal to support a 19th and 20th century iron industry. Today, SSHO is a relatively pristine forest and good wildlife habitat with little human impact. The basin is primarily available for recreation, education and research. The Penn State forest, of which the basin is a part, is managed for timber with set-asides for research.

There are a number of active PSU research projects within the Penn State Forest.

**Current Research** Our interdisciplinary team works collaboratively at the Susquehanna-Shale Hills CZO to advance methods for characterizing regolith, to provide a theoretical basis for predicting the distribution, properties and evolution of regolith, and to theoretically and experimentally study the impacts of regolith on fluid pathways, flow rates, solute residence times, and response to climate change.

*Climate and Hydrometeorology:* This research focuses on investigation of explicit coupling and feedback for subsurface-landsurface-atmosphere interaction using fully coupled models over meteorologic and climatic time scales. A long history of hydrologic research at the site has stimulated reanalysis research to reprocess and assimilate observational data collected during experimental campaigns conducted over a 40+ year span, into an integrated watershed reanalysis product.

*Weathering:* Weathering fronts, mineral transformation reactions, and long-term physical-chemical weathering fluxes are elucidating the important physical, biological and hydrogeochemical processes that operate within this shale dominated catchment.

*Hydropedology:* Using use a suite of non-invasive imaging techniques (X-ray tomography, ground penetrating radar, and electromagnetic induction) in combination with real-time soil monitoring we are able to detect and model subsurface flow networks and their dynamics.



Figure 2. Shale Hills CZO sampling sites.

*Ecological Research*: In this study patterns of tree water use and water availability across the watershed influence trees at the physiological, community and evolutionary time scales; and how a temperate forest affects water, energy and weathering rates.

*Stable Isotope Hydrology:* The stable isotope network takes a comprehensive approach to determine space-time signatures in all stores of the watershed and to elucidate fluid pathways and time scales from source to sink.

*Watershed Modeling:* The stable isotope network is also being used to evaluate the "age" and residence times of stable isotopes at Shale Hills as part of an integrated hydrodynamic model for water, solutes and sediments. The Penn State Integrated Hydrologic Model for water and energy budgets has been implemented at Shale Hills and the sediment transport and solute transport are in final stages of completion. A landscape evolution model is planned for implementation in year 5.

*Soil Biogeochemistry:* This research focuses on quantification of soil respiration rates and investigation of how water movement/storage and soil texture lead to variability in soil-atmosphere CO2 exchange. Ecological Research: In this reseach patterns of tree water use and water availability across the watershed influence trees at the physiological, community and evolutionary time scales; and how a temperate forest affects water, energy and weathering rates.

*Geomorphology:* Sediment erosion, transport, and deposition are being incorporated into the Penn State Integrated Hydrologic Model. Efforts include development of a hillslope sediment flux model that incorporates tree-throw and freeze-thaw creep.

*Hydrogeophysics:* In field-scale and lab-scale tracer tests both soils and shale material show preferential pathways that may be indicative of dual-domain solute transport behavior.

The Observation Network The Shale Hills watershed has a comprehensive base of instrumentation for physical, chemical and biological characterization of stable isotopes and geochemical water, energy, conditions. This includes a dense network of soil moisture observations at multiple depths (120), a shallow observation well network (25 wells), soil lysimeters at multiple depths (+80), a research weather station including eddy flux measurements for latent and sensible heat flux, CO2, and water vapor, radiation, barometric pressure, temperature, relative humidity, wind speed/direction, snow depth sensors, leaf wetness sensors, a load cell precipitation gauge. A laser precipitation monitor (LPM: rain, sleet, hail, snow, etc.) was installed in 2008, as were automated water samplers (daily) for precipitation, groundwater, and stream water

for chemistry and stable isotopes with weekly sampling of lysimeters. Arrays of sapflow measurements are carried out each year as a function of tree species (25 species in the watershed). Geochemical measurements for solution chemistry, isotopes, electrical conductance and potential are carried out weekly on the soil lysimeter profiles, stream, groundwater and precipitation. Real time observations for soil moisture, groundwater level, streamflow, and weather are at 10 minute intervals. A multi-hop wireless sensor network (eKo-Array) has been deployed and is gradually replacing the real-time soil moisture, groundwater level, ground temperature, and electrical conductance at 25 observation well locations.

The Shale Hills watershed and the larger Shaver Creek watershed has had 3 airborne lidar flights to date with the most recent flights at 1 m resolution to evaluate micro-topography and tree species identification. Bedrock elevation surveys have been carried out with ground-penetrating radar and verified with rotary airdrilling and hand augering. Ground-based lidar and totalstation surveys have been carried out for all instrument elevations and tree surveys (trees > 8 inches) for species, biomass, crown height have been completed. Leaf Area Index (LAI), greenness index, microbial composition, distribution and CO2 flux are regularly carried out. A complete suite of borehole logging was done at 3 locations to 17m. These include: (1) spectral gamma; (2) caliper- borehole diameter log to locate broken and fractured zone; (3) fluid resistivity- total dissolved solids in the water column (4) fluid temperature; (5) heat-pulse flowmeter- rate and direction of vertical flow in a borehole; and (6) optical tele-viewer for continuous, oriented, true-color  $360^{\circ}$  image of the borehole wall. Additionally hydraulic and tracer tests were done to estimate the effective hydraulic properties in all wells in the field.

**CZO Site Infrastructure:** This section describes power, communications and sensor array infrastructure at Shale Hills.

*Power:* A 15 amp, 120 volt service was completed in July 2008, including lightning and surge protection. Power was tied off at a newly constructed small communications building located at the entrance to the watershed. Extensions of that tie-off have been run to the eddy flux and wireless communication tower, the stream gauge at the Shale Hills outlet, and the sap flow experiment. Other outlets have been requested and were installed in 2009-10 and continue to he installed.

**Backhaul Communications & Power:** A 30m tower was installed in 2008 to provide backhaul link from the watershed to the university for real-time observations. A 5.7 GHz Motorola multipoint access wireless system

was installed by a local IP to serves Shale Hills and the larger Penn State Forest with internet communications. The tower, located 300m from the power lines and communication building, is also our main met-research site. Ethernet and power was installed in 2008-09. In Dec. 2010 the Ethernet was replaced with a 3-mode fiber optic cable in response to several failures of the buried Ethernet due to lightning. Financial resources for the tower came from the 3 Penn State colleges that are involved in the CZO. The system also supports the Shaver's Creek Environmental Center for which they have their own access point where they will create a virtual classroom for K-12 education onsite at the center.

*Wired & Wireless CSI Network:* From 2005-2009 the main observing network was based on Campbell Scientific data loggers that are maintained manually except for the RTH\_NET sites which use a Free Wave 900 MHz radio. The 900MHz antennas and radios connects the RTH\_NET arrays to the backbone. These sites include a below-canopy met station, groundwater levels, soil moisture profiles and stream stage observations. Although this network should be real-time in 2011. A 3<sup>rd</sup> CSI manual network has recently been implemented for redox and dissolved oxygen measurements and this CSI system is expected to be real-time in 2011.

Adaptive Sensor Network: A 25 node adaptive sensor network is presently being tested at Shale Hills for all sensors currently in use. Each node in eKo.NET can moisture. monitor: soil matric potential. soil temperature, soil electrical conductance, groundwater level, groundwater temperature, groundwater electrical conductance, and snow depth with an acoustic range sensor. eKo.NET provides communication capability with each node, and the ability to examine our sensors from any browser. The system is intended to provide a simple to operate, low-power, real-time network with each node and in fact each sensor accessible over the web. The nodes or "motes" are based on Crossbow data acquisition and radio technology (http://memsic.com/). Wireless ad-hoc networks are packet based, multi-hop, radio networks consisting of mobile wireless nodes communicating over a shared wireless channel.

Contacts: Christopher Duffy <u>cxd11@psu.edu</u> Principal Investigator Sue Brantley <u>brantley@geosc.psu.edu</u> Co-Principal Investigator Timothy White <u>tsw113@psu.edu</u> National CZO Coordinator Website: www.czo.psu.edu/shale hills.html

# 2011 Annual Reporting for SSHCZO

# Discipline: Geomorphology Team

Rudy Slingerland, Eric Kirby, Nicole West

**Research Progress:** 

Overall, our efforts to understanding the geological evolution of regolith in the SSHO advanced significantly during the past year. Progress occurred on two primary fronts: 1) characterization of the timescales of regolith formation, rates of downslope transport, and processes controlling long-term landscape evolution, and 2) development and implementation of a numerical model encoding these processes

From an observational standpoint, data collection focused on:

- 57 bulk soil samples were collected from the north and south planar hillslopes and were analyzed for meteoric <sup>10</sup>Be concentrations at Lawrence Livermore National Laboratory (LLNL). This effort was completed to determine soil residence times, erosion rates, and establish a measure of variance for meteoric <sup>10</sup>Be. Meteoric <sup>10</sup>Be inventories from the two planar hillslopes will be used to determine whether an aspect control exists for erosion rates at SSHO.
- 2. 15 sediment cores collected across the valley fill near the mouth of the SSHO watershed were logged in order to characterize the nature of the shallow subsurface at SSHO.
- 3. 12 bulk soil samples from 6 partner watersheds will be processed analyzed in Fall of 2011 for meteoric <sup>10</sup>Be concentrations. Data from these analyses will provide estimates of soil residence times, erosion rates and downslope soil flux rates along the Rose Hill climate transect. Ridgetop and mid-slope samples will be analyzed from the New York, Marcellus, Virginia, Tennessee, Alabama, and Puerto Rico partner sites.
- 4. 2 charcoal samples collected from the soil core in the valley fill were sent for <sup>14</sup>C analysis and age dating. These data will provide an exact chronometer of the shallow subsurface.

Model development focused on:

1. Transforming the hydrologic model PIHM into a true morphodynamic landscape evolution model. In PIHM the various governing equations are transformed into ordinary differential equations through a finite differencing of selected terms. We have tested various control volume solution methods to obtain mass-conserving forms and arrived at our best approximation. Various solutions have been obtained for a 2D model of landscape evolution that includes tree-throw and weathering of bedrock as a function of regolith thickness.

# Significant Findings:

Using meteoric <sup>10</sup>Be measurements at SSHO, we have estimated that the residence time of soils on the southern ridge top is ~10-11 ky, while soils further downslope have greater inventories consistent with slow rates of downslope creep. Sediment cores collected from the valley fill at SSHO suggest the presence of buried hillslope colluvium along the southern side of the valley floor. The combination of stratigraphic observations and <sup>10</sup>Be residences suggest that regolith presently mantling ridgetops has formed over at least the Holocene, whereas colluvium and soils toward the valley floor are inferred to be older, perhaps even relict from glacial times in the Late Pleistocene.

Training/Development:

Nicole West, a PhD student working with the Geomorphology team, continued her research and training in landscape analysis, cosmogenic isotopes, and geochemistry.

# Outreach Activities (broadening participation of under-represented / under-served groups):

In May of 2011, Nicole West of the Geomorphology team assisted with the Hydrogeophysics Field Experience, led by Kamini Singha. Nicole West led a ground penetrating radar (GPR) demonstration and assisted in subsequent radar data work up as part of the camp. The Hydrogeophysics Field Experience included students from a number of colleges and universities that serve under-represented groups such as Fort Valley State University and Jackson State University.

# Conference Abstracts:

West, N., Kirby, E., Bierman, P., Slingerland, R., Ma, L., Jin, L., Brantley, S., 2011, Toward an understanding of landscape change in the Susquehanna Shale Hills Critical Zone Observatory, Critical Zone Observatory All Hands Meeting, Oracle, AZ, May, 2011.

West, N., Kirby, E., Bierman, P., Rood, D., 2011, Preliminary estimates of regolith generation and mobility in the Susquehanna Shale Hills Critical Zone Observatory, Pennsylvania, using meteoric <sup>10</sup>Be. International Symposium on the Geochemistry of the Earth's Surface, Boulder, CO, June, 2011.

West, N., Kirby, E., Bierman, P., Using meteoric <sup>10</sup>Be to estimate soil residence times and erosion rates at the Susquehanna Shale Hills Critical Zone Observatory, PA, European Science Foundation Conference on Cosmogenic Nuclides, Obergurgl, Austria, August, 2011.

## **Publications:**

West, N., Kirby, E., Bierman, P., Rood, D., 2011, Preliminary estimates of regolith generation and mobility in the Susquehanna Shale Hills Critical Zone Observatory, Pennsylvania, using meteoric <sup>10</sup>Be. Applied Geochemistry, Volume 26, Supplement 1, Pages S146-S148.

West, N., Kirby, E., Bierman, P., plus others?, Timescales of soil residence in the Susquehanna Shale Hills Critical Zone Observatory: constraints from soil stratigraphy and meteoric <sup>10</sup>Be, Earth Surface Processes and Landforms, in prep.

# 2. Geomorphology

The geomorphology working group is examining three fundamental questions at the Shale Hills CZO and in the surrounding region (Fig. 1):

- 1) What are the primary processes and rate laws that set the shape of the landscape and the thickness & properties of the Critical Zone?
- 2) What are the dynamics of feedbacks between hydrology, biology, weathering, and physical erosion?
- 3) How have the processes and products of the SHO regolith mill changed in response to past climatic, base level, and land-use perturbations?



Figure 1. Perspective view of a shaded-relief image generated from high-resolution LiDAR topographic data. The relict braided stream in the foreground with alluvial terraces is interpreted to have formed during earlier time periods of increased sediment yield associated with active hillslope transport under periglacial conditions. Adjustments in this trunk stream are suspected to have changed base level for the SHO watershed.

# Question 1: Primary processes and rate laws

We are approaching the question of what controls soil erosion and downslope transport from both a theoretical and empirical perspective. Ongoing theoretical efforts include development of a hillslope sediment flux model that incorporates treethrow and freeze-thaw creep. Model development also includes improvement of overland and channel flow formulations to simulate unsteady non-uniform flows. Validation experiments will employ LiDAR and regolith thickness data being collected onsite.

We are also conducting field-based experiments designed to quantify the rate of regolith formation, the role of tree-throw in the downslope transport of material, and the residence time of material in regolith. These experiments combine two types of data: 1) high-resolution topographic surveys obtained by terrestrial laser scanning (Fig. 2a) to characterize the spatial density of pit-and-mound topography associated with tree-throw; and 2) field calibration of the material transported per event (Fig. 2b). In addition, we are using the spatial distribution of meteoric <sup>10</sup>Be along hillslope transects (Fig. 3) to estimate the residence time of regolith materials near the surface and the rate at which these move downslope.



Figure 2a. Close-up perspective view of a shaded relief image of the SHO watershed, with an overlay generated from terrestrial laser scanning of topography. Note the sub-meter scale roughness associated with pit-andmound topography interpreted to represent relict tree-throw events.

Figure 2b: Geometric properties of pitand-mound topography.

# Question 2: Feedbacks in the landscape/regolith system

Transport laws relating sediment transport, erosion, and deposition are being incorporated into the Penn State Integrated Hydrologic Model (PIHM) and implemented in numerical simulations designed to illuminate the nature and direction of feedbacks among processes acting within the Critical Zone. The fully integrated hydrologic/sediment flux model (PIHMSed) includes feedbacks between soil thickness, downslope sediment

flux due to rate of tree-throw, rate of regolith conversion from bedrock, evolving soil moisture, and solute fluxes. Three domains (Fig. 4) all co-evolve to produce different steady-state landscapes, depending upon the external forcing conditions.



Figure 3. Schematic representation of the use of meteoric 10Be as a tracer of sediment flux on hillslopes. Meteoric 10Be is produced by cosmic-ray reactions in the atmosphere and delivered to the ground surface via precipitation. Accumulation in regolith over geologic time is a function of both delivery rate, and the residence time of regolith material in the watershed.

# Question 3: Dynamic evolution of the SHO over geologic time

The thickness of regolith and the efficiency of the weathering engine in the SHO has been influenced by perturbations in both the geologic and recent past. Ongoing efforts are focused on understanding the response of Critical Zone processes to enhanced sediment production and hillslope transport during periglacial times. Analysis of high-resolution digital elevation models (generated from airborne laser altimetry surveys) reveals abundant periglacial features such as solifluction lobes in



Figure 4. Definition sketch of hillslope where z = ground surface elevation (m), e = bedrock interface elevation (m), f = fracture zone thickness (m), h = regolith thickness measured in the vertical (m), U = rock uplift rate (m yr<sup>-1</sup>), E = net erosion/deposition rate (m yr<sup>-1</sup>) on the surface by overland flow, and  $q_{sx}$  = volumetric flux of regolith (m<sup>3</sup> m<sup>-1</sup> yr<sup>-1</sup>). These form the basis for transport laws implemented in PIHM.

the region, as well as evidence for previous periods of aggradation along fluvial systems (Fig. 1). Using a combination of coring and subsurface imaging (using groundpenetrating radar), we are currently exploring whether these processes generated deposits

that are present in the subsurface of SHO, and, if so, to what degree they influence chemical and isotopic measures of weathering and soil production.

We anticipate that these investigations will inform our understanding of the degree to which antecedent conditions "preconditioned" the landscape and materials now incorporated in the Critical Zone. For example, hillslopes along east-west oriented hillslopes within the CZO and nearby catchments exhibit systematic differences in gradient. We speculate that this difference reflects more efficient hillslope transport during vigorous periglacial activity in the past, but acknowledge that such differences may still be reflected in the modern transport and weathering regime.

Geomorphology team: <u>Rudy Slingerland</u> (PI), <u>Eric Kirby</u> (PI), <u>Nicole West</u> (Ph.D. student)

Collaborators: Paul Bierman (University of Vermont)

# 2011 Annual Reporting for SSHCZO

# <u>Choose your Discipline</u>: Hydropedology

# **Participants:**

- Henry Lin, Associate Professor of Hydropedology
- Chris Graham, Research Associate of hydrology
- Danielle Andrews, PhD student of soil science
- Jun Zhang, PhD student of soil science
- Doug Baldwin, Master student of soil science
- Will Burger, REU student
- Jialiang Tang, Visiting Scholar from Chinese Academy of Sciences

# **Research Progress:**

- We have installed a new set of 26 automatic soil moisture and temperature monitoring sites, which completes the coverage for the entire catchment (including south and north-facing slopes, all soil types and landform units).
- We have installed a set of 4 automatic cameras that records snow cover and tree phenology by taking a photo once per day at 4 different locations/angles in the catchment.
- We have developed a new toolbox called Hydropedograph for comprehensive and streamlined analysis of automatic soil moisture monitoring datasets, which allows the revealing of soil and hydrologic information in efficient and visually appealing ways.
- We have also developed a customized software to process time-lapsed Ground Penetrating Radar (GPR) images.
- We have continued to explore the combined use of time-lapsed GPR imaging and real-time soil moisture monitoring to identify subsurface flow pathways in contrasting soil transects in the Shale Hills Critical Zone Observatory.
- We have continued to analyze extensive soil moisture monitoring datasets collected for many years and to couple that with other datasets collected for the Shale Hills CZO, especially geochemical and ecological datasets.

# Significant Findings:

- The Hydropedograph Toolbox we developed will greatly facilitate cross-CZO studies as this will significantly enhance the comprehensive and streamlined analysis of automatic soil moisture monitoring datasets. We look forward to apply the methodology developed at other CZOs for cross-site comparisons. Sites with different land cover, precipitation regimes, soil types, and topographic features are expected to have different controls on soil moisture dynamics and preferential flow initiation and occurrence. Such information will provide a valuable foundation for improving hydrologic models and their predictions as well as biogeochemical hot spots and hot moments that are often dictated by soil hydrologic conditions.
- First simultaneous determination of the temporal and spatial patterns of in situ preferential flow and its underlying controls has been made in a forested catchment. Our results show that preferential flow is common throughout the Shale Hills catchment, occurring at one or more

sites during at least 90% of the 175 precipitation events that we monitored in the past three years.

- Based on the four-year database consisting of catchment-wide soil moisture measurements at 78 locations from the surface down to 1.1-m depth, we found that soil moisture spatial variability increases exponentially with catchment-wide wetness across all measurement depths and various soil-landform units. This is significant for guiding soil moisture monitoring campaigns as well as for interpreting and scaling remote sensing footprints of soil moisture during different times of a year.
- Swales are confirmed to be hot spots of soil organic carbon (SOC) storage and dissolved organic carbon (DOC). Soil pore water DOC also show elevated concentrations at restrictive subsurface layer interfaces (i.e., preferential flow pathways).
- Stream water DOC concentration is found to significantly correlate with stream discharge and stream water temperature, with hot moments observed during snowmelt and late summer to early fall wet-up.
- Five Hydropedological Functional Units (HFUs) have been delineated for the entire Shale Hills CZO based comprehensive datasets (LIDAR terrain attributes, soil properties, soil moisture storages, soil water retention parameters). These units reflect well soil moisture storage and hydrologic processes, and will significantly facilitate the modeling and future data collections in the Shale Hills CZO. The methodology developed is applicable in other CZOs.

# Training/Development:

- Andrews, D. 2011. Coupling Dissolved Organic Carbon and Hydropedology in the Shale Hills Critical Zone Observatory. Ph.D. dissertation, Penn State Univ.
- Zhang, J. 2011. Integrated Approach to Identifying Subsurface Flow in a Forest Catchment. Ph.D. dissertation, Penn State Univ.
- Baldwin, D. 2011. Catchment-Scale Soil Water Retention Characteristics and Delineation of Hydropedological Functional Units in the Shale Hills Catchment. Master thesis, Penn State Univ.
- Burger, W. REU student. Summer 2011.
- The Shale Hills CZO was used as a field laboratory for Soils 405 Hydropedology class in Fall 2010. There were a number of field trips to the site.

# **Outreach Activities (broadening participation of under-represented/under-served groups):**

• Participating in "The Life Cycle of Water" video shooting for NSF at the Shale Hills.

# **Conference Abstracts:**

- Zhang, J., and H.S. Lin. 2011. Evidence of Subsurface Lateral Flow in the Shale Hills CZO as Revealed by Real-Time Soil Moisture Monitoring. CZO All-Hands Meeting in Biosphere 2, Tucson, AZ, May 2011.
- 2. Graham, C., H.S. Lin, and D. Baldwin. 2011. Modeling Shale Hills catchment soil hydrology using distributed soil-terrain properties. CZO All-Hands Meeting in Biosphere 2, Tucson, AZ, May 2011.
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- 4. Naithani, K., K. Gaines, D. Baldwin, H.S. Lin, and D. Eissenstat. 2010. Spatial and temporal dynamics of vegetation and hydrological properties at Shale Hills Critical Zone Observatory in central Pennsylvania. AGU Fall meeting, Dec. 13-17, 2010, San Francisco, CA.
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# 3\_Hydropedology

# March 2011

**Hydropedology Studies at the Shale Hills CZO:** Hydropedology research being conducted at the Shale Hills CZO is multi-faced, cross-scale, and interdisciplinary. Two fundamental questions we seek to answer are:

1) How do soil architecture and the distribution of soils over the landscape exert a first-order control on hydrologic processes (and associated biogeochemical and ecological dynamics) across spatio-temporal scales?

2) How does landscape water (and the associated transport of energy, sediment, chemicals, and biomaterials by flowing water) influence soil genesis, evolution, variability, and functions?



Fig. 1. Soil hydrologic monitoring network in the Shale Hills.

We focus on interactive hydrologic and pedologic processes at the pedon, hillslope, and catchment scales. The following several studies have

been ongoing:

# Soil Moisture Spatial-Temporal Patterns across

Scales: A spatially intensive network of soil hydrology monitoring has been implemented at the Shale Hills since 2004 (Fig. 1). This includes (1) a total of 106 sites (covering all soil types, topographic positions, and landform units in the catchment) where approximately weekly measurements of soil volumetric water content, matric potential, and water



Fig. 2. Soil moisture spatial patterns and their temporal stability.

table are conducted manually from soil surface down to bedrock, and (2) a total of 12 stations where real-time soil moisture, matric potential, temperature, and water table are monitored automatically at 0.5-10 minutes interval. An example of soil moisture spatial pattern and its temporal stability is illustrated in Fig. 2. We continue to investigate the controls of soil moisture spatial-temporal patterns and related processes (including soil type, depth to bedrock, landform,



Fig. 3. Non-invasive imaging of the Shale Hills subsurface and its soils.

topography, vegetation, and climate).

Subsurface Flow Pathways and

Processes: We use a suite of non-invasive imaging techniques (Xray tomography, ground penetrating radar or GPR, and electromagnetic induction or EMI) in combination with realtime soil hydrologic monitoring to detect and model subsurface flow networks and their dynamics (Fig. 3). In particular, we use timelapsed approaches to reveal complex subsurface architecture and its relationships to

hydrologic functions. A large geophysical database has been developed over the years.



Defining and Delineating Hydropedological Functional Units: These are soil-landscapes units

Fig. 4. Major elements constituting the conceptual foundation for defining Hydronedological Functional Unite in the Shale Hille

(Knocking Pole, GPR)

with Biogeochemistry with a Focus on Carbon dynamics: We are evaluating the coupling of hydropedological properties (soil type, depth, moisture content, water table, and redox dynamics) and biogeochemistry through the quantification of carbon dynamics. Soil pore waters from nested lysimeters in four hillslope transects (swales and planar hillslopes on both north and south sides of the catchment) in different landscape positions (ridge-top, mid-slope, and valley floor) are being continuously collected, along with bulk soil samples and stream and ground water samples, for analyzing dissolved organic carbon (DOC) and major cations and anions. Daily export of DOC from the stream and its flushing mechanism are also being investigated, as well as the role of metals in stabilizing DOC to enhance carbon storage in the catchment soils (Fig. 5).



Contacts: <u>Henry Lin</u> (PI), Chris Graham (postdoc), Danielle Andrews (PhD student), Jun Zhang (PhD student), Doug Baldwin (MS student)

Collaborators: Jim Doolittle, Chris Duffy, Sue Brantley, Lixin Jin

Fig. 5. DOC in soil solution in relation to metal concentrations (AI, Fe, Mn) in the Shale Hills.

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Waleska Castro, Lin Ma, Molly Holleran, Lixin Jin, Ashlee Dere, Laura Liermann, Susan Brantley, Jennifer Williams, Aaron Regburg, Megan Carter, Henry Gong, Beth Herndon, Tiffany Yesavage

**Sources and cycling of Mn:** Located in the heart of a historic iron producing region, the Susquehanna Shale Hills CZO provides a model system to investigate anthropogenic metal inputs to soils. Detailed geochemical studies have shown that excess manganese (Mn) contaminates the soils at SSHO due to past atmospheric deposition (Herndon et al., 2011). This Mn, emitted as a byproduct of iron and steel production, coal combustion, and other industries, remains in the soil as the legacy of Huntingdon County's industrial past.

We are currently evaluating the role of vegetation in retaining Mn within the watershed (Figure 1). Low concentrations of Mn are found in soil pore fluids, indicating that losses to chemical weathering are small. In contrast, high concentrations of Mn are found in tree leaves, suggesting that Mn is being rapidly taken up from soil by the trees.



Figure 1. A box model shows mass reservoirs of Mn (boxes) and the Mn fluxes that impact SSHO (arrows; values in µg cm-2 y-1). Emissions from anthropogenic activity have resulted in a net gain of Mn in SSHO soils (mMn, w = 47 mg cm-2). Rates of Mn uptake into trees (83 µg cm-2 y-1) currently outpace removal through chemical weathering (1 µg cm-2 y-1), indicating that vegetation may retain Mn within the catchment.

In this way, vegetation acts as a "capacitor" that stores Mn and releases it slowly to the



Figure 2. X-ray fluorescence spectroscopy (XRF) and X-ray absorption spectroscopy (XAS) are used to characterize the location and speciation of manganese within leaf biomass. Left: Red oak leaves examined with XRF exhibit discrete areas of high Mn, ROIs (regions of interest), as shown in red and white. Right: XAS was used to analyze Mn hot spots within foliar tissue. Mn spectra obtained from these ROIs (shown in blue) are most consistent with trivalent, organically-complexed Mn. Standards for the oxides MnO, Mn2O3, and MnO2 are also shown.

environment over time. We are using X-ray absorption spectroscopy (XAS) to characterize Mn in soils and vegetation. Preliminary results show that Mn in foliar tissue is reduced and complexed with organic compounds (Figure 2), while Mn in soils is present as a tri-/tetravalent oxide, indicating that Mn is oxidized and immobilized as tree leaves fall to the soil and are decomposed.

Additionally, we are coupling our study of Mn at SSHO with analysis of global Mn contamination. Data gathered from multiple geochemical databases show that Mn addition is common in soils, but patchy in distribution. Air and water data indicate that air concentrations of Mn peaked in the 1960s before declining by an order of magnitude, while riverine outputs of Mn peaked ~1980 before also declining.

This research is spearheaded by Elizabeth Herndon. [Herndon, E.M., Jin, L., and Brantley, S.L. (2011) Soils reveal widespread manganese enrichment from industrial sources, Environmental Science & Technology 45(1), 241-247.]

Iron Isotopes: This research involves understanding how Fe is transformed and cycled as a result of weathering and soil formation in the Shale Hills watershed. In order to investigate this question, a series of soil samples were collected from along a transect and analyzed for bulk chemistry and Fe(II) concentrations. Chemical weathering results in a moderate but incomplete loss of both total Fe and Fe(II) from soil profiles. Furthermore, mass balance calculations are used to evaluate fluxes of these two constituents from different topographic positions along the transect.





In order to better elucidate microbiological processes that may be cycling Fe within the catchment, both Fe-oxidizing and Fe-reducing bacteria were cultured. The abundance of Fe-reducing bacteria is well predicted by soil moisture level, while Fe-oxidizing bacteria are often prevalent near the soil/bedrock interface.

A final goal of this research involves understanding how different processes associated with Fe weathering and cycling may fractionate the stable isotope values of Fe in soils. Previous experimental work suggests that many common processes (including bacterial Fe reduction and the ligand-promoted dissolution of minerals) tend to produce Fe isotope signatures in bulk soils that are isotopically heavy relative to starting material. In contrast, although the overall extent of Fe fractionation in SSHO soils is low, we observe a very different type of trend that involves isotopic depletion with increased weathering extent toward the valley floor (Figure 1). At the moment, we are not fully sure of how to explain this trend. It may result from the preferential uptake of isotopically light Fe by vegetation over time or from the loss of isotopically enriched dissolved Fe from the watershed. This research is spearheaded by graduate student Tiffany Yesavage.

**Uranium-series disequilibrium isotopes:** U-series disequilibrium isotopes (<sup>238</sup>U, <sup>234</sup>U, and <sup>230</sup>Th) of shale rocks and soils are being analyzed at the Shale Hills catchment to derive the soil production function and estimate the residence time of regolith particles using mass balance models (Figure 1). The activity ratios observed in the soils are explained by loss of U-series isotopes during water-rock interactions and re-precipitation of <sup>234</sup>U and <sup>238</sup>U downslope. Regolith



production rates calculated with these isotopes decrease exponentially from 45 to 15 m/Myr (regolith residence times increase from 6.7 to 45 kyr) on the south planar transect. with increasing soil thickness from the ridge top to the valley floor. By contrast.

regolith production rates from the north planar transect are ~40-52 m/Myr (regolith residence times are 8-10 kyr). The regolith profiles on the northern, sun-facing slope are thus characterized by faster regolith production rates and shorter duration of chemical weathering compared to the southern, more shaded slope. These observations are consistent with the conclusion that aspect

exerts an important control on the regolith formation at the Shale Hills catchment. The aspect asymmetry induces different microclimatic conditions that affect slope stability and erosion and set the residence time for the materials available for chemical weathering. Given that the SSHO experienced a peri-glacial climate ~15 ky ago, we conclude that the hillslope retains regolith formed before that glacial period and that the hillslope is not at



geomorphological steady state. This research is spearheaded by postdoctoral scholar Lin Ma (present address: Department of Geological Sciences, University of Texas at El Paso, El Paso, TX 79968). [Ma, L., Chabaux, F., Pelt, E., Blaes, E., Jin, L., and Brantley, S.L., Regolith production rates calculated with Uranium-series isotopes at Shale Hills Critical Zone Observatory, Earth and Planetary Science Letters vol 297, 211-225; Ma, L., Chabaux, F., Pelt, E., Jin, L., and Brantley, S., North versus south: Implications from U-series isotopes about regolith formation at Shale Hills, to be submitted]

U-series isotopes and trace element concentrations were also measured in a basaltic andesite weathering rind from the Bras David watershed in Guadeloupe to study chemical weathering under a tropical climate. These measurements allow us to directly quantify rind formation rates in Guadeloupe and to further independently test the hypothesis that the curvature of core-rind boundary controls the rind growth rate. Based on the measured U-series activity ratios, rind formation rate is determined and increases to a factor of about 1.4 (0.23 to 0.31 mm/kyr) from a low curvature transect to a high curvature transect of the clast (Figure 2). The observation of a higher rate of rind formation on a higher curvature interface is expected with a diffusion-limited weathering rind formation, as a higher curvature interface experiences a more active and faster exchange between the weathering fluids and clast compared to a low curvature site. U-series geochronmetry is thus proven to be an effective dating tool to study rind formation rates and also provides the first directly evidence that the curvature of the interface controls the rate of the rind formation on the clast scale [Ma, L., Chabaux, F., Pelt, E., Granet, M., Sak, P., Gaillardet, J., Lebedeva, M., and Brantley, S., Control of curvature on rind formation rates: evidences from Uranium-series isotopes in basaltic andesite weathering clasts in Guadeloupe, to be submitted].



Figure 1. Mg2+, Mg\*, and Mg\* (Cl-normalized) concentrations in the pore water as a function of depth at the SPRT (A, D, G), SPMS (B, E, H) and SPVF (C, F, I) sites. Shaded areas highlighted the variations of Mg concentrations in soil waters from different depths. The Mg2+ concentration is that measured in the soil water; Mg\* is Mg concentration in soil water after correcting for atmospheric input; and Mg\* (Cl-normalized) is Mg concentration corrected for atmospheric input and evapotranspiration. Notice changes in scale between Mg2+/Mg\* and Mg\* (Cl-normalized).

Water Chemistry: An intense field study was conducted at the Susquehanna/Shale Hills Critical Zone Observatory to use water chemistry to probe the subsurface hydrogeochemical conditions and water flow dynamics. Soil pore water sampled through tension lysimeters suggest that contemporary reaction rates depend on preferential flowpaths and solute residence times, and are limited by dissolution kinetics. Thus weathering processes are strongly coupled with hydrological features of shale rocks and soils. The chemistry of ground- and streamwater is being analyzed in relation to that of the soil porewaters to elucidate the mineral reactions occurring below the soils and to derive elemental fluxes over the whole catchment.

Soil water solutes are predominantly contributed by shale weathering, which is limited by clay dissolution kinetics. As such, solute concentrations are primarily controlled by the residence time of water in soil. Translocation and

deposition of secondary clays created B-horizons that are more conductive to lateral flow right above or below it than vertical flow. Consistent with soil moisture monitoring data, water flows out of the steep-sloping hillslope predominantly laterally through preferred pathways that include soil horizon and soil-bedrock interfaces, and vertically via macropores. As a consequence, much higher concentrations of major cations are observed in porefluids within the B-horizon because water flows more slowly and mineral-water contact time is much longer. The amplitude of seasonal variations in O and H isotopes decreases in the order: precipitation>> soil water > stream > groundwater, suggesting water becomes progressively older as rainfall infiltrates the soil and eventually recharges to ground water. Interestingly, Mg concentrations increase with the residence time of the water due to increasing contact time with minerals (clay and ankerite). Stream water is a mixture of groundwater and shallow soil water where the relative proportions change seasonally. The discharge of the first-order stream responds to precipitation closely, documenting the rapid release of both old groundwater and relatively young soil water during storms.



Figure 2. Conceptual hydrological flow model on pedon (A) and hillslope (B) scales. In A, large wide black arrows indicate preferential flow paths, narrow black arrows indicate vertical flow through macropores formed for example by tree roots, and white curly arrows indicate solute exchange between low-flow zone and macropores via diffusion. In B, black arrows indicate water and Mg transport through rainfall and snowmelt input, advection along the hillslope through the preferential flow paths (high-flow domain, squares) and recharge to stream from vadose zone and groundwater. Grey arrows mean diffusion of Mg2+ from restrictive layers (low-flow domain, eclipse) to flow paths (high-flow domain). The Mg2+ concentrations in each reservoir are calculated by averaging those measured at corresponding sites/depths and used to determine the chlorite dissolution rates (see text for details). It is assumed that the annual precipitation is 1000 mm and half of it returns to the atmosphere via evapotranspiration. Thus the Mg concentration in water that penetrates to the soil doubled (=0.88 \*2=1.76 mM).

Jin, L., Andrews, D.M., Holmes, G.H., Duffy, C.J., Lin, H and Brantley, S.L. (2011) Water chemistry reflects hydrological controls on weathering in Susquehanna/Shale Hills Critical Zone Observatory (Central Pennsylvania, USA). In review for Vadose Zone Journal.

**Neutron Scattering:** We use neutron scattering techniques to characterize the evolution of nanoscale features (e.g., nano-porosity, surface area, surface roughness) in shales and to reveal



Figure 1. Variations of power law Porod exponent (A), porosity (B), specific surface area (C), and ferrous and total Fe contents as a function of depth (D), for shales that have been weathered to different extents. The exponent, n, indicates the type of fractal (2 < n < 3, mass fractal; 3 < n < 4, surface fractal). that changes of these physical properties are coupled with chemical weathering reactions. At  $\sim 20$  m depth, dissolution is inferred to have depleted the bedrock of ankerite and all the chips investigated with neutron scattering are from above the ankerite dissolution zone. Scattering data documents that 5-6% of the total ankerite-free rock volume is comprised of isolated, intraparticle pores. At 5 m depth, an abrupt increase in porosity and surface area corresponds with onset of feldspar dissolution in the

saprock and is attributed mainly to peri-glacial processes from 15 ka. At tens of centimeters below the saprock-regolith interface, the porosity and surface area increase markedly as chlorite and illite begin to dissolve. These clay reactions contribute to the transformation of saprock to regolith. Throughout the regolith, intraparticle pores in chips connect to form larger interparticle pores and scattering changes from a mass fractal at depth to a surface fractal near the land surface. Pore geometry also changes from anisotropic at depth, perhaps related to pencil cleavage created in the rock by previous tectonic activity, to isotropic at the uppermost surface as clays weather. In the most weathered regolith, kaolinite and Fe oxyhydroxides precipitate, blocking some connected pores. These precipitates, coupled with exposure of more quartz by clay weathering, contribute to the decreased mineral-pore interfacial area in the uppermost samples.

These observations are consistent with conversion of bedrock to saprock to regolith at SSHO due to i) transport of reactants (e.g., water, O2) into primary pores and fractures created by tectonic events and peri-glacial effects, ii) mineral-water reactions and particle loss that increase porosity and the access of water into the rock. From deep to shallow, mineral-water reactions may change from largely transport-limited where porosity was set largely by ancient tectonic activity to kinetic-limited where porosity is changing due to climate-driven processes.



Figure 1. Depth profiles of major elements (a, SSRT; b, SSMS; c, SSVF), Ca and Na (d, SSRT; e, SSMS; f, SSVF) and REEs (g, SSRT; h, SSMS; i, SSVF)  $\tau$  value as a function of depth. The uncertainties in  $\tau$  calculations were estimated by error propagation and averaged at approximately 0.07  $\tau$  unit.

Jin, L., Rother, G., Cole, D.R., Mildner, D.F.R., Duffy, C.J. and Brantley, S.L. (2011) Characterization of deep weathering and nanoporosity development in shale – a neutron study. In press for American Mineralogist.

Swale Chemistry: The soil chemistry data (major and REEs) from a swale transect are characterized for comparison to similar measurements on a planar transect for the Susquehanna/Shale Hills critical zone observatory. Similar reaction fronts are observed: plagioclase dissolution is indicated by Na and Ca depletion and a negative Eu anomaly; clay dissolution followed by particle loss is accompanied by loss of Mg, K, Fe, Al and Si. However, different from the planar transect, soils along the swale transect, especially in the topographically depressional site, do not show smooth elemental profiles. This documents both residuum soils and accumulation of colluvium sediments. The soils at the swale transect are thicker and on average wetter than those along the planar transect; however, the Ce anomaly

observed in the swale soils is consistent with a generally oxic environment. Thus, preferential flowpaths are an important mechanism for water transport, preventing swale soils from water saturation.

Jin, L. and Brantley S.L. (2011) Soil chemistry and shale weathering on a hillslope influenced by convergent hydrologic flow regime at the Susquehanna/Shale Hills Critical Zone Observatory. Abstract submitted to the 9th International Symposium on Geochemistry of the Earth's Surface (GES-9).

**Deep shale weathering:** Molly Holleran is a senior undergrad in the Geosciences Department, who has been working as a field assistant at Shale Hills for the past three years. She assists with lysimeter sample collection during the spring, summer and fall seasons. Molly is now working on her senior thesis based at Shale Hills, on the quantification of deep shale weathering. Research goals include evaluating the change of mineralogy with depth, and determining if changes seen can be attributed to chemical weathering or heterogeneity in the lithology. Carbonate, pyrite, feldspar, and illite/chlorite reaction fonts are being investigated, from the ridge top to the valley floor. Overall, a goal of this study is to be able to relate the process of shale weathering and associated reaction fronts with the overall water-table in the catchment.



Figure 1. Molly Holleran (undergraduate student, Geosciences) works with Danielle Andrews (graduate student, Crop and Soils Sciences) to collect water samples from lysimeters installed at the SSHCZO.



Figure 2. Holleran has assisted with water and soil collection for three years and is currently working on a senior thesis based at SSHO.

Contacts: Susan Brantley (PI), Carmen Enid Martinez

### 2011 Annual Reporting for SSHCZO

### Discipline: Biogeochemistry Team

### **Research Progress:**

In coordination with the Ecophysiology group, I have been collecting vegetation samples from the SSHCZO. This includes taking 160 tree cores, constructing and placing 35 litter traps, and climbing trees to obtain upper canopy branches. We intend to conduct chemical analyses of these samples, which will complement soil chemistry, pore fluid chemistry, and water usage studies. Additionally, I am continuing X-ray Absorption Spectroscopy studies at the Advanced Photon Source in order to characterize the chemical forms of manganese, enriched in soils at SSHCZO due to past industrial pollution, in soils and vegetation.

## Significant Findings:

We have found that standing vegetation is actively recycling Mn vegetation, potentially increasing its residence time within the SSHCZO. Analyzed foliar tissue contains elevated levels of Mn, approaching ranges considered toxic to most tree species. Visible dark concretions on tree leaves were found to contain high levels of a Mn-compound that is chemical different from the Mn found in bulk leaf tissue.

Training/Development:

Outreach Activities (broadening participation of under-represented / under-served groups):

#### Conference Abstracts:

Herndon E.M., Eissenstat D., Martinez C.E., and Brantley S.L. (2011, oral) "Biogeochemical characterization of contaminant Mn sequestration." 20<sup>th</sup> V.M. Goldschmidt conference, Prague, Czech Republic.

#### **Publications:**

Herndon, E.M., and Brantley S.L. (2011) Movement of manganese contamination through the Critical Zone. *Appl. Geochem* **26**, S40-S43. doi: 10.1016/j.apgeochem.2011.03.024.

## 3. Biogeochemistry

## **March 2011**

Soil Biogeochemistry: We are

investigating the distribution of total soil carbon, soil  $CO_2$  concentrations, dissolved organic carbon (DOC), and soil microorganisms along hillslopes and with soil depth at the Shale Hills Critical Zone Observatory. These measurements will help us predict how soil development affects soil carbon storage and transport in this watershed. Jason Kaye (Department of Crop and Soil Sciences) and Susan Brantley (Geosciences) are interested in soil respiration rates at the Shale Hills Critical Zone Observatory. Soil respiration is the release of  $CO_2$  from



Left: Graduate student Danielle Andrews collects pore water samples for chemical analysis. Right: Graduate student Tiffany Yesavage studies microbiology in the Shale Hills catchment.

plant roots and soil heterotrophic organisms to the atmosphere. Kaye's group is working to quantify how water movement, water storage, and soil texture affect soil-atmosphere exchange rates of  $CO_2$ . The flux of  $CO_2$  from soil is a critical component of the global carbon cycle, yet factors affecting this flux remain unclear.



Figure 1. Concentrations of dissolved organic carbon (DOC) in a valley soil profile consistently show patterns of variation with depth. DOC levels tend to be elevated around 30 cm, which likely corresponds to the interface between the Bw and Bt horizons.

Work by Danielle Andrews (advised by Henry Lin of Crop and Soil Sciences) examines how soil and landscape characteristics affect the movement of dissolved organic carbon (DOC) within the Shale Hills watershed. These studies indicate that DOC concentrations are correlated with topographic position. For instance, soil pore fluids in swale sites have elevated DOC relative to planar hillslope sites. Swales contain deeper soils than the planar hillslopes and are regions of convergent water flow that may facilitate organic matter collection and breakdown. Additionally, DOC concentrations were found to vary within the soil profile. For example, DOC increases above restrictive soil interfaces

such as the clay-rich Bt horizon (Figure 1). Graduate student Tiffany Yesavage (advised by Susan Brantley of Geosciences) is investigating how variations in DOC and total carbon

concentrations in turn may affect the distribution of different groups of microorganisms at different depths and topographic positions (Figure 2).

The ultimate goal of this work is to understand how environmental parameters such as rates of regolith formation can be used to explain the distribution of  $CO_2$  and DOC in soils throughout the catchment. By creating this interdisciplinary team consisting of members from Crop and Soil Sciences and Geosciences, we hope to provide a theoretical basis for predicting soil carbon dynamics in shale-derived watersheds around the world.



Soil CO<sub>2</sub> concentrations: Total cell counts: Total carbon and nitrogen:

Figure 2. Soil CO2, heterotrophic microorganisms, and nutrients (e.g. carbon and nitrogen) vary as a function of depth and topographic position in the watershed. Current research seeks to quantify interactions amongst these parameters.

Contacts: Jason Kaye (PI) and Susan Brantley (PI)

# 4. Hydroclimatology



**Subsurface-land surface-atmosphere interaction:** The instrument array at Susquehanna Shale Hills Critical Zone Observatory (SSHO) enables an unprecedented investigation of the subsurface-land-surface-atmosphere interaction. A fully-coupled hydrologic-land-surface model is developed and tested on SSHO to study the subsurface-land-surface interaction. The questions being researched include:

1) How does the hydrologic modeling system, driven by satellite observations and meteorological reananalyses improve the prediction of flood and drought conditions?

2) How does the fully-coupled hydrologic-land-surface modeling system improve the prediction of surface energy balance (SEB)?

3) What are the impacts of upland recharge, groundwater redistribution, root uptake of water, and water table fluctuations on SEB?

4) What are the impacts of vegetation (vegetation fraction, leaf area index, etc.) on hydrologic and land-surface systems?



Figure 1 Grid setting for SSHO model domain. Locations of RTHnet wells, flux tower, weather station and outlet gauge are also presented.

5) How do the model parameter

values affect the coupled processes in the modeling system?

Groundwater, land surface and atmosphere are closely related to each others. A barrier to studying the subsurface-land-surface-atmosphere interaction is the lack of sufficient numerical model. Traditional hydrologic models have relatively simple land-surface schemes, while traditional land surface models (LSMs) are limited to vertical moisture transport in the soil column and ignore the deeper soil moisture processes and groundwater. The combination of local sensor arrays at SSHO provides valuable information for advance modeling. In particular, the eddy-covariance flux tower provides an opportunity to investigate the SEB and turbulence properties at SSHO and a primary means to evaluate model SEB simulations. A groundwaterland-surface model system has been developed from the Penn State Integrated Hydrologic Model (PIHM) by incorporating a land-surface component into PIHM. This land-surface scheme is mainly adapted from the Noah LSM, which is widely used in mesoscale atmospheric models and has undergone extensive testing. Because PIHM is capable of simulating lateral water flow and has deep groundwater, the new model is able to represent some of the land-surface heterogeneity caused by topography. At the same time, the robust land-surface scheme provides accurate sensible heat flux and evapo-transpiration rates. The new model has been implemented for the SSHO (Figure 1). It is manually calibrated to enhance its performance at this watershed. Model parameters including soil hydraulic conductivity, macropore hydraulic conductivity, soil porosity, van Genuchten soil parameters, and minimum stomatal resistance are tuned to fit the model outputs with both hydrologic and land-surface measurements. The model is driven by in situ measurements and North American Regional Reanalysis (NARR) dataset.



Figure 2 Flowchart of calibration and evaluation process.

The model reproduces realistic topographically-induced distributions of water table, soil moisture, and skin temperature. The simulated river discharge shows good agreement with outlet



Figure 3 Comparison of hourly river discharge between model simulation and RTHnet measurements from 01

gauge measurements (Figure 3). The sensible and latent heat fluxes simulated by the new LSM compare well with the eddy-covariance flux measurements on most days (Figure 4). Errors are relatively large when NARR fails to provide realistic radiation data. The model is able to capture the fluctuation of saturated and unsaturated water reasonably well. It therefore provides more realistic soil moisture variations which benefits the simulation of surface energy balance. The simulated sensible heat flux, latent heat flux, ground heat flux, and skin temperature are correlated with water table depth and are affected by soil type and land cover as well (Figure 5). The impact of soil type and land cover strengthens with the increase of water table depth.





Figure 4 Comparison of sensible heat flux (H), latent heat flux (LE), and net radiation (Rn) (from top to bottom) between model and flux tower from 01 Aug to 01 Sep 2009.

Figure 5 Simulated sensible heat flux, latent heat flux, ground heat flux (G), and surface skin temperature (Tskin) as functions of water table depth.

This fully-coupled model of the atmosphere, land surface and subsurface may yield significant improvements in both flood/drought forecasting and in weather forecasting, and provide a valuable chance to study the subsurface-land surface-atmosphere interactions.

Hydroclimatology team: <u>Kenneth Davis</u> (PI, davis@meteo.psu.edu), <u>Yuning Shi</u> (PhD student, yshi@psu.edu), <u>Burkely Twiest</u> (undergraduate student, blt5086@psu.edu)

# 7. Isotope Hydrology

## **March 2011**

## Stable Isotope Network: An isotopic

sampling network has been implemented at the Susquehanna Shale Hills Critical Zone Observatory. This site has been approved as a node in the IAEA Global Network of Isotopes in Precipitation (GNIP) database. This research is an attempt to determine oxygen-18 and deuterium signatures and time scales in all stores of the watershed. Some of the questions to be researched include:

1) Can the isotope network be used to determine the continuous mean age of the system, and how does this mean age change over time?

2) What are the dominant modes controlling each phase of the hydrologic cycle, and how do these change over time?



Figure 1. Examples of the instruments used to sample the isotopes at Shale Hills. a) Eigenbrodt NSA-1815 wet only precipitation collector, b) Suction-cup lysimeter nest for weekly soil water, c) ISCO automatic sampler for daily groundwater, d) Groundwater well sites for weekly samples, e) ISCO automatic sampler sites for daily stream water, and f) Vegetation sites for synoptic isotope sampling.

## 3) How are macro-pores affecting water flow paths in the subsurface?

#### 4) How does vegetation affect the hydrologic cycle?

The stable isotope network covers all phases of the hydrologic cycle, including precipitation sampled on an event basis with an Eigenbrodt NSA-181S wet only collector (four-hour samples), soil water sampled weekly along four transects with suction-cup lysimeters, groundwater sampled daily at two wells with ISCO automatic samplers and weekly at 15 wells, vegetation sampled during the growing season, and stream water sampled daily with an ISCO automatic sampler. An example of the instruments used at the different sampling locations is shown in



Figure 2. Layout of the Shale Hills CZO showing the location of the sampling sites.

figure 1, and the location of the instruments is shown in figure 2.

The comprehensive sampling of the catchment is possible because of the DLT-100 liquid water stable isotope analyzer from Los Gatos Research. The DLT-100, shown in figure 3, is a new machine that uses off-axis integrated cavity output spectroscopy (laser-absorption spectroscopy) to determine absolute isotope abundances. The machine has a reproducibility of  $\pm 0.2\%$  for oxygen-18 and  $\pm 1.0\%$  for deuterium, and the capability to run approximately 30 samples per day. This machine is simpler to use, quicker, and cheaper than a traditional isotope ratio mass spectrometer (IRMS).

The goal of this research is to identify flow paths and time scales of water from precipitation input through stream flow output from the catchment. Although results are preliminary

precipitation, soil water, groundwater and stream water can be visualized with a local meteoric water line (figure 4). The soil water, groundwater and stream water plot in the same region, suggesting that the source of the stream is primarily soil water and groundwater. It is also clear that the stream water, soil water, and groundwater all depart from the local meteoric line. The reason for this is unknown, but it can possibly be due to evaporation or the influence of snow recharging the system. Time series analysis and spatial principal component analysis is used to "classify" dominant modes and processes affecting stable isotope



Figure 4. Local meteoric water line for Shale Hills



Figure 3. DLT-100 liquid water stable isotope analyzer, with auto-injection unit, from Los Gatos Research.

dynamics in the watershed. Time series analysis will be used on the daily stream water and groundwater record to determine how these phases evolve through time. Spatial principal component analysis will be used on the records of weekly groundwater and soil water samples to determine how these phases evolve spatially. Principal component analysis will also be used on the watershed as a whole, to determine how all the phases of the hydrologic cycle are related spatially. The stable isotope network, real time hydrologic network, real time soil moisture network, real time groundwater network and sap flow network are

being used to quantitatively estimate the continuous mean age of the water in the catchment. An age model is being developed by Duffy (unpublished), that incorporates transient hydrodynamics, and determines the continuous mean age of the system from the moments of the tracer age distribution function. The tracer at Shale Hills will be <sup>18</sup>O and <sup>2</sup>H, which are ideal tracers because they are part of the water molecule, and conservative at the low temperatures

found in the watershed. The ultimate goal of the isotope research can be summarized as: where is the water going, what controls its movement, and how long will it be in the system?

Written by Kevin Dressler and George Holmes

For more information about Isotope Hydrology at the Shale Hills CZO contact:

Christopher Duffy (PI): cxd11@psu.edu

Kevin Dressler (senior personnel): kxd13@psu.edu

George Holmes (masters student): ghh108@psu.edu

### 2011 Annual Reporting for SSHCZO

#### Discipline (Please choose team and list current team members): Ecology Team

David Eissenstat, Frederick C. Meinzer, David Woodruff, Margot Kaye, Tom Adams, Katie Gaines, Kusum Naithani, Jacy Marshall-McKelvey (undergraduate researcher)

Research Progress:

- Leaf area index measurements on a weekly to biweekly schedule occurred in April and May 2011 to capture leafing out and complement the previous year's data collection prior to publication of data on leaf area index and soil moisture (see Conference Abstracts below).
- Trees that were used for sapflux in 2010 were measured for diameter at breast height and height, and trees without XY coordinates were surveyed with a Trimble Total Station unit in order to facilitate data for publication (see Conference Abstracts and Publications below).
- Plant water isotope samples were extracted on a cryogenic vacuum distillation line in the
  Eissenstat lab and analyzed via isotope ratio mass spectroscopy at the Center for Stable Isotope
  Biogeochemistry at University of California, Berkeley for <sup>18</sup>O and <sup>2</sup>H. This recent data is now
  being analyzed statistically to look for trends in the source of water used by trees according to
  tree-level and environmental variables.
- Two graduate students one from the ecology group (Katie Gaines), and another from the biogeochemistry group (Elizabeth Herndon), undertook an effort to collect canopy branch samples to analyze for water isotopes and leaf chemistry, respectively, along a slope transect. Two species of trees were sampled, *Quercus prinus* (chestnut oak) and *Acer saccharum* (sugar maple) to investigate changes in water source and potentially rooting depth with slope position as well as seasonal variation. Sampling will continue through September at which point samples will be cryogenically extracted and analyzed via isotope ratio mass spectrometry.
- A coring effort was undertaken to collect cores from a total of 180 trees in order to measure sapwood depth for the purposes of scaling sap flux data with sapwood depth for the dominant species in the catchment. Trees were also measured for diameter at breast height and height.
- An undergraduate student, Jacy Marshall-McKelvy, has been working with the research team to collect tree cores and analyze them to complete an undergraduate research project to quantify the growth of the dominant tree species at Shale Hills and analyze how it varies with location in the catchment.
- Litter traps were constructed and set out at 35 locations to collect leaf litter beginning in September. The ecology team will collect litter on a weekly basis throughout the fall and sort the leaves by species. This data will be used to begin building a catchment carbon budget. The biogeochemistry group was also involved in the construction and installation of the litter traps and will perform chemical analyses on the litter.

Significant Findings:

- We measured sap flux during the 2010 growing season in three ring-porous species (oaks), two • diffuse-porous species and two conifers. There were substantial differences among the species studied in stomatal regulation of sap flux in response to changes in soil water availability and atmospheric evaporative demand. As a group, the three oaks studied behaved similarly and their water use was considerably less responsive to soil drying than that of either the two angiosperm or two coniferous species both in terms of the relative decline in sap flow during a given soil drying cycle and in recovery from successive soil drying cycles. Stomatal regulation in the oaks was also less responsive to increased vapor pressure deficit than in the other four species. These differences in responsiveness to changes in the below- and aboveground environment imply that regulation of leaf water potential in the oaks was less stringent than in the other species. Regardless of whether differences in this suite of functional traits are associated with differences in wood anatomy per se, they enabled the ring-porous oaks to more effectively exploit soil water resources over a broader range of soil water availability and atmospheric dryness than either the diffuse-porous angiosperms or the tracheid-bearing conifers.
- We measured leaf area index (LAI) and quantified its spatial structure. Our results show an
  exponential increase (90-600 m) in spatial range of LAI from leaf onset (April) to leaf maturity
  (July) and subsequent decline (600-100 m) in spatial range from leaf maturity (July) to leaf
  senescence (October). Soil water content (at all measured depths) decreased from leaf onset to
  maturity and subsequently increased from leaf maturity to senescence. Results from this study
  suggest that the landscape canopy area and soil water become more homogenized and coupled
  from leaf onset to maturity (increasing spatial dependence and decreasing water content) and
  the landscape becomes more heterogeneous and uncoupled from leaf maturity to senescence
  (decreasing spatial dependence and increasing water content)
- A note on methods for plant water isotope samples: Test runs were performed on two different laser instruments in addition to the mass spectrometer when plant water samples were analyzed at UC Berkeley. The laser instruments were found to produce unreliable results for these samples. The lab plans to send any remaining sample to the manufacturers of these instruments to aid in the testing of methods to remove organic contaminants and improve reliability of laser spectrometer results for plant water. As a result, we will continue using the isotope ratio mass spectrometry for plant water isotopes.

#### Training/Development:

- Katie Gaines has advanced to candidacy after passing the Ecology Program candidacy exam in the spring.
- Jacy Marshall-McKelvey (Sr in Geography) did an undergraduate research project on tree growth variation among species and aspect at the critical zone.

Outreach Activities (broadening participation of under-represented / under-served groups):

• Katie Gaines assisted with Summer Field School activities in June 2011 including giving a talk at Shale Hills about the research being done by the Ecology Team, and providing feedback during field school student presentations at the conclusion of the field school.

### Conference Abstracts:

## (Presenting author is in bold)

- Naithani K. J., K. Gaines, D. Baldwin, H. Lin, & D. M. Eissenstat. Spatio-Temporal Dynamics of Vegetation Structure and Hydrology at Shale Hills Critical Zone Observatory in Central Pennsylvania. CZO All Hands Meeting, Arizona. May 8-12, 2011. [Poster]
- Naithani K. J., K. Gaines, D. Baldwin, H. Lin, & D. M. Eissenstat. Spatio-Temporal Dynamics of Vegetation Structure and Hydrology at Shale Hills Critical Zone Observatory in Central Pennsylvania. Postdoctoral Research Exhibition, The Pennsylvania State University. April 12, 2011. [Poster]
- Naithani K. J., K. Gaines, D. Baldwin, H. Lin, & D. M. Eissenstat. Spatio-Temporal Dynamics of Vegetation Structure and Hydrology at Shale Hills Critical Zone Observatory in Central Pennsylvania. 1<sup>st</sup> Conference on Spatial Statistics, Enschede, Netherlands. March 23-25, 2011. [Poster]
- Naithani K., K. Gaines, D. Baldwin, H. Lin & D. Eissenstat. Spatial and Temporal Dynamics of Vegetation and Hydrological Properties at Shale Hills Critical Zone Observatory in Central Pennsylvania. Fall meeting of the American Geophysical Union. San Francisco, CA, USA. December 13-17, 2010. [Poster]
- Meinzer F.C., D. Woodruff, T.A. Adams & D. M. Eissenstat. Tree transpiration at the Shale Hills Critical Zone Observatory. CZO All Hands Meeting, Arizona. May 8-12, 2011. [Poster]

## Spatial and Temporal Dynamics of Vegetation and Hydrological Properties at Shale Hills Critical Zone Observatory in Central Pennsylvania

Kusum J. Naithani<sup>1,2,3</sup>, Katie Gaines<sup>3,4</sup>, Doug Baldwin<sup>5</sup>, Henry Lin<sup>5</sup>, David Eissenstat<sup>3,4</sup>

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#### ABSTRACT

Understanding the interaction of vegetation and hydrology and determining the changes in this relationship across spatial and temporal domains is critical for modeling landscape hydrology. Trees

release water into the atmosphere via stomatal pores in exchange for carbon dioxide and play an important role in landscape hydrology. Our objective was to investigate the coupled spatial and temporal dynamics of vegetation and hydrological properties in a forested catchment covering 7900  $m^2$ area in central Pennsylvania at the Shale Hills Critical Zone Observatory. During 2010, we measured leaf area index (LAI) and canopy closure to characterize vegetation properties and measured soil water content, soil water tension and water table depth to characterize hydrological properties at a spatial grid of 70 sampling points across an entire watershed at 15-day intervals. We used geostatistical techniques to quantify spatial structure (semi-variograms) and visualize spatial patterns (Kriging) of vegetation and hydrological properties and their relationship to each other. Our results show an exponential increase (90-600 m) in spatial range from leaf onset (April) to leaf maturity (July) and subsequent decline (600-100 m) in spatial range from leaf maturity (July) to leaf senescence (October). Soil water content (at all measured depths) decreased from leaf onset to maturity and subsequently increased from leaf maturity to senescence. Results from this study suggest that the landscape canopy area and soil water become more homogenized and coupled from leaf onset to maturity (increasing spatial dependence and decreasing water content) and the landscape becomes more heterogeneous and uncoupled from leaf maturity to senescence (decreasing spatial dependence and increasing water content). Our results provide insight into tight coupling between vegetation and hydrology across space and time; incorporating these spatial and temporal feedbacks in hydrological models will improve current and future landscape modeling of temperate forests.

## **Publications:**

- Johnson, DM, McCulloh, KA, Meinzer, FC, Woodruff, DR, Eissenstat, DM (2011) Hydraulic patterns and safety margins, from stem to stomata, in three eastern US tree species. Tree Physiology 31: 659-668.
- Meinzer, FC, Woodruff, DR, Eissenstat, DM, Lin, HS, Adams, TS, McCulloh, KA (2011) Above- and belowground controls on water use by trees of different wood types in an eastern United States deciduous forest. Agricultural and Forest Meteorology (in review).
- Kusum J. Naithani, Katie Gaines, Doug Baldwin, Henry Lin, & David Eissenstat. Spatial and Temporal Dynamics of Vegetation and Hydrological Properties at Shale Hills Critical Zone Observatory in Central Pennsylvania. [in preparation for Journal of Hydrology]

## 8. Ecology



**Ecological studies** at the Shale Hills Observatory include patterns of tree water use across the water shed, and how water availability may influence trees at the physiological, community and evolutionary time scales. Measurements include:

- Mapping of tree species distribution, sapwood area and leaf area index
- Transpiration by sap flux
- Tree hydraulic parameters for conducting water and tolerating water stress
- Sources of water uptake

using natural abundance of  ${}^{18}$ O and  ${}^{2}$ H

From this work we hope to improve hydraulic models and our understanding of how water availability shapes the ecology of temperate forest trees.

We characterized the woody vegetation in the watershed by surveying all canopy trees greater than 8" diameter at breast height (DBH). From this data we gained information about the presence, distribution, and dominance of species within the watershed. These data are



Figure 1. Distribution map for Oak species (Quercus spp.) at Shale Hills Critical Zone Observatory. Notice that the species occur preferentially on wetter or drier soils. Maps of soil moisture (blue wetter) are after a period of limited rainfall in August 2005.



Figure 2. Seasonal courses of sap flow (black lines) and soil water potential (red lines) in tree species representing three contrasting wood types: ring-porous (*Quercus prinus*), diffuseporous (*Acer saccharum*) and coniferous (*Pinus virginiana*). While all species exhibit reduced sap flux with reductions in soil water availability, the ring-porous oak is much less adversely affected in recovering sap flux with rewetting later in the season. In contrast, the other two species, show a steady decline in their transpiration rates across the growing season with successive soil drying/ rewetting cycles.

being used to better understand how water availability may influence the ecology of tree species as well as permit scaling of individual estimates of tree transpiration (Figure 1).

Sap flow sensors (heat dissipation probes) have been installed at multiple locations in the watershed in multiple tree species. Data are being continuously logged and transmitted to the web. Trees of different vascular anatomy (ring-porous vessels, diffuse porous vessels, trachieds only - coniferous) seem to have very different responses to wetting and drying events (Figure 2).

Small branch samples have been collected to measure specific conductivity, capacitance, and xylem vulnerability. These parameters make it possible to characterize the hydraulic architecture of the tree and to determine which species make more or less conservative use of water. Six species within the three dominant genera of the watershed were sampled at four different sites. By sampling all species at both wet and dry sites, environmental variation is reduced and we are able to begin to differentiate between genetic adaptation by a species and an individual's plasticity.

When trees take up water from the soil, the water maintains the same concentration of <sup>18</sup>O and <sup>2</sup>H isotopes while it is transported through the tree. By extracting the xylem water from small branches in the canopy, it is possible to determine the isotopic signature of the water taken from the soil. This signature is then compared with the signatures of surface-shallow soil water and deeper ground water. Because each source has a unique signature, we can determine which water source the tree is relying on by how similar the tree's signature is to a source's signature.

Contact: David Eissenstat (PI)

## 9. Watershed Modeling

# March 2011

Hypothesis: When compared to similar but less intensive observations for watersheds chosen along environmental gradients, the observed and predicted rates of regolith formation at Shale Hills provides the basis for quantification of hydrologic and hydrochemical prediction as well as identification of storage reservoirs and preferential pathways in shale-dominated landscapes.

In order to test the hypothesis above and to evaluate our "predictive understanding" of water, solute, energy, and sediment cycles, it was necessary to rapidly implement a first-class observing system at the Susquehanna-Shale Hills CZO and to continue to build a new generation of environmental models capable of simulating pathways, time scales and feedbacks of the system processes. It is not widely recognized that watershed modeling is a data-intensive process. Our approach to synthesis of experimental data and computational models began by developing webbased GIS tools that allow rapid model prototyping and archiving by, with fast access to terabytes of CZO and national data with online data mining, and visualization tools geared to users that are not modelers or scientists but rather focus on policy, planning and decision making. The CZO LIDAR VIEWER (http://pihm.ics.psu.edu/CZO NOSL/Default.aspx) is one example. Although the process is still underway, a model-data integration framework is presently being tested at the Penn State Institute for CyberScience facility for data intensive computing using the Shale Hills testbed. The facility will provide support on-line access to visualization, data analysis tools and other resources necessary for model setup, simulation, scenario building and CZO science support. We have downloaded the necessary national data sets so that model input for weather, climate, soil, land cover and geology for all watersheds in the US. The basic workflow is illustrated in Figure 1. In principal all data and models would reside in a private "CZO-cloud" accessible by all with most technical details transparent to users. The hardware is designed for data-intensive web-based applications and model analysis that are connected to a private cloud to distribute the work load and make the details of model input preparation transparent to the user.

PIHM Model: The Penn State Integrated Hydrologic Model (PIHM) is a multi-process, multiscale hydrologic model for Numerical Watershed Prediction (NWP), where the major hydrological processes are fully coupled using the semi-discrete finite volume method. Instead of coupling through artificial boundary conditions, major hydrological processes are fully coupled by the semi-discrete finite volume approach. For those processes whose governing equations are partial differential equations (PDE), we first discretize in space via the finite volume method. This results in a system of ordinary differential equations (ODE) representing those processes within the control volume. Within the same control volume, combining other processes whose governing equations are ODE's, (e.g. the snow accumulation and melt process); a local ODE system is formed for the complete dynamics of the finite volume. After assembling the local ODE system throughout the entire domain, the global ODE system is formed and solved by a state-of-art ODE solver. PIHM represents a simulation strategy for the solution of process equations at the watershed and river basin scales, and includes a tightly coupled GIS tool for data handling, domain decomposition, optimal unstructured grid generation, and model parameterization. Atmospheric forcing for the watershed from 1979 to present uses the North American Land-Data Assimilation System (NLDAS-2). We have completed the first goal for this element of our research to assimilate the historical and modern measurement data to produce a

complete 30 year hydroclimatic history for the site, with all important land surface and subsurface states simultaneously simulated in space and time. The future of environmental observing systems will certainly utilize embedded sensor networks with continuous real-time measurement of hydrologic, atmospheric, and ecological variables across diverse terrestrial environments. However, the value and contribution of historical data must also be assessed and preserved where it adds to our understanding of the terrestrial water cycle.



**Figure 1.** Typical workflow for PIHM within the Model-Data Integration Framework we are developing at Penn State. Other physical models and tools can be added as required (Phase 5 CBM would be done first under Activity#2). Note that the data and model are accessible as a web service with online GIS and visualization tools. Versioning of simulations, scenarios and the models are handled through Git version control system (<u>http://git-scm.com/</u>) or similar. A desktop interface is also available for modeling and GIS data handling locally using open-source software (<u>http://www.pihm.psu.edu/</u>), which integrates with the web service for model input setup and local model execution.

**Reanalysis 1979-2011:** Watershed reanalysis research is being carried out at the Susquehanna-Shale Hills Critical Zone Observatory (CZO) in central PA to reprocess and assimilate observational data collected at various periods at Shale Hills over a 40+ year span, into a fully coupled integrated hydrologic model at the testbed. Early observations in the 1970's consisted of a spatial array of 40 groundwater level sites measured daily, daily soil moisture records, and 15 minute streamflow records. These data was used for empirical studies by forest hydrologists to resolve the role of antecedent moisture in runoff peak flows within a forest canopy. Over the last 3 years the CZO effort has followed up the early experimental research by deploying a real-time and spatially distributed embedded sensor network (30 sites as of Dec 2010) of soil moisture, soil temperature, soil conductance, groundwater levels, -temperature, -conductance, matric potential, snow depth (15 minute sampling). Shale Hills has a 30m tower with eddy covariance, net radiation, IR surface temperature, and for precipitation a disdrometer, load cell gauge along with a network of tipping bucket rain gauges (10 minute data). Results of hydrologic reanalysis are shown in the figure below for the 2009 calibration period and for the watershed response of a series of storms at Shale Hills after Hurricane Isabel.



Figure 3. Shale Hills Hydrologic Reanalysis for streamflow. Upper plot is the 2009 calibration, lower plot is the are simulations of rainfall-runoff after hurricane Isabel in 2003.

**Real-time hydrologic forecast system (now-cast):** The future of hydrologic forecast system will utilize monitoring station networks with continuous real-time measurement of a branch of informatics, including hydrologic, atmospheric, and pedologic variables across diverse terrestrial water cycle. The research provides a framework to implement a physical-based integrated hydrologic model (Penn State Integrated Hydrologic Model) for real-time hydrologic forecast, and targets a feedback strategies gaining model improvement from forecasting results. Two research questions are being asked:

1) How can we continuously improve the model simulation error and forecast efficiency?

2) How should we optimize the monitoring station networks to improve performance of the real-time hydrologic forecast system?



Figure 1. Real-Time Forecast System framework

Forcing data and initial conditions are major inputs of hydrologic model. A real-time hydrologic monitoring network has been developed to support data observation. The preliminary Real-time Forecast Framework will incorporate a data monitoring system with a hydrologic modeling



Figure 2. Discharge rate from Jan 1 - 6, 2011 Click link for most recent discharge data.

system. There are two modeling systems involved (one for forecast, one for real-time simulation) running independently. Both the systems keep checking if the forcing data is updated. Once forcing data is updated, the corresponding system will restart from the last stop of real-time simulation with the state variable of real-time simulation as initial condition, and move forward until the end of the updated forcing data.

## **Forecast Results**

2009 data is used as a prototype, before we implement the actual weather forecast.

The model started at 2009-1-1. Weather forecasting data came from the observation data with a slight random fluctuation in precipitation and temperature. We are adding to forcing data with one-day records every hour. The forcing data for forecast is three days longer than that of real-time simulation, which represents the weather forecasting results. So we are doing one-day real-time simulation and three-day forecast. A simple webpage of discharge rate shows system output in Figure 2. Real-time simulation starts one day ahead, and forecast model ends three days after.

http://cataract.cee.psu.edu/rt/plot/webpages/index.html

**Age Modeling for Stable Isotopes:** There is now a wide literature on the use of tracer age and transit time distributions to diagnose transport in environmental systems. Theories have been proposed using idealized tracer age modelling for ocean ventilation, atmospheric circulation, soil, stream and groundwater flow. Most approaches assume a steady flow regime and stationarity in the concentration (tracer) distribution function for age, although recent work shows that this is not a necessary assumption. In this paper (Duffy, 2010), dynamic model for flow, concentration, and age in volume-averaged and a spatially distributed watershed system are derived in terms of the moments of the underlying distribution function for tracer age, time, and position. Several theoretical and practical issues are found:

(1) The low-order moments of the age distribution function are sufficient to construct a dynamical system for the mean age and concentration under steady or transient flow conditions.

(2) Solutions to the coupled system of equations for flow, concentration and age show that 'age' of solutes stored within the watershed or leaving the watershed is a dynamic process which depends on flow variations as well as the solute or tracer dynamics.

(3) Intermittency of wetting and drying cycles leads to an apparent increase in the tracer age in proportional to the duration of the 'dry' phase.

(4) The question of how mobile/immobile flow may affect the age of solutes is examined by including a low permeable, passive store that relaxes the well-mixed assumption.

(5). A spatially distributed advective and dispersive transport solution for age evolution over a simple 1-D hillslope is developed to demonstrate the age theory for a distributed source of water and tracer, and the solution is shown to have very similar input–output behaviour when compared to the volume-average model for comparable parameters.

The SSHO\_CZO stable isotope network is currently being used to evaluate the "age" and residence times of stable isotopes at Shale Hills as part of an integrated hydrodynamic model for water, solutes and sediments.

For more information contact:

Christopher Duffy (PI),

Xuan Yu (Ph.D student), Gopal Bhatt (Ph.D student), Lorne Leonard (Ph.D student)

## References

Ek, M. B. 2003, Implementation of Noah land surface model advances in the National Centers for Environmental Prediction operational mesoscale Eta model, JOURNAL OF GEOPHYSICAL RESEARCH, VOL. 108, 8851, 16 PP., 2003, doi:10.1029/2002JD003296

Duffy, C. J. 2010, Dynamical modelling of concentration-age-discharge in Watersheds, Hydrol. Process. 24, 1711–1718 (2010), DOI: 10.1002/hyp.7691

### 2011 Annual Reporting for SSHCZO

### Discipline (Please choose team and list current team members): Hydrogeophysics

#### **Research Progress:**

Last year we completed a suite of borehole logging in wells at the Shale Hills Critical Zone Observatory, including (1) spectral gamma, which measures gamma rays emitted by isotopes of the uranium decay series, the thorium decay series, and potassium-40; (2) caliper, which measures the borehole diameter to locate broken and fractured zone; (3) fluid resistivity, which measures the total dissolved solids in the water column (4) fluid temperature; (5) heat-pulse flowmeter, which indicates the rate and direction of vertical flow within a borehole; and (6) optical televiewer, which provides a continuous, oriented, true-color 360° image of the borehole wall. These data, as well as slug and pump tests to estimate the effective transmissivity of subsurface at this site, were used to determine where to conduct a sodium chloride tracer test in the shale saprolite. We additionally collected soil cores from a continuous hole that extended through the soil profile to quantify also how solute transport behavior changes with depth and weathering.

We have modeled a series of tracer tests in the soil columns, and have begun modeling the field-scale tracer test using fracture flow models to compare with mobile-immobile domain models. We have also been analyzing the resistivity profiles taken during the tracer test to look for improved configurations for follow-on testing using resistivity tomography. The borehole logs have been analyzed using WellCad.

#### Significant Findings:

From the data collected at the SHCZO, we can make the following conclusions: there is substantial variability in the quality of the shale above 6-7 m, after which the shale becomes more homogeneous and less fractured. Pump and slug test indicate a hydraulic conductivity of the shale material on the order of 10-6 m/s. Many of the bedding plane partings seen in the optical televiewer data are not flowing, as indicated from heat-pulse flowmeter data, and hydraulic conductivity and porosity are as low as 10<sup>-15</sup> m/s and 0.035, respectively, in the unfractured shale bedrock. Hydraulic conductivity and porosity of the shallow soils are notably higher, around  $10^{-5}$  m/s and 0.45, respectively. Bromide breakthrough curves from the SHCZO demonstrate significant tailing in soil cores and field tracer experiments, which do not fit classical advection-dispersion processes. To quantify the behavior, numerical simulation of solute transport is carried out with both a mobile-immobile (MIM) model and a continuous-time random walk (CTRW) approach. 1-D MIM modeling results yield low mass transfer rates (<1/d) coupled with large immobile domains. MIM modeling results also suggest that immobile porosity is a combination of soil texture, fractures, and porosity development on shale fragments. 1-D CTRW results yield a parameter set indicative of a transport regime that is consistently non-Fickian within the soil profile and bedrock. These modeling results confirm the important role of preferential flow paths, fractures, mass transfer between more- and less-mobile fluid domains, and advances the need to incorporate a continuum of mass transfer rates to more accurately quantify transport behavior within the SHCZO, as well as estimating age of water, a fundamental variable of interest to geochemists

working at this site. The field-scale tracer test conducted at the soil/shale interface also shows non-Fickian behavior and the expected long tailing.

The borehole logs and fracture flow modeling both show reduced fracture spacing with depth. There is improved fit in the tail of the breakthrough using fracture flow models, but also indications that the fracture network may be nested (both large and small scale fractures).

## Training/Development:

A new masters student started work on the project: Matthew Mercuri, Temple University. Two other masters students have been supported by the project: Brad Kuntz, Penn State University, and Mitchell Johnson, Penn State University.

## Outreach Activities (broadening participation of under-represented / under-served groups):

A diverse group of students from Penn State and two historically black colleges (Jackson State University and Fort Valley State University) participated in a 3-week research experience at the Penn State campus from mid-May to early June. The students conducted tracer, slug, and pump tests, collected ground-penetrating radar and electrical resistivity data, and learned to use wellbore logging tools such as the optical televiewer and spectral gamma logs. They also analyzed and interpreted data, which included creating numerical models of water flow and solute transport using Comsol Multiphysics to extrapolate their field findings to other systems. The field portion of the class was held at the Shale Hills Critical Zone Observatory near the Penn State Campus. Information on the program is available at www.geosc.psu.edu/hydrocamp.

## Conference Abstracts:

CZO All hands meeting, Tuscon AZ May 2011:

Laboratory, Field and Modeling Analysis of Solute Transport Behavior at the Shale Hills Criitcal Zone Observatory (Brad W. Kuntz, Shira Rubin, Brian Berkowitz, Kamini Singha, Laura Toran)

GSA Annual Meeting (submitted), Minneapolis, Oct 2011

Using Groundwater Models to Understand the Effects of Fractures on the Transport of Solutes at the Shale Hills Critical Zone Observatory (Matthew Mercuri, Laura Toran, Jonathan Nyquist, Kamini Singha, and Brad Kuntz)

#### Publications:

Kuntz, B., Rubin, S., Berkowitz, B., and Singha, K. (2011). Quantifying Solute Transport Behavior at the Shale Hills Critical Zone Observatory. *Vadose Zone Journal*, 10, doi:10.2136/vzj2010.0130, 15 p.

# **10. Hydrogeophysics**



**Hydrogeophysics:** The hydrogeology group at the Shale Hills CZO has been exploring solute transport in the shale and shaleproduced soils.

1) What is the importance of the interface between the shale bedrock and the regolith above with respect to flow within the watershed? Is the shale bedrock "impermeable"?

2) How does dead-end pore space affect estimated ages of water at the site?



## 3) How do the parameters controlling solute transport operate within the watershed?

To answer these questions we have been coupling lab and field studies. We have drilled four 17m deep bedrock wells using a portable drill, and have completed a suite of borehole logging in these wells, including (1) spectral gamma, which measures gamma rays emitted by isotopes of the uranium decay series, the thorium decay series, and potassium-40; (2) caliper, which measures the borehole diameter to locate broken and fractured zone; (3) fluid resistivity, which measures the total dissolved solids in the water column (4) fluid temperature; (5) heat-pulse flowmeter, which indicates the rate and direction of vertical flow within a borehole; and (6) optical televiewer, which provides a continuous, oriented, true-color 360° image of the borehole wall. We additionally conducted slug and pump tests to estimate the effective transmissivity of



Figure 2a) Terryl Daniels (PSU undergrad) drills wells with the Portadrill Mini.

subsurface at this site. We have also been conducting tracer tests at the field and lab scale.

From the drilling and wireline logs, we can make the following conclusions: there is a "slow drilling" zone around 6-7 m below land surface, above which is highly weathered shale that is reddish in color, beneath which is largely unfractured blue-grey shale. The natural gamma data similar indicate a higher percentage of clays with depth than in the top 6 m that shows variability in shale bedrock density down to about 6 m.

In field-scale and lab-scale tracer tests, observed transport behavior appears inconsistent with the standard advective-dispersive model. We have collected and

analyzed breakthrough curve (BTC) data to identify the parameters controlling transport. A series of undisturbed fully saturated soil cores were collected in a continuous hole extending across the soil profile vertically at one location to quantify how solute transport behavior changes with physical and chemical weathering. Additionally, we performed a field scale doublet tracer test to determine transport behavior within the weathered shale bedrock. Hydraulic conductivity and porosity are as low as 10<sup>-15</sup> m/s and 0.035, respectively, in the shale bedrock and range as high as 10<sup>-5</sup> m/s and 0.45, respectively, in the shallow soils. Bromide BTCs demonstrated significant anomalous tailing in soil cores and shale bedrock, which do not fit classical advection-dispersion processes. To quantify the behavior, numerical simulation of solute transport was carried out with both a mobile-immobile (MIM) model and a continuous-time random walk (CTRW) approach. 1-D MIM modeling results on the soil cores yielded low



Figure 2b) One of many logging tool. the optical televiewer. Nate Wysocki (PSU undergrad) and Maurice Dukes (Fort Valley State undergrad) control operation.

mass transfer rates (< 1/d) coupled with large immobile domains and revealed that solutes were transported within only 30-40% of the total pore space. MIM modeling results also suggested

that immobile porosity is a combination of soil texture, fracture spacing, and porosity development on shale fragments. Similarly, the field scale doublet tracer test between boreholes indicated fractures are controlling transport and the surrounding shale matrix has a large potential to store and retard solute movement. 1-D CTRW results yielded a parameter set indicative of a transport regime that is consistently non-Fickian across the vertical length of the soil profile, identified solute tracer velocities are up to 50 times greater than the average fluid velocity, predicted that anomalous transport behavior could extend for significant periods of time, and identified the need to incorporate a continuum of mass transfer rates to accurately predict and describe the observed tailing behavior. These modeling results confirmed the important role of preferential flow paths, fractures, and mass transfer between more- and less-mobile fluid domains, and established the need to incorporate a mass transfer process that



utilizes a distribution of mass transfer rates.

Figure 3a (left). Preliminary wireline logs from the four new groundwater wells, with gamma on left and caliper on right. Well CZMW1 is plotted in blue, CZMW2 in green, CZMW3 in yellow, and CZMW4 in red.

Figure 3b (right). Optical televiewer logs shown. CZMW1 is on the left and CZMW4 is on the right.



Contact: Kamini Singha (PI)
#### 2011 Annual Reporting for SSHCZO

#### Discipline: Shale Transect Team

Tim White, Ashlee Dere, Rich April, Elizabeth Knapp, Larry McKay, Mezemir Wagaw, Tom Miller

#### **Research Progress:**

Soil and rock samples have been collected from ridgetops (1-D sites) at all shale satellite sites and analyzed for major elemental chemistry. Quantitative mineralogy for these samples is ongoing. This summer soil samples were collected from 2-D sites (backslope) in New York, Tennessee and Alabama. Analyses of these samples is ongoing.

#### Significant Findings:

Initial results show soil depth increases as a function of temperature, with shallow (~30 cm) profiles in Wales and Pennsylvania varying up to 630 cm deep in Puerto Rico. Depletion profiles of Na, a proxy for feldspar dissolution, are less than 20 % depleted at the surface in Wales and Pennsylvania, 50-60% depleted in Virginia and Tennessee, and 100% depleted at the surface in Puerto Rico. Using estimated soil residence times, apparent activation energies for Na depletion were calculated using different assumptions to range from 15-19 kcal mol-1, values that are slightly higher than those reported for Na plagioclase dissolution in the laboratory

Outreach Activities (broadening participation of under-represented / under-served groups):

An REU summer field school was conducted from June 5 – June 25 in which seven undergraduates, representing Penn State, Juniata College, Washington and Lee University, University of Tennessee, Alabama A&M University and the University of Puerto Rico – Mayaguez, participated in two weeks of field work followed by one week of laboratory work and data processing.

#### **Conference Abstracts:**

Brantley, S.L., Dere A.L. and White T.S. Quantifying rates and mechanisms of shale weathering across a continental-scale climosequence. Mineralogical Magazine *75*:575.

#### **Cross-site Activities**

#### The COsmic-ray Soil Moisture Observing System (COSMOS) successfully deployed the catchment

A non-invasive, intermediate scale soil moisture measurement network consisting initially of 50 probes is up-scaling to 500 probes distributed across the contiguous USA. Recent research progress has determined soil moisture can be inferred from measurements of cosmic-ray neutrons that are generated within soil and emitted back to the atmosphere.

Postdoctoral Research Associate Dr. Trenton Franz, Department of Hydrology and Water Resources at the University of Arizona, has successfully installed the COSMOS probe at Shale Hills. The probe consists of two gas filled chambers and a datalogger, which count and record the number of cosmic-ray neutrons, respectively. Neutrons counted over a period of time are correlated to the volumetric water content over a 700 m diameter circle at 10 cm depth intervals from 10-70 cm of soil. Our instrument is number 39 (See Figure) of the initial 50 to be deployed across the continental United States, with all real-time data freely available to the public to view and download at

<u>http://cosmos.hwr.arizona.edu/Probes/probemap.php</u>. Additional CZO probes are located at Mount Lemmon, AZ part of the Jemez River Basin and Santa Catalina Mountains CZO.



# Location of COSMOS Probes

Click on balloons for site descriptions and data access (site list).

 Soil Moisture (V=volumetric, G=gravimetric, U=uncalibrated)

 ● 0 - 05%
 ● 05 - 15%
 ● 15 - 25%
 ● 25 - 35%
 > 35%
 ○ mixed

#### Additional Collaborations

Infrastructure improvements have been designed in conjunction with the Applied Research Laboratory here at PSU to protect against lightening damage. The lightening isolation and protection equipment (RS485?) is currently being installed on each datalogger with upgrades to complete real-time status of each. Completion of upgrades expected fall 2011.

## 11\_Satellite Site Research

## **March 2011**

#### **Undergraduate Thesis Abstract (2011)**

#### Critical Zone Studies of Shale Weathering in Lares, Puerto Rico

Lorena Vázquez Albelo, Department of Geology, University of Puerto Rico - Mayaguez; Advisor - Thomas E. Miller

As part of the Critical Zone Exploration Network, the University of Puerto Rico at Mayagüez and Penn State University are in collaboration to collect and exchange data to be related to the Critical Zone studies. Textural analysis of two hand dug profiles along with field description has shown that soils above shales in Lares, Puerto Rico are Ultisols with udic moisture regime and excessive development that has an iso-hyperthermic temperature regime. Dominant soils for both, eastern U.S. and west PR are Ultisols. This investigation shows that shale weathering progresses similarly in different climates since soils above shales in Puerto Rico (tropical climate) and soils above shales on Eastern US (template climate) behave similarly in terms of geochemistry. In both places, eastern US and western PR soils have a very low percentage of soluble cations like CaO and K<sub>2</sub>O and shows accumulation of sesquioxides.



Figure 1. Calcium oxide average percentage from Puerto Rico and eastern US



Figure 2. Iron and Aluminum Oxides average percentage from Puerto Rico and Eastern US

## Geological Society of America (GSA) Abstracts 2010

# A Study of Physical and Chemical Weathering of the Marcellus Shale in Central Pennsylvania

J. Paul, R. Mathur\*, S.L. Brantley, and L. Jin

CEKA and Dept. of Geology, Juniata College, Huntingdon, PA 16652 (\*correspondence: mathur@juniata.edu)

The Marcellus shale is well known as a natural gas play in the northeastern United States of America. A fracture density and geochemical study was conducted on Marcellus outcrops in central Pennsylvania to better understand physical and chemical weathering processes and



relationships within the weathering profile of the Marcellus.

For the fracture density study, fifty by fifty centimeter boxes were drawn on various outcrops with chalk. Columns of boxes starting from the bottom of the exposed outcrop to the bottom of the soil profile were produced to obtain a representative sample at the outcrop. Sketches were then constructed depicted all bedding partitions and joints within each individual box. A fracture density value was calculated by adding the

lengths of all the bedding partitions and joints and divided by the area of the box (x / cm). The data shows interesting trends. Joint fracture density values remain constant in respect to depth at all outcrops studied, while bedding partition and total (joints and bedding partitions) fracture density values increase closer to the soil profile at all outcrops studied.

To understand the chemical weathering process, lysimeters were installed to collect water from Marcellus regolith. Lysimeter "nests" located on the ridge top, mid slope, and valley floor of a hill and at depths ranging from 0 to 100 cm were used to quantify concentrations of major and trace elements in soil water. These concentrations are important to understanding the extent of weathering taking place at different depths and topographic locations on the same hill.

#### Goldschmidt Conference Abstracts 2010

#### Clay mineral weathering in shales and soils in the critical zone

#### S. MACDONALD, R.H. APRIL\* AND D.M. KELLER

Geology Department, Colgate University, Hamilton, NY 13346 (\*correspondence: rapril@colgate.edu)

As part of the Shale Hills Critical Zone Observatory (SHCZO) research project, we studied the weathering characteristics of Clinton group (Silurian) shale and overlying soils in a research site in central New York State. This site is the northern-most of six SHCZO satellite sites making up a NS climate-transect that extends from New York to Puerto Rico. We were especially interested in the weathering characteristics of the clay minerals of these deposits, some of which tend to

undergo mineralogical transformations via mixed-laver intermediates. X-ray diffraction analysis (XRD) of bulk shale samples reveals that the shale is composed of quartz, Fe-rich chlorite and illite (mica). Some shale beds contain calcite or dolomite, or both, and feldspar is present in minor amounts. Modelling with NEWMOD© [1] suggests that illite is the most abundant phyllosilicate in the  $<2\mu m$ clay-size fraction (~90%), with chlorite constituting the remainder. Both phyllosilicates are well crystallized.

#### Soils at our study site contain



abundant fragments of Clinton group shale. [Most soils in central New York have developed from glacial sediments (e.g. till and stratified drift) comprising aggregates of sand, silt, clay, and rock fragments derived from ice-scoured bedrock units. The mineralogy of the glacial debris is often heavily influenced by the mineralogy of the local bedrock.] XRD reveals that the bulk soil contains abundant quartz with lesser amounts of feldspar, mica and chlorite. The <2µm clay-size fraction contains illite, illite-vermiculite, chlorite (possibly chlorite-vermiculite) and vermiculite with hydroxy-aluminum interlayers. Kaolinite may be present in minor amounts. Modelling with NEWMOD© reveals that the proportions of soil clays change with depth in the soil profile. For example, illite consitutes 60% of the clay fraction in the 65-70 cm depth interval and decreases in abundance to about 45% in the 0-5 cm interval where near-surface weathering is more intense. Artificial weathering experiments with the shale show that the Fe-rich chlorite is more susceptible to decomposition in a weak acid solution than illite. Clays exfoliated (by

sonification) from the surface of shale fragments collected from the soil were analyzed by XRD and show incipient weathering of clay minerals.

[1] Moore & Reynolds (1997) X-Ray Diffraction and the Identification & Analysis of Clay Minerals, Oxford, p.378.

# 12. Education and Outreach



formation by investigating a series of soils on shale from Wales to New York to Puerto Rico. Each of these "satellite sites" is run with a partner institution and many of these are primarily undergraduate-serving institutions. This work thus provides opportunities for faculty and students at other institutions to interact with scientists from Penn State. Students from each satellite institution spent two weeks this past summer (2010) at PSU learning about Shale Hills and the instrumentation used in

# Shale Satellite Sites

Ashlee Dere (Geoscience, Penn State) and her advisors, Tim White and Sue Brantley, are working to understand the influence of climate on rates of shale weathering and rates of soil

**March 2011** 



the catchment. Those students were taught how to set-up and collect data from a weather station as well as how to describe soils and collect samples. Ashlee and Nicole West (Geoscience, Penn State) have visited almost all the sites to date, working with students and faculty at the corresponding institutions.

Figures: above - Ashlee and Sarah Lemon (Colgate University) collect soil samples at 10 cm intervals; right - Nikki and Karen Lease (University of Tennessee) work to complete a 1m x 1m x 1m soil pit.

#### **International Student Experience**

Lin Ma (Geoscience, Penn State) measured U disequilibrium isotopes on Shale Hills samples at the Univ of Strasbourg with Francois Chabaux. Beth Herndon (Geosciences, Penn State) learned to run mesocosm experiments at Univ of Sheffield. Jennifer Williams and Ashlee Dere

(Geoscience, Penn State) visited Plynlimon, Wales, a shale site that will become part of our satellite sites. During their UK visit, Jennifer and Ashlee were hosted by the British Geological Survey, and encouraged to explore the records room and observe some of Charles Darwin's notebooks.

George Holmes (MS CEE Dept. Penn State) participation in the International CZO Experience started in Vienna, Austria with two weeks visiting scientists at the IAEA (International Atomic Energy Agency). The first week was spent at a short course demonstrating how to operate a Los Gatos



Research Liquid Water Stable Isotope Analyzer. The second week was spent working with Brent Newman on the GNIR (Global Network of Isotopes in Rivers) database. The database was made public this year and Brent is encouraging publishing papers using the data. He also spent time with Tomas Vitvar and Luis Araguas concerning the Shale Hills CZO. The next three weeks were spent in Zurich, Switzerland working with Manfred Staehli at WSL (Swiss Federal Institute for Forest, Snow and Landscape Research). While visiting, he was able to talk with many scientists about the Shale Hills CZO and discuss related projects like the BigLink Damma Glacial Forefield and the Cottbus Watershed in Germany. At WSL he gave a presentation that outlined all three CZO projects with focus on Shale Hills. He was able to visit the Damma Glacier Forefield and see the set up of the instrumentation and travel to the Rietholzbach research catchment. The final week was spent in Davos, Switzerland at the Goldschmidt Conference with many talks related to the Shale Hills CZO.

Bryn Kimball (Geosciences, Penn State) visited Stockholm University, the Royal Institute of Technology (RIT) in Stockholm, Sweden and the University of Sheffield, UK to share and learn of recent research projects focused on mineral dissolution rates. Discussions of chalcopyrite dissolution rates and variability by orders of magnitude helped to further her understanding of rock dissolutions and what minerals likely contribute the most elemental release. A formal presentation of Bryn's chalcopyrite dissolution project was delivered to Dr. Malmstrom (RIT) and Dr. Wold (RIT). Additional mineral dissolution data was compiled from experiments conducted in laboratories (Dr. Sara Holmstrom) and field projects (Dr. Birgitta Kalinowski) in Stockholm and Sheffield (Dr. Steven Banwart). The minerals thus far include olivine, biotite, biogenic Mn-oxides, and Mn-substituted goethite, pyrite, illite, kaolinite, albite and quartz.



#### Hydrology Field Camp

A diverse group of students from Penn State and two historically black colleges (Jackson State University and Fort Valley State University) participated in a 3 week research experience at Penn State campus from Mid-May through early June. Students conducted tracer, slug and pump tests, collected ground penetrating radar and electrical resistivity data and learned to use wellbore logging tools such as the optical televiewer spectral gamma logs. They also analyzed and interpreted data, which included developing numerical models of water flow and solute transport using Comsol Multiphysics to extrapolate their field findings to other systems. The field portion of the class was conducted at the Shale Hills Critical Zone Observatory. *Figure: Claudia Shuman (Penn State) and Tramond Baisden (Fort Valley State) introduce tracer into a stream at Leading Ridge*.

## **CZO Field School**

The Shale Hills CZO is a research and teaching platform open to the academic community that supports general environmental education especially as it relates to environmental information, modeling and earth systems infrastructure. The inaugural field school was offered May 31 - June 9 and attracted 16 participants (undergraduate to post-doc) from 9 countries. During the two week school, the junior scientists experienced field techniques, instrumentation set-up and deployment, as well as modeling and database utilization. The data and models generated at Shale Hills and the



Taru Lehtinen (left), Silviya Yordanova (middle) and Georg Lair (right) discuss soil horizon classification.

surrounding region are widely used in the classroom by CZO scientists and grad students as well as non-CZO researchers through the real-time capability. To date, several of the international participants have begun collaborative research projects initiated during the school.

#### **PIHM Workshop**

As part of our Critical Zone cross-site activities, the Shale Hills CZO helo a workshop August 2-4, 2010 titled: Multiscale Modeling Using the Penn State Integrated Hydrologic Modeling System (PIHM). PIHM is multi-process, multi-scale hydrologic modeling tool, where the physical processes are fully coupled using the semi-discrete finite volume method (http://www.pihm.psu.edu). This workshop provided hands-on experience in using PIHM for modeling watershed dynamics. Participants learned to use a customized GIS interface to PIHM (called PIHMgis) for *i*) automated ingestion of model parameters from national databases, *ii*) conditional domain decomposition of the model domain, *iii*) performed multistate simulations and calibration and *iv*) visualized model results. A goal of the workshop was to stimulate crosssite CZO modeling activities.

The Departments of Anthropology and Civil and Environmental Engineering hosted Jaime J. Carrera-Hernández, PhD, Professor of Applied Geosciences at Instituto Potosino de Investigación Científica y Tecnológica (IPICyT) in San Luis Potosí, México on August 4, 2010. Dr. Carrera's nterests are in the analysis of the impact that human activities have on the hydrological cycle and on the development of tools to analyze water management policies. He is also interested in the use of remotely sensed imagery for the development of physically-based, distributed hydrogeological modeling along with the use of Relational Databases for the efficient development of these models, as exemplified in the Basin of Mexico Hydrogeological Database (BMHDB). Carrera has applied some of these tools to estimate potential aquifer recharge in the Basin of Mexico and to analyze the impact that urban growth has had on aquifer recharge.



## **STEM Field School**

The State College Area School District, SCASD, has formed a summer STEM Academy, a new initiative that uses field and experiential instructional techniques to engage our students in STEM areas. The goal of this Academy was to improve the middle school to high school transition by engaging students early in their high school career with academic experiences of the highest caliber. Incoming first year high school students along with preservice and master teachers learned how to measure and monitor soil moisture, collect GPS

data, install a weather station, and observe the hydrologic cycle through rain and groundwater simulation systems. Data collected from school premises will be compared to data streaming from the catchment to develop STEM curriculum modules, thus engaging students in relevant, project-based collaborative research.

#### REU 2008-2010

<u>2010</u> - Two ecology REU's, Shelley Pickett and John Govannicci, studied the spatial and temporal dynamics of vegetation structure in relation to hydrology. Initial measurements of spatial data from the beginning of the growing season (April, 2010) for leaf area index (LAI), canopy closure, and tree height were collected. The students worked with Dr. Eissenstat and Katie Gaines (PhD student) and developed a model code to predict spatial processes. Based on the spatial map of LAI we selected regions of low, intermediate and high LAI to study the inter- and intra-specific differences in maximum light use efficiency (REU Project: John figure right) and leaf structure (REU Project: Shelly figure left) of plants living in different light environments.



One additional REU, Gabrielle Dernier (REU - Hydrology) from Rose Hulman College carried out hydraulic tests on 20 wells at Shale Hills and compiled a report showing the mean distribution of hydraulic conductivity with depth for the watershed. This work is critical to modeling study.

<u>2009</u> - Nick Kaiser's summer REU project focused on the measurement of soil respiration in the Shale Hills catchment. He was mentored by Dr. Jason Kaye, Dr. Lixin Jin (postdoc), and Danielle Andrews (graduate student). Over the summer, Nick tested hypotheses regarding





relationships among soil CO2 concentrations, soil respiration, and soil microclimate. He made weekly trips to the field site where he used soil access tubes to sample soil gas from multiple depths. At the same locations he measured soil moisture using at TDR probe, and surface soil respiration using a portable infrared gas analyzer and soil cover (a chamber used to capture CO2 diffusing out of the soil). Using Fick's law of diffusion he predicted soil CO2 flux throughout the profile and compared these values to soil moisture, soil temperature, and surface soil flux measured with the soil cover. His work has led to important insights on the role of soil water in

controlling gas diffusion, and has inspired the possible use of simple gas access syringes for cheap, highly replicated measurements of soil respiration. At the end of the summer, Nick attended the Ecological Society of America meeting in Albuquerque where he was exposed to a wide array of carbon cycling talks that provide context for his work at Shale Hills. Nick was a student at Gannon University in northwestern PA where he double-majored in math and chemistry.

Three additional students, Kristen Jurinko, Jose Morales, and Shaquandra Wilson engaged in projects ranging from the quantitative relationships between soil moisture, geology, tree distribution, and topography to metal concentrations in leaf vegetation to developing new membranes for use in root boxes to image enzyme production around roots.

<u>2008</u> - Susquehanna Shale Hills, a forested, temperate-climate catchment in central Pennsylvania, has been designated a Critical Zone Observatory. Through analysis of hydrologic, geochemical, geomorphologic, and biological processes at Shale Hills, our goal is to understand how natural processes interact and shape this site. However, until recently, the biological characteristics of Shale Hills had not been adequately considered.

Therefore, the goal of this study was to take initial steps in characterizing the microbial community of Shale Hills. John Fleming, an REU student at PSU in the summer of 2008, collected soil samples from various depths at a valley floor location at Shale Hills. Through selective culturing, chemical and biological analyses, the presence of iron-related bacteria (iron reducers and oxidizers), sulfate-reducing bacteria, and various aerobic heterotrophic bacteria were indicated throughout the depth profile.



Two additional students, Melissa M. Melendez-Oyola (University of Puerto Rico, Rio Piedras Campus - Environmental Science) and Colin Duffy (Pennsylvania College of Technology, Electronics, and Computer Engineering Technology) learned research techniques through the Horticulture Department and Civil and Environmental Engineering Department, respectively.

#### 13. In the Press

#### July 2011

#### July 6, 2011 Deployment of Non-Invasive Soil Moisture Instrumentation a Success

Postdoctoral Research Associate Dr. Trenton Franz, Department of Hydrology and Water Resources at the University of Arizona, has successfully installed the COSMOS probe at Shale Hills. The probe consists of two gas filled chambers and a datalogger, which count and record the number of cosmic-ray neutrons, respectively. Neutrons counted over a period of time are correlated to the volumetric water content over a 700 m diameter circle and 10-70 cm of soil. Our instrument is number 39 of the initial 50 to be deployed across the continental United States, with all real-time data freely available to the public to view and download at <a href="http://cosmos.hwr.arizona.edu/Probes/probemap.php">http://cosmos.hwr.arizona.edu/Probes/probemap.php</a>.

## June 4, 2011 – Nine Undergraduates Complete the 3rd Annual Hydrogeophysics Field Camp

The 3rd annual hydrogeophysics field camp, offered by Dr. Kamini Singha, has come to completion. Nine undergraduate participants, from rising sophomores to rising seniors, spent three weeks collecting a wide range of data from the CZO and nearby Lake Perez. New data included images from the optical televiewer and gamma logs, GPR, pumping/slug tests and electrical resistivity measurements. Using COMSOL, a multiphysics software designed for analysis and visualization, the students built numerical models and learned the intricacies of field data interpretation.

# June 1, 2011 – CZO REU Summer Field School Brings 7 Undergraduates from Collaborating Institutions

This summer, the CZO Field School adds a new dimension with two weeks of field work followed by one week of data analysis. Undergraduate participation includes two students from the University of Puerto Rico Mayaguez, one student from Alabama A&M Univ., one from University of Tennessee, one from Washington & Lee University, one from Juniata College and one from Penn State. Field work, organized by Dr. Tim White and Ashlee Dere (PhD Candidate), will complete research at the CZO Shale Transect sites in New York, Virginia, Tennessee and Alabama. Work will include sampling and digging soil pits on hillslopes, GPR transects, shale fracture density and tree throw measurements.

# May 16, 2011 - National CZO All Hands Meeting hosted by University of AZ takes place at the Biosphere 2

Team members from each of the 6 national CZO's gathered at the Biosphere 2 to share research progress and develop new directions for cross CZO research. The program included 2 full days of oral and poster presentations in addition to a tour of the Santa Catalina Mountains including stops at Soldier Canyon, Mt. Bigelow eddy covariance tower and Marshall Gulch catchment experiments. Created as a model for Biosphere 1, our Earth, the Biosphere 2 was an ideal locale to host scientists who study the zone where rock meets life, The Critical Zone. To learn more about Biosphere 2.....click here.

# March 21, 2011 - The COsmic-ray Soil Moisture Observing System (COSMOS) is coming to the catchment

A non-invasive, intermediate scale soil moisture measurement network consisting initially of 50 probes is upscaling to 500 probes distributed across the contiguous USA. Recent research progress has determined soil moisture can be inferred from measurements of cosmic-ray neutrons that are generated within soil and emitted back to the atmosphere. Probe deployment is targeted for summer 2011 with the real-time data available to for the public to view.

## February 22, 2011 - The passing of Kelly Cherrey has touched the SSHCZO community

It is with sadness yet great appreciation we pay tribute to one of our own, Kelly Cherrey. Cherrey worked tirelessly to build the communication and backbone physical structure at the Shale Hills watershed. He made things work and work well, which is an art unto itself. Through his work, the CZO team gained reliability in data and communication that we are using and building on today. We are grateful for all of the hard work Kelly contributed mostly on his own and to our benefit, for which we say - Thank you. You left this Earth much too soon and it enlightens all of us of how very precious every life is. For words most fitting by Alfred Lord Tennyson.....<u>click here</u>.

# December 20, 2010 - Environmental DNA from SSHCZO soil to be analyzed in international study

The DNA Sequencing Research Group (DSRG) of the Association of Biomolecular Resource Facilities (ABRF), an international group of scientists from 140 core laboratories, is conducting a comparison of high-throughput parallel sequencing technologies on selected environmental DNA samples. On the recommendation of Mary Ann Bruns, PSU Associate Professor of Crop and Soil Sciences, soil DNA from the SSHCZO (Rushtown series, A/A2 horizons) will be included in the study. According to Bruns, the wealth of soil biogeochemical data collected at the CZO site adds value to the "metagenome" information obtained by DSRG. Provision of key soils information is consistent with the mission of the Genomics Standards Consortium for international DNA sequence databases. The Bruns lab will obtain DNA using two different soil extraction methods. Deb Grove, Director of the Huck Institutes of Life Sciences Genomics Core Facility at Penn State, will be involved in high-throughput sequencing of two "pools" of environmental DNA-small subunit ribosomal RNA genes and shotgun metagenome fragments. Results will be presented at 2011 ABRF meeting Feb 19 in San Antonio, TX.

## December 13, 2010 - Paper highlights manganese contamination in soils

Elizabeth Herndon, PhD candidate in Geosciences, and co-authors have determined that iron furnaces in operation during the 1700s and 1800s may have left toxic levels of manganese in Pennsylvania soils. Researchers identified the manganese enrichment after sampling various sites within the Susquehanna Shale Hills CZO. By examining soil chemistry from around the world, the team concluded the increased manganese levels were the result of industrialization. For the full story, visit: Penn State Live - SciTech or NSF News.

# November 11, 2010 - Best Paper Award for 2010 SSSA Forest, Range and Wildland Soils Session

Danielle Andrews, PhD candidate in Crop and Soil Science, was recognized for her research accomplishments at this year's Soil Science Society of America annual meeting in Long Beach, CA. Her paper entitled "*The Carbon Story at the Shale Hills Critical Zone Observatory*" was selected as the best paper in Session 328: Soil Carbon Dynamics. Her accomplishment will be rewarded with a certificate from the Soil Science Society of America in the S7 Business Meeting at next years SSSA Meeting in San Antonio, TX.

# October 25, 2010 - Shale Hills CZO featured article in Research|PennState

Members of the University Research Magazine Association and the National Association of Science Writers focused a September article on the Critical Zone, specifically Shale Hills. Weekly features, designed to inform and inspire the University community, highlight current research by telling the story. Interviews with Dr. Chris Duffy and Dr. Susan Brantley shed light on the various research questions posed by different disciplines and how the watershed has sparked interest from other Penn State researchers. For the complete article, visit <u>Research|Penn</u> <u>State</u> or download the pdf <u>Critical Zone</u>.

## October 8, 2010 - CZO hosts students and faculty from University of Pittsburgh

The Pitt Chapter of IAHR, the International Association of Hydro-Environment Engineering and Research, spent a day in the catchment visiting with Professor Christopher J. Duffy, Civil and Environmental Engineering, about ongoing research projects, instrumentation and technology. This student group has specific interests in research with engineering applications. Although the engineers focus is primarily water resources and sediment transport, forward progress suggests the interactions of river and coastal hydraulics, risk analysis, energy, environment, disaster prevention, and industrial processes must be taken into consideration when addressing future societal needs. Students are seeking to expand their knowledge base through interactions from neighboring disciplines, with Shale Hills an ideal laboratory for collaborative projects.

## August 10, 2010 - State College Area School District teams with PSU for STEM studies

The SCASD has formed a summer STEM Academy, a new initiative that uses field and experiential instructional techniques to engage our students in STEM areas. The goal of this Academy is to improve the middle school to high school transition by engaging students early in their high school career with academic experiences of the highest caliber. Incoming first year high school students along with pre-service and master teachers will learn how to measure and monitor soil moisture, collect GPS data, install a weather station, and observe the hydrologic cycle through rain and groundwater simulation systems. Data collected from school premises will be compared to data streaming from the catchment to develop STEM curriculum modules, thus engaging students in relevant, project-based collaborative research.

# August 9, 2010 - PI's from CZO organizing AGU session on hydrologic processes

As scientists from all over the world converge in San Francisco, CA this fall for the annual meeting of the American Geophysical Union, PI's from Penn State (Chris Graham, Kevin Dressler, and Chris Duffy) will convene a hydrology session "The Role of Isotope Networks in Environmental Observatories." This session is envisioned as bringing together researchers who are using stable isotope measurements (water, carbon and other isotopes) in the fields of surface hydrology, ecohydrology, tree physiology and groundwater hydrology. It is of special interest to anyone who is working at some of the hydrological observatory networks (such as CZO, LTER, NEON etc...). Abstracts for presentations are now being accepted on topics ranging from determining flow patterns and flow rates to the design and implementation of isotope networks. Additional session details can be found at <u>2010 AGU Fall Meeting</u>. Search for session H84.

# August 2, 2010 - Sanders Seminar Series hosts Jaime J. Carrera-Hernández, PhD

The Departments of Anthropology and Civil and Environmental Engineering will host Jaime J. Carrera-Hernández, PhD, Professor of Applied Geosciences at Instituto Potosino de Investigación Científica y Tecnológica (IPICyT) in San Luis Potosí, México on August 4, 2010. Dr. Carrera is interested in the analysis of the impact that human activities have on the hydrological cycle and on the development of tools to analyze water management policies. He is also interested in the use of remotely sensed imagery for the development of physically-based, distributed hydrogeological modeling along with the use of Relational Databases for the efficient development of these models, as exemplified in the Basin of Mexico Hydrogeological Database (BMHDB). Carrera has applied some of these tools to estimate potential aquifer recharge in the Basin of Mexico and to analyze the impact that urban growth has had on aquifer recharge.

# July 26, 2010 - Airborne LiDAR survey completed for Susquehanna Watershed

Last week, NCALM, NSF's National Center for Airborne Laser Mapping completed an airborne laser mapping flight over the Susquehanna/Shale Hills Critical Zone Observatory. The area flown was ~200 km<sup>2</sup> for the purpose of a leaf-on survey of the Shaver Creek watershed which includes the Shale Hills catchment. The goal of the survey is to identify tree species distribution, leaf area and abundance over the watershed. Extensive ground-based validation sites were surveyed during the campaign in conjunction with LiDAR survey. This most recent fly-over will provide high-resolution imagery at the 0.5 m scale. Data collected from this flight will be available for use in conjunction with maps of the regional geology, soils, instrumentation site surveys and PASDA (the Pennsylvania Spatial Data Access). An interactive version is currently under development with accessibility from this website in the future.

# June 29, 2010 - Multiscale Modeling Workshop will be hosted by Shale Hills CZO

As part of our Critical Zone cross-site activities, the Shale Hills CZO will be holding a workshop August 2-4, 2010 titled: Multiscale Modeling Using the Penn State Integrated Hydrologic Modeling System (PIHM). PIHM is multi-process, multi-scale hydrologic modeling tool, where the physical processes are fully coupled using the semi-discrete finite volume method (http://www.pihm.psu.edu). This workshop will provide hands-on experience in using PIHM for modeling watershed dynamics. Participants will learn to use a customized GIS interface to PIHM (called PIHMgis) for *i*) automated ingestion of model parameters from national databases, *ii*)

conditional domain decomposition of the model domain, *iii*) performing multistate simulations and calibration and *iv*) visualization of model results. A goal of the workshop is to stimulate cross-site CZO modeling activities.

# June 1, 2010 – 1st CZO Field School Brings 16 Participants from 14 Institutions across 9 Countries

The first week of a two week field school opened on Monday with 16 participants, including both undergraduates and graduates/post-docs. Field school attendees will experience a range of activities such as: discussions of Critical Zone science, SSHO and CZO modeling, laboratory tours, regional geology, field instrumentation and GIS applications. Each of the disciplines with active projects in the catchment will provide hands-on activities to introduce and train the junior scientists. The overarching goal of the school is to develop a new international interdisciplinary cadre of Critical Zone scientists.

# May 25, 2010 - Collaborations with outside institutions to begin Spring 2011

Princeton scientists, <u>Dr. Francois Morel</u> and <u>Dr. Anne Kraepiel</u>, will collaborate at Shale Hills to advance our understanding of nitrogen fixation in the laboratory and the catchment. The fertility of ecosystems is often limited by the amount and availability of nitrogen. PI's will investigate how aerobic soil bacteria acquire metals and how the kinetics of that reaction limit N2 fixation in terrestrial systems.

# April 16, 2010 - Hydrogeophysics Field Camp Returns for 2nd year

This summer, nine undergraduate students will be taking Geosc 397A: The Hydrogeophysics Field Experience with Dr. Kamini Singha from May 17 to June 4. Four students will be from Penn State, two from Jackson State University in MS and three from Fort Valley State University in GA. These students will combine field experimentation, data analysis, and numerical modeling with in-class instruction during the three-week program to develop and test hypotheses regarding the processes controlling solute transport. The Shale Hills Critical Zone Observatory near Shaver's Creek Environmental Center is the "home base" for this field camp due to its proximity to the Penn State campus and its facilities.

Environmental consultants, government employees, and researchers from small companies will be coming through the field camp to demonstrate hydrogeophysical field equipment and highlight jobs in environmental fields. The students will learn basics of pumping tests, tracer tests, and slug tests as well as have exposure to geophysical techniques such as electrical resistivity, wireline logging, and ground-penetrating radar. Any students, staff, or faculty, interested in hydrology or environmental science are welcome to attend field demonstrations if they are interested; please contact Kamini Singha at kxs55@psu.edu.

# April 1, 2010 - Terrestrial LIDAR Comes to the Catchment

PI's Eric Kirby and Rudy Slingerland and PhD student, Nicole West, hosted A.J. Herrs (University of Kansas) from March 21st – 23rd to conduct high-resolution imaging of micro-

topography along hillslopes within the Shale Hills CZO catchment. Herrs used a terrestrial, tripod-mounted LiDAR (Light Detection and Ranging) to scan the topography of the catchment from multiple points; geodetically referenced prisms and reflectors were used to tie multiple scans into a single image. Measurements from the ground-based LiDAR are collected at much finer resolution (decimeter scale) than airborne LiDAR (approximately 1.5 meter). This resolution will enable the researchers to characterize pit-and-mound topography characteristic of soil mixing by tree-throw.

## **14. Journal Publications**

# 2011

Lin, Henry, Hopmans, Jan W., deB Richter, Daniel. Interdisciplinary Sciences in a Global Network of Critical Zone Observatories. *Vadose Zone Journal* 10:781-785, doi:10.2136/vzj2011.0084.

Graham, C., and H.S. Lin. Controls and Frequency of Preferential Flow Occurrence: A 175event Analysis. *Vadose Zone Journal* doi:10.2136/vzj2010.0119.

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Jin, L., Andrews, D.M., Holmes, G.H., Lin, H., and Brantley, S.L. Opening the "Black Box": Whater Chemistry Reveals Hydrological Controls on Weathering in th Susquehanna Shale Hills Critical Zone Observatory. *Vadose Zone Journal* 10:928-942, doi:10.2136/vzj2010.0133.

Andrews, D.M., H. Lin, Q. Zhu, L. Jin, S.L. Brantley. Hot Spots and Hot Moments of Dissolved Organic Carbon Export and Soil Organice Carbonn Storage in the Shale Hills Critical Zone Observatory. *Vadose Zone Journal* 10:943-954, doi:10.2136/vzj2010.0149

Nicole West, Eric Kirby, Paul Bierman, Dylan Rood. Preliminary estimates of regolith generation and mobility in the Susquehanna Shale Hills Critical Zone Observatory, Pennsylvania, using meteoric <sup>10</sup>Be. *Applied Geochemistry* 26:S146–S148, doi:10.1016/j.apgeochem.2011.03.053.

Xianzeng Niu, Kerstin A. Lehnert, Jennifer Williams, Susan L. Brantley. CZChemDB and EarthChem: Advancing management and access of critical zone geochemical data. *Applied Geochemistry* 26:S108–S111, doi:10.1016/j.apgeochem.2011.03.042

Lin Ma, Lixin Jin, Susan L. Brantley. Geochemical behaviors of different element groups during shale weathering at the Susquehanna/Shale Hills Critical Zone Observatory. *Applied Geochemistry* 26:S89–S93, doi:10.1016/j.apgeochem.2011.03.038.

Lixin Jin, Susan L. Brantley. Soil chemistry and shale weathering on a hillslope influenced by convergent hydrologic flow regime at the Susquehanna/Shale Hills Critical Zone Observatory. *Applied Geochemistry* 26:S51–S56, doi:10.1016/j.apgeochem.2011.03.027.

Elizabeth M. Herndon, Susan L. Brantley. Movement of manganese contamination through the Critical Zone. *Applied Geochemistry* 26:S40–S43, doi:10.1016/j.apgeochem.2011.03.024.

S.L. Brantley, H. Buss, M. Lebedeva, R.C. Fletcher, L. Ma. Investigating the complex interface where bedrock transforms to regolith. *Applied Geochemistry* 26: S12–S15, doi:10.1016/j.apgeochem.2011.03.017.

Shuangcai Li and Christopher J. Duffy. Fully coupled approach to modeling shallow water flow, sediment transport, and bed evolution in rivers. *WATER RESOURCES RESEARCH* VOL. 47, W03508, doi:10.1029/2010WR009751.

Zhang, J. H.S. Lin, and J. Doolittle. Subsurface Lateral Flow as Revealed by Combined Ground Penetrating Radar and Real-Time Soil Moisture Monitoring. Submitted to *Hydrological Processes*.

Takagi, K. and H.S. Lin. Soil-Terrain Attributes in Relation to Surface and Subsurface Soil Moisture in the Shale Hills Catchment. Submitted to *Geoderma*.

Laura J. Liermann, Ryan Mathur, Laura E. Wasylenki, Jochen Nuester, Ariel D. Anbar, and Susan L. Brantley. Extent and isotopic composition of Fe and Mo release from two Pennsylvania shales in the presence of organic ligands and bacteria. *Chemical Geology* vol 281, 167-180.

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Anderson, S.A., R. C. Bales, and C. J. Duffy. Critical Zone Observatories: Building a network to advance interdisciplinary study of Earth surface processes. *Mineralogical Magazine*, 72(1), pp 7-10.

Brantley, S. L. Understanding Soil Time. Science 321, 1454-1455.

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Kumar, M., G. Bhatt, and C.J. Duffy, An efficient domain decomposition framework for accurate representation of geodata in distributed hydrologic models. *International Journal of Geographical Information Science*, 23(12):1569-1596.

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# **Books, Theses and Other One-time Publications**

# 2011

Holmes III, G.H., Usings  $\delta^2$ H AND  $\delta^{18}$ O To Determine The Flowpaths and Timescales of Water at the Susquehanna Shale Hills Critical Zone Observatory, Master of Science, Pennsylvania State University, p. 70.

Holleran, M.E., A Quantitative Analysis of Deep Shale Weathering at the Shale Hills Critical Zone Observatory, Bachelor of Science, Pennsylvania State University, p. 38.

Andrews, D.M., Coupling Dissolved Organic Carbon and Hydropedology in the Shale Hills Critical Zone Observatory, Doctor of Philosophy, Pennsylvania State University, p. 233.

### 2010

Kuntz, B., Laboratory, Field, and Modeling Analysis of Solute Transport Behavior at the Shale Hills Critical Zone Observatory, Master of Science, Pennsylvania State University, p. 73.

Li, W., Implementing the Shale Hills Watershed Model in Application of PIHM, Master of Science, Pennslyvania State University, p. 97.

Mizsei, D., Rates and Mechanisms of Soil Carbon Sequestration at the Shale Hills Critical Zone Observatory, Bachelor of Science, Pennsylvania State University, p. 51.

Wubbles, J., Tree species distribution in relation to stem hydraulic traits and soil moisture in a mixed hardwood forest in central Pennsylvania, Master of Science, Pennslyvania State University, p. 39.

## 2009

Herndon E.M., Jin L., and Brantley S.L., Impact of aeolian deposition on Mn cycling in soils. 19th V.M. Goldschmidt conference, Davos, Switzerland.

Jin, L., Rother, G., Cole, D., and Brantley, S. L., Characterizing weathering fronts of shales by small angle neutron scattering: pores and interconnectivity. American Chemical Society annual meeting, Washington DC.

Kumar, M., Toward a Hydrologic Modeling System, Doctor of Philosophy, Pennsylvania State University, p. 251.

Takagi, K., Static and Dynamic Controls of Soil Moisture Variability in the Shale Hills Catchment, Master of Science, Pennsylvania State University, p. 68.

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Zhang, J., H.S. Lin., and J. Doolittle. Identification of subsurface flow pattern using a combination of Ground Penetrate Radar and real-time soil moisture monitoring. The 1st International Conference on Hydropedology, July 28-31, 2008, Penn State, University Park, PA.

A set of 3 DVD for The 1st International Conference on Hydropedology held July 28-31, at Penn State Univ. in University Park, PA.

## 2007

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