Annual Report for Period: 11/2009 - 10/2010 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: 07/31/2010 Award ID: 0725019

#### **Project Participants**

# **Senior Personnel** Name: Duffy, Christopher Worked for more than 160 Hours: Yes **Contribution to Project:** 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: Toran, Laura Worked for more than 160 Hours: Yes **Contribution to Project:** Hydrogeophysics Name: Singha, Kamini Worked for more than 160 Hours: Yes **Contribution to Project:** Hydrogeophysics Name: Davis, Kenneth Worked for more than 160 Hours: Yes **Contribution to Project:** Meteorology Name: Eissenstat, David Worked for more than 160 Hours: Yes **Contribution to Project:** 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
Contribution to Project:	
Nome: Tuttle Michelle	
Worked for more than 160 Hours:	No
Contribution to Project.	110
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.	110
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
<b>Contribution to Project:</b>	
Geochemistry Informatics	
Name: Miller, Tom	
Worked for more than 160 Hours:	Yes
<b>Contribution to Project:</b>	
Name: Fedo, Chris	
Worked for more than 160 Hours:	Yes
Contribution to Project:	

# Post-doc

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

#### Training and Development:

Opportunities for Training, Development, and Mentoring

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

Name: Andrews, Danielle, PhD Soil Science
Name: Baldwin, Doug, MS Soil Science
Name: Bhatt, Gopal, PhD (2010) Civil and Environmental Engineering
Name: Herndon, Beth, Geoscience
Name: Holmes, George, (2010) MS Civil and Environmental Engineering
Name: Jun Zhang, PhD (2009) soil science
Name: Ken Takagi, MS (2009) soil science
Name: Kumar, Mukesh\*, PhD (2009) Civil and Environmental Engineering
Name: Brad Kuntz, MS (2010) Geosciences
Name: Fuller, Robert, PhD Geosciences
Name: Li, Wenfang, MS (2009) Civil and Environmental Engineering
Name: Li, Shuangcai\*, PhD (2008) Civil and Environmental Engineering
Name: Yesavage, Tiffany, PhD Geosciences
Name: Williams, Jennifer PhD Geosciences
Name: Yu, Xuan, PhD Civil & Environmental Engineering

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. S Riggins (Univ of CO, Boulder) visited the British Geological Survey. As a graduate student working on the Shale Hills Critical Zone Observatory she was able to travel to both Austria and Switzerland for a total of six weeks. While in both countries she was able to create a relationship with scientists working on projects similar to the Shale Hills CZO, and was able to further her 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.

Undergraduate Students working on the Shale Hills CZO:

Nick Kaiser , Geosciences PSU Jose Morale , 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 Morale

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 Contribution to Project: (see Geophysics)

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. This summer, 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.

2. 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 ~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 )

3. 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.

4. 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.

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5. 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.

6. 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.

7. 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.

7. 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).

8. Collaboration is occurring with the Shaver's Creek Environmental Center to share our new 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.

9. 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 identifying 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,

Lin, H.S.;;Vogel, H.J.;;Seibert, J.;, "Towards holistic studies of the Earth's Critical Zone: Hydropedology perspectives", Hydrology and Earth System Science, p. 479-480, vol. 14, (2010). Published,

Lin, H.S.; Fluhler, H.; Otten, W.; Vogel, H.J.;, "Soil Architecture and Preferential Flow across Scales", Journal of Hydrology, p., vol., (2010). Published,

Zhang, J.;;Lin, H.S.;;Doolittle, J.;, "Subsurface Lateral Flow as Revealed by Combined Ground Penetrating Radar and Real-Time Soil Moisture Monitoring", Hydrologic Processes, p., vol., (2010). Submitted,

Graham, C.G.; Lin, H.S., "Spatial-temporal patterns of preferential flow occurrence in the Shale Hills CZO based on real-time soil moisture monitoring", Vadose Zone Journal special issue, p., vol., (2010). to be submitted for special issue,

Lin, H.S., "On the study of soils and the Critical Zone: Time vs. space, evolution vs. conservation, biology vs. physics, and beyond", Soil Science Society of America Journal, p., vol., (2010). in revision,

Takagi, K.; Lin, H.S., "Temporal Evolution of Soil Moisture Spatial Variability in the Shale Hills Catchment", Journal of Hydrology, p., vol., (2010). Submitted,

Takagi, K.; Lin, H.S., "Temporal Evolution of the Correlations between Soil-Terrain Attributes and Surface-Subsurface Soil Moisture", Geoderma, p., vol., (2010). Submitted,

Duffy, Christopher, "Dynamical modelling of concentration-age-discharge in watersheds", Hydrological Processes, p. 1711, vol. 24, (2010). Published, 10.1002/hyp.7691

# **Books or Other One-time Publications**

Brantley, S. L., White, T. S., Ragnarsdottir, K. C, "The Critical Zone: Where Rock Meets Life", (2007). Book, Published Editor(s): Brantley, S. L., White, T. S., Ragnarsdottir, K. C. Collection: Elements Bibliography: 3

Lin, H.S., E. Brook, P. McDaniel, and J. Boll, "Hydropedology and Surface/Subsurface Runoff Processes", (2008). Book, Accepted Editor(s): M. G. Anderson Collection: Encyclopedia of Hydrologic Sciences Bibliography: John Wiley & Sons, Ltd.

Bhatt, G. M. Kumar, and C.J. Duffy, "Bridging the Gap between Geohydrologic Data and Distributed Hydrologic Modeling", (2008). Book, Published Editor(s): M. S?nchez-Marr?, J. B?jar, J. Comas, A. Rizzoli and G. Guariso Collection: Integrating Sciences and Information Technology for Environmental Assessment and Decision Making

Information Technology for Environmental Assessment and Decision Bibliography: Proceedings iEMSs 2008: International Congress on Environmental Modelling and software

Kumar, M. and C.J. Duffy, "Shared Data Model to Support
Environment Sensor Network Data in
Hydrologic Models", (2008). Book, Published
Editor(s): M. S?nchez-Marr?, J. B?jar, J. Comas, A.
Rizzoli and G. Guariso
Collection: Proceedings International Congress on Environmental Modelling
and Software
Information Technology for
Environmental Assessment and
Decision Making
Bibliography: Integrating Sciences and Information Technology for Environmental Assessment

Lin, H.S., E. Brook, P. McDaniel, and J. Boll, "Hydropedology and Surface/Subsurface Runoff Processes", (2008). Book, Published Editor(s): M. G. Anderson (Editor-in-Chief) Collection: In Encyclopedia of Hydrologic Sciences. John Wiley & Sons, Ltd. Bibliography: DOI: 10.1002/0470848944.hsa306

Lin, H.S., K. Singha, D. Chittleborough, H-J. Vogel, and S. Mooney, "Inaugural International Conference on Hydropedology Offers Outlooks on Synergistic Studies of Multi-Scale Soil and Water Processes", (2008). Book, Published Collection: IUSS Bulletin Bibliography: 113:51-54

Lin, H.S., K. Singha, D. Chittleborough,

H.-J. Vogel, and S. Mooney, "Advancing the Emerging Field of Hydropedology", (2008). Abstract, Published Collection: Eos Trans. AGU Bibliography: 89(48), 490 doi:10.1029/2008EO480009

Lin, H.S., E. Brook, P. McDaniel, and J. Boll, "Hydropedology and Surface/Subsurface Runoff Processes", (2008). Book, Published Editor(s): M. G. Anderson Collection: Encyclopedia of Hydrologic Sciences Bibliography: John Wiley & Sons, Ltd. DOI: 10.1002/0470848944.hsa306

Lin, H.S., "Hydropedology and the Earth?s Critical Zone", (2009). Book, Submitted Editor(s): Ratten Lal Collection: Encyclopedia of Soil Science Bibliography: Taylor and Francis Group. (In process)

Takagi, K., H.S. Lin., "Soil Moisture Response to Year-round Storm Events and Dominant Subsurface Flow Processes in a Steep Forested Catchment", (2008). Book, Published Collection: The 1st International Conference on Hydropedology Bibliography: uly 28-31, 2008, Penn State, University Park, PA.

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", (2008). Book, Published Collection: The 1st International Conference on Hydropedology Bibliography: July 28-31, 2008, Penn State, University Park, PA.

Andrews, D., L. Li, H.S. Lin, and S. Brantley, "Using manual and automated monitoring systems to study soil water movement in a small forested watershed", (2008). Book, Published Collection: The 1st International Conference on Hydropedology Bibliography: July 28-31, 2008, Penn State, University Park, PA.

Lin, HS., J. Zhang, L. Luo, K. Takagi, Q. Zhu, and J. Doolittle, "Heterogeneous World Underfoot: Visualizing Soil-Water Interactions in the Critical Zone", (2008). Abstract, Published Bibliography: Joint annual meetings of GSA and SSSA in October 5-9, Houston, TX.

Kumar, M., "Toward a Hydrologic Modeling System", (2009). Thesis, Published Bibliography: Civil Engineering, University Park, Pennsylvania State University, Doctor of Philosophy, p. 251 Li, W, "Implementing the Shale Hills Watershed Model in Application of PIHM", (2010). Thesis, Published Bibliography: Civil Engineering, University Park, Pennslyvania State University, Master of Science, p. 97

Mizsei, D, "Rates and Mechanisms of Soil Carbon Sequestration at the Shale Hills Critical Zone Observatory", (2010). Thesis, Published Bibliography: Geosciences, University Park, Pennsylvania State University, Bachelor of Science, p. 51.

Takagi, K, "Static and Dynamic Controls of Soil Moisture Variability in the Shale Hills Catchment", (2010). Thesis, Published Bibliography: Crop and Soil Science, University Park, Pennsylvania State University, Master of Science, p. 68.

Wubbels, J, "Tree species distribution in relation to stem hydraulic traits and soil moisture in a mixed hardwood forest in central Pennsylvania", (2010). Thesis, Published Bibliography: Horticulture, University Park, Pennslyvania State University, Master of Science

# 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:**

Software (or netware)

#### **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, 4-hourly 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 Hills.

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, SoilGeochemDB, 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, although currently password protected according to embargo. We are currently working with investigators at Colorado to input data using a spreadsheet template. We are offering webinars this summer/fall for outside PSU investigators to learn how to input data into the template and demonstrate functionality of the database to expand utilization.

#### 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.

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.

# **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 everchanging, 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 communitygenerated, 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.

# 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 Any Conference

# **Activities and Findings 2010**

# Biogeochemistry Team (Jason Kaye, Lixin Jin, Susan Brantley):

Soil respiration is the  $CO_2$  flux from soils to the atmosphere, which originates from two sources, plant roots and soil heterotrophic organisms. Respiration from roots and heterotrophs causes  $CO_2$  to accumulate in soil profiles, providing a strong diffusion gradient promoting movement of  $CO_2$  out of soils and into the atmosphere. This flux is one of the largest terms in the global C cycle, and small changes in this flux due to global climate change such as soil warming, changes in precipitation, or soil disturbance, could have a significant impact on atmospheric  $CO_2$  concentrations.

As a result of extensive soil mapping and moisture and temperature monitoring, we have the opportunity to significantly increase our understanding of the effects of soil moisture and soil physical properties (e.g. porosity) impart spatial variation in soil respiration. To constrain the magnitude of this flux at Shale Hills, we have made thousands of direct soil respiration measurements and also calculated fluxes based on soil CO<sub>2</sub> gradient. Models are being developed to study the controls on soil respiration rates and up scale it to the ecosystem, stand, watershed, or region.

[Jin, L., Andrews, D., Kaiser, N., Kaye, J., Lin, H., and Brantley, S. L. (2009) Interaction between nutrient dynamics and chemical weathering at Shale Hills catchment, a Critical Zone Observatory in Pennsylvania, USA. Geological Society of American meeting, Portland, OR.]

Mizsei, Daniel (2010) Rates and Mechanisms of Soil Carbon Sequestration at the Shale Hills Critical Zone Observatory. Bachelor of Science, Geoscience, University Park, Pennsylvania State University, p. 51.

Ecology Team (Dave Eissenstat, Jane Wubbels, Rebekah Zimmerer, Jim Savage, Fredrick Meinzer, Kate McCulloh, Matt Peoples, Tom Adams, Kelly Cherrey, Katie Gaines, Kusum Naithani, Shelly Pickett – REU, and John Govannicci - REU ):

Research Progress:

# Spatial and temporal dynamics of vegetation structure at Shale Hills:

We laid out a spatial grid for data collection to study the spatial and temporal dynamics of vegetation structure in relation to hydrology. We have started collection of spatial data from the beginning of the growing season (April, 2010) for leaf area index (LAI), canopy closure, and tree height.

We developed a model code to predict spatial processes (Fig. 1 – model output). Based on the 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.



Figure 1. Kriged map of leaf area index at Shale Hills on May 20, 2010. Green circles represent sampling location and different colors represent the gradient of LAI from low (red) to high (yellow). The numbers associated with contour lines represent LAI of that area.

We are in the process of collecting field data and developing a Bayesian spatial model to study the temporal dynamics of uncertainty associated with LAI and canopy closure at Shale Hills. We also developed a model code to study the spatial point patterns (tree locations) and to analyze it in the context of hydrology (soil moisture data from Dr. Lin's group).

# Vegetation survey to coordinate with LiDAR flight of the watershed

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.

# Sap flow

In May of this year collaborators for Oregon State University (Dr. Frederick Meinzer and Dr. David Woodruff) visited the Shale Hills CZO and assisted in installing a completely new set of 76 sap-flow probes in 7 tree species at 3 locations within the watershed. Sensors need to be replaced annually, because in most tree species the outermost new sapwood growth represents a substantial portion of the water movement in the tree. If probes are not reinstalled to monitor this new sapwood, much of the water use by the tree will be missed. The data from these newly installed probes is continuously monitored and initial sap-flow radial profiles have been generated (**Figure 2**). Additionally, at our common garden tree planting at the Russell E. Larson Agricultural Research Center we installed sap-flow probes in 3 individual trees of 4 of the same tree species which are being monitored at the Shale Hills CZO. We hope that using the trees at the common garden will allow us to examine sap-flow without the environmental differences encountered between sampling locations at the Shale Hills CZO.





Also in May of 2010, Jane Wubbles defended her Master's thesis, "Tree Species Distribution in Relation to Stem Hydraulic Traits and Soil Moisture in a Mixed Hardwood Forest in Central Pennsylvania". The study examined six co-occurring tree species at the Shale Hills CZO, within three genera (3 congeneric contrasts; *Carya glabra* and *C. tomentosa*, *Pinus strobus* and *P. virginiana*, *Quercus alba* and *Q. prinus*) under naturally occurring soil moisture gradients. Within each genus, species differed significantly in distribution along gradients of soil moisture (*P* < 0.003), with one species preferentially occupying wetter sites and the other occupying drier sites. To test the hypothesis that hydraulic architecture might partially explain variation in the distribution of species, Jane measured a suite of hydraulic architecture parameters including maximum specific hydraulic conductivity (ks max), leaf specific hydraulic conductivity (LSC), and xylem vulnerability at three levels of percent loss of maximum hydraulic conductivity (P20, P50, and P70). The congeneric contrasts within oaks and within hickories showed no significant differences for any of the parameters. For pines, the species associated with drier sites, *P. virginiana*, was more resistant to cavitation, which was consistent with the hypothesis. In general, species that preferentially occurred on drier sites tended to have higher maximum specific conductivity (P = 0.0039), which was opposite from the expected water-conserving strategy hypothesized for drought-adapted species. These results suggest that these measures of hydraulic architecture of stems in mature trees may play only a minor role in explaining species-level variation in distribution on the landscape.

# Significant Findings:

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*)

# Training/Development:

Two undergraduate students are trained to operate field instruments and are conducting their independent projects (See Research Progress) to inform the spatial modeling of vegetation structure.

One M.S. student defended her thesis and additional training was provided for a postdoctoral fellow (Kusum Naithani) and a PhD graduate student (Katie Gaines).

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

We participated in CZO Summer School "show and tell" and trained participants in a variety of techniques used in our research at Shale Hills. For instance, LI2200 (to measure LAI), densiometer (to measure canopy closure) and Pressure chamber (to measure water potential and generating vulnerability curves).

We also organized a 3 day workshop for CZO Summer School participants. First two days for field data collection and third day for spatial modeling.

- 1. Field component was focused on data collection, and
- Modeling was focused on: 1) introduction to LI2200 software and data download; 2) introduction to spatial modeling at landscape scale; 3) introduction to a statistical modeling software R and using example data to create spatial maps.

Conference Abstracts: none to report

Publications:

Wubbels, J.K., 2010, Tree Species Distribution in Relation to Stem Hydraulic Traits and Soil Moisture in a Mixed Hardwood Forest in Central Pennsylvania. Master's Thesis in Horticulture. The Pennsylvania State University, 39 pp.

# Geomorphology Team (Rudy Slingerland, Eric Kirby, Nicole West)

Research Progress:

Activities focused on data collection and model development and included:

- 1. Collected field data on tree-throw
- Analyzed meteoric 10Be concentrations in 30 samples of regolith along a downslope transect in SHO;
- 3. Collected 17 one to three m long regolith cores along a transverse valley-transect at SHO;
- 4. Collected 2.79 Gb of terrestrial lidar data at SHO to capture microtopography associated with tree-throw pits and mounds; and
- 5. Continued development work on incorporating sediment erosion, transport, and deposition into the Penn State Integrated Hydrologic Model (PIHM).

# Significant Findings:

We 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.

# Training/Development:

This project supported one female PhD student, Nicole West.

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

We organized and led two activities during the summer 2010 CZO Field School that gave participants experience measuring tree-throw and using ground-penetrating radar. These results allowed students to better understand the nature and distribution of regolith and processes controlling its downslope movement.

Conference Abstracts:

NONE

Publications:

NONE

# Hydrogeophysics Team (Kamini Singha, Kamini Singha, Brad Kuntz (PSU MS Student), Terryl Daniels (PSU BSc student) and about 20 summer field students)

# **Research Progress:**

Last year we completed a suite of borehole logging in four new 17-m deep wells near the watershed outlet, 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 have also nearly completed a series of lab-scale tracer tests in soil core. Ten-cm diameter soil columns have been retrieved from the field site from the soil surface down to the saprolite using a geoprobe. These cores have been fitted to a peristaltic pump to flow water vertically from the base of the column, and strontium bromide has been injected into the soil column and the effluent monitored with an electrical conductivity sensor. In the shale matrix, we have estimated the permeability in a triaxial cell, and used BET to quantify the distribution of pore sizes.

# Significant Findings:

From the data collected at the Shale Hills Critical Zone Observatory, 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. The tracer test conducted at the soil/shale interface shows the expecting long tailing, and we are in the process of building comparison models, using a simple dual-domain mass transfer approach as well as using continuous-time random walks (CTRW) to explain these data. We additionally have been testing the use of mobile-immobile models and electrical data to explore solute transport in stream settings in a sister watershed to the CZO.

Preliminary modeling of the soil cores 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.

Training/Development:

One masters student has been funded on this project.

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 groundpenetrating 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:

- Singha, K., Kuntz, B.\*, and Toran, L. (2009). Exploring Lithologic Controls on Solute Transport at the Shale Hills Critical Zone Observatory. EOS Trans. AGU 90(52), Fall Meet. Suppl. Abstract. EP52B-03 (*Invited*).
- 2. Kuntz, B.\*, and Singha, K. (2009). Solute transport in shale and shale-derived soils at the Shale Hills CZO. EOS Trans. AGU 90(52), Fall Meet. Suppl. Abstract. H33H-0987.

# Publications:

Kuntz, B., Rubin, S., Singha, K., and Berkowitz, B., in preparation for Vadose Zone Journal, Solute transport in shale and shale-derived soils at the Shale Hills Critical Zone Observatory. To be submitted in late August.

Hydropedology Team (Henry Lin, Chris Graham, Danielle Andrews, Jun Zhang, Doug Baldwin and Ken Takagi)

# **Research Progress:**

• We have characterized the relationship between soil moisture spatial variability and catchmentwide wetness to assess the uncertainty in estimating spatially-averaged soil moisture. We have examined temporal evolution of soil moisture spatial variability in different soil-landform units and temporal changes in soil moisture profile along topographic gradient to identify processes that influence soil moisture variability.

- We continue to explore the combined use of time-lapsed Ground Penetrating Radar (GPR) imaging and real-time soil moisture monitoring to identify subsurface flow pathways in two contrasting soil transects in the Shale Hills Critical Zone Observatory.
- We have developed new understanding of controls on preferential flow at the Shale Hills CZO. We analyzed over 3 years of soil moisture monitoring, and identified 166 distinct storms. Using continuous soil moisture monitoring, for each storm we have categorized the response as preferential flow vs. non-preferential flow. From these analyses, in conjunction with analysis of the precipitation and soil moisture dynamics prior to and during the storm, we are able to develop a comprehensive understanding on the controls on preferential flow at the Shale Hills CZO.

# Significant Findings:

- Soil moisture spatial variability increased exponentially with increasing catchment-wide wetness across all measurement depths (from surface down to 1.1 m) and soil-landform units. This relationship led to the widening of confidence intervals for estimating spatially-averaged soil moisture and an increase in the number of sites required to obtain 95% confidence in estimating spatially-averaged soil moisture. During the winter through spring, the emergence of shallow water table in the valley and spatially-temporally limited concentrated lateral subsurface flow along hillslopes increased catchment-wide soil moisture spatial variability during wet periods. Conversely, during dry periods in the summer to fall, an increase in hydrological processes operating across the watershed, particularly evapotranspiration, acted to decrease the overall catchment-wide soil moisture variability. The results of this study would be particularly useful for guiding soil moisture monitoring campaigns in complex terrains and have implications for remote sensing footprint of soil moisture.
- 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.

# Training/Development:

• The Shale Hills CZO was used as a field laboratory for Soils 405 Hydropedology class in fall 2009. There were a number of field trips to the site.

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

# **Conference Abstracts:**

- Zhang. J, H. Lin, J. Doolittle. 2009. Combining time-lapsed GPR and real-time soil moisture monitoring to detect subsurface lateral flow. Annual meetings of SSSA in November 1-5, Pittsburg, PA.
- Graham, C. B., H.S. Lin. 2009. Pressure vs. Particle velocities from the pedon to the hillslope scale, SSSA Anual Meeting, 2009
- Graham, C. B., H.S. Lin. 2009. A framework for predicting spatial patterns of soil moisture dynamics at the catchment scale, AGU Fall Meeting, 2009
- Danielle M. Andrews, Lixin Jin, Susan Brantley, and Henry Lin. Influence of catchment topography on carbon and dissolved metal concentrations in the Shale Hills Critical Zone Observatory. 2009. Soil Science Society of America Annual Meeting. Pittsburgh, Pennsylvania. USA.
- Lixin Jin, Danielle Andrews, Nicholas Kaiser, Jason Kaye, Henry Lin and Susan Brantley. Interactions between nutrients dynamics and chemical weathering at Shale Hills catchment, a Critical Zone Observatory in Pennsylvania, USA. 2009. Geological Society of America Annual Meeting. Portland, Oregon, USA.

# **Publications:**

- 1. Lin, H.S. 2010. Earth's Critical Zone and hydropedology: Concepts, characteristics, and advances. *Hydrology and Earth System Science* 14:25-45.
- 2. Lin, H.S., H.J. Vogel, and J. Seibert. 2010. Towards holistic studies of the Earth's Critical Zone: Hydropedology perspectives. *Hydrology and Earth System Science* 14:479-480.
- 3. Lin, H.S. 2010. Comments on energy-based pedogenic models by Field and Minasny (2008) and Rasmussen (2008). *Soil Science Society of America Journal*. 74:337-339.
- 4. Lin, H.S. 2010. Linking principles of soil formation and flow regimes. *Journal of Hydrology.* (In press)
- 5. Takagi, K. and H.S. Lin. 2010. Temporal Evolution of Soil Moisture Spatial Variability in the Shale Hills Catchment. Submitted to *Journal of Hydrology*.
- 6. Takagi, K. and H.S. Lin. 2010. Temporal Evolution of the Correlations between Soil-Terrain Attributes and Surface-Subsurface Soil Moisture. Submitted to *Geoderma*.
- 7. Zhang, J. H.S. Lin, and J. Doolittle. 2010. Subsurface Lateral Flow as Revealed by Combined Ground Penetrating Radar and Real-Time Soil Moisture Monitoring. Submitted to *Hydrologic Processes*.
- 8. Lin, H.S. 2010. On the study of soils and the Critical Zone: Time vs. space, evolution vs. conservation, biology vs. physics, and beyond. *Soil Science Society of America Journal*. (in revision).

9. Graham, C. G. and H.S. Lin. 2010. Spatial-temporal patterns of preferential flow occurrence in the Shale Hills CZO based on real-time soil moisture monitoring. *Vadose Zone Journal* special issue. (To be submitted Aug 2010)

Lin has 1 invited talk:

"Overarching Scientific questions pertaining to the Critical Zone: Challenges to the Soil and Geologic Sciences Community" Invited Talk SSSA Annual Meeting, Long Beach, CA, Nov 1, 2010

1 Thesis:

Takagi, K., 2009. Static and Dynamic Controls of Soil Moisture Variability in the Shale Hills Catchment, Pennsylvania State University, University Park, 68 pp.

# Hydrology and Land Surface Modeling Team (Chris Duffy, Ken Davis, George Holmes, Yuning Shi, Gopal Bhatt, Mukesh Kumar, Lorne Leonard, Colin Duffy, Wenfang Li, Kevin Dressler, Gabrielle Dernier (REU student)

# **Research Progress:**

*Isotope Hydrology:* The installation of SI.net is complete (stable isotope network for O<sup>18</sup> and D<sup>2</sup>). The network which is maintained by George Holmes (MS, 2010) who is collecting daily stream samples (1 site), daily groundwater samples (2 sites), 6 hour interval precipitation samples at the automated rainfall sampler, weekly soil water (12 sites) and ground samples at (20 sites). We have nearly 1.5 years of daily data now, sufficient to begin analysis and modeling. Our primary goal for SI.net is to begin to verify the age of all waters within the watershed for soil, groundwater and streamflow. Age here is defined as the time since the water entered the system as rainfall. Duffy (2010) published the first paper on this subject for our CZO with a theory paper for constructing age models under transient hydrologic flow conditions. A second paper is under way with Peter Lichtner a CZO partner concerning age modeling for reactive species. A third paper is under development by George Holmes who is developing an application of the age model in Duffy (2010) for Shale Hills stable isotope data.

*Penn State Integrated Hydrologic Model:* During the last several years the <u>Penn State Integrated Hydrologic Modeling System (PIHM; <u>http://www.pihm.psu.edu/</u>) has been under development as an open-source community modeling project presently funded by NSF EAR/GEO and formerly by NSF CBET/ENG. PIHM represents a strategy for the formulation and solution of fully-coupled process equations at the watershed and river basin scales, and includes an integrated GIS tool for data handling, domain decomposition, optimal unstructured grid generation, model parameterization, and visualization. The Penn State Integrated Hydrologic Model (<u>PIHM</u>) is a multiprocess, multi-scale hydrologic model where the major hydrological processes are fully coupled using the semi-discrete finite volume method. The model itself is "tightly-coupled" with <u>PIHMgis</u>, an open-source Geographical Information System designed for PIHM. The PIHMgis provides the interface to PIHM, access to the digital data sets (terrain, forcing and parameters) and tools necessary to drive the model, as well as a</u>

collection of GIS-based pre- and post-processing tools. As the main code for PIHM has been completed our main activities during this year are:

- Develop web services for automated downloading and file formatting for running PIHM anywhere in the US and Mexico using national databases for geology, soil, topography, land cover, and atmospheric forcing. This project is being led by Lorne Leonard.
- Complete the PIHMgis tool for domain decomposition and parameter formatting using the web services described above. This project is led by Gopal Bhatt who expects to complete his dissertation later this year.
- A new project has begun to develop PIHM in a Cloud, or server, where the entire modeling process is perfomed on-line. This will integrate with the two projects above.
- Distributed solute and age model with PIHM is now complete and being tested by G. Bhatt. We expect in the next 6 months to implement the model at Shale Hills as part of Bhatt's dissertation.
- Yuning Shi a PhD candidate under the direction of Ken Davis has implemented a new land surface scheme for PIHM that computes a full energy budget. Yuning has implemented the scheme at Shale Hills and 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.

*Embedded Sensor Network:* At Shale Hills we are deploying environmental sensor arrays with the latest sensor network technology. Figure 3. shows the WSN nodes that exist as of July 2010. Figure 4 is a representation of the WSN and communications deployed at Shale Hills. At the present the Thredds sever has not been implemented. The goal is to assimilate environmental sensor data into PIHM in near-real time to allow us to understand and predict the detailed space and time over the course of the CZO field experiment.

The simulation system described above with fully-coupled physical models of the atmosphere-land-vegetation-subsurface system will be fully linked during the first 5-yrs of this effort. The sensor and simulation system have the following elements:

- Extensive, spatially-distributed, non-invasive, smart sensor networks to gather massive geologic, hydrologic, and geochemical data
- Support stochastic information fusion/assimilation methods
- Spatially-explicit multi-physics models for the land-vegetation-atmosphere system
- Asynchronous, parallel, distributed, adaptive algorithms for rapidly simulating the states of a basin at high resolution
- Signal processing tools for data mining and parameter estimation
- Visualization tools for process and prediction assessments

# Significant Findings

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 below illustrates the calculated water budget from PIHM using a simulation for 2009. At this point we are still calibrating the model so this result should be considered preliminary. 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.



Preliminary annual mean water budget as a percentage of precipitation using PIHM to partition the fluxes. Throughfall is net precipitation delivered to the land surface. Note that infiltration balances a positive recharge to the water table and a negative recharge or loss by capillary rise and evapotranspiration supplied by the water table. The latter component is important at Shale Hills when and where the water table is less than 1.5 m below land surface (Shi, 2010). The runoff ratio is ~39%.

# Training, Development and Outreach

 1<sup>st</sup> ANNUAL MULTISCALE MODELING USING THE PENN STATE INTEGRATED HYDROLOGIC MODELING SYSTEM (PIHM). 2-4 August, 2010, State College, PA. As part of our Critical Zone cross-site activities a workshop was held 2 - 4 August 2010. <u>PIHM</u> is multi-process, multi-scale hydrologic modeling tool, where the physical processes are fully coupled using the semi-discrete finite volume method. This workshop provided hands-on experience in using PIHM for modeling watershed dynamics. Participants learned to use a customized GIS interface to PIHM (<u>PIHMgis</u>) 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. The workshop was supported by the NSF-funded <u>Critical Zone Observatory program at Penn State</u>.

- Mukesh Kumar, a major developer of PIHM during his PhD at Penn State, after a 6-month Post-Doc at UC Santa Barbara took an assistant professor position at Duke University in the Nicholas School of the Environment & Earth Sciences.
- 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.
- We participated in CZO Summer School may 31- June 9 coordinating well testing and sampling at Shale Hills, and hands-on drilling and installation of 2 observation wells by the field school participants. Hydraulic testing for all wells installed over the last 2 years proved to be a useful exercise for students and for CZO research as well.

# Invited Talks, Workshops and Conference Abstracts:

Duffy, C. J. and G. Holmes, The age of recharge in hydrologic flow systems: the Shale Hills Critical Zone Observatory. Chesapeake Modeling Symposium, May 10-11, 2010.

Duffy, C. J. Invited Talk: The Shale Hills Critical Zone Observatory, The Soil TrEC (Soil Transformations in European Catchments), Workshop 27-29 January, 2010.

Duffy, C. J. 2010, Simulation and Sensing at the Shale Hills Critical Zone Observatory, Feb 5, 2010, invited department talk at the Stroud Water Center and Christina River CZO.

Duffy, C. J. invited talk: The age of recharge in mountain-front flow systems, AGU Chapman Conference: Examining Ecohydrological Feedbacks of Landscape Change Along Elevation Gradients in Semiarid Regions; Sun Valley, Idaho, 5-8 October 2009

Duffy, C. J. 2009, Invited talk: The Shale Hills Critical Zone Observatory for Embedded Sensing and Simulation, Interagency Steering Committee on Multimedia Environmental Models (ISCMEM) Workshop, 13-15 Oct. 2009. WDC

# **Publications:**

2 Theses and 3 journal publications:

- Kumar, M., 2009. Toward a Hydrologic Modeling System, PhD Dissertation in Civil & Environmental Engineering Dept. Pennsylvania State University, University Park, 251 pp.
- Li, Wenfang., 2010. Implementing the Shale Hills Watershed Model, MS thesis in Civil & Environmental Engineering Dept. 97 pp. Pennsylvania State University, University Park.
- Kumar, M., Bhatt, G. and Duffy, C.J., 2009. An efficient domain decomposition framework for accurate representation of geodata in distributed hydrologic models. International Journal of Geographical Information Science, 23(12): 1569-1596.
- Kumar, M., Bhatt, G. and Duffy, C.J., 2010. An object-oriented shared data model for GIS and distributed hydrologic models. International Journal of Geographical Information Science, 24(7): 1061-1079.
- Duffy, C.J. 2010, C. J. Dynamical modelling of concentration-age-discharge in watersheds, Hydrological Processes, Volume 24 Issue 12, 1711-1718.

# Soils and Weathering Geochemistry (Susan Brantley, Lixin Jin (postdoc), E Herndon (grad), Lin Ma (postdoc), T Yesavage (grad), X Yuan (faculty visitor, Hohai University, Nanjing, China), Ashlee Deere (grad), Tim White)

We have 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.

Brantley had 2 invited talks:

"Bedrock to Soil: where rock meets life in the Critical Zone" Plenary Talk Goldschmidt, Knoxville, TN June 17, 2010

"The movement of rock particles up and water pores down through weathering bedrock" Invited Talk Goldschmidt, Knoxville, TN June 18, 210

Jin had 1 invited talk:

"How pores grow in shale during rockwater interaction: A SANS/USANS study" Invited Talk, Goldschmidt, Knoxville, TN June 14, 2010

Two journal publications and 1 thesis:

- Jin, L. et al., 2010. Mineral weathering and elemental transport during hillslope evolution at the Susquehanna/Shale Hills Critical Zone Observatory. Geochimica et Cosmochimica Acta, 74: 3669-3691.
- Ma, L. et al., (accepted) Regolith Production Rates Calculated with Uranium-series Isotopes at the Susquehanna/Shale Hills Critical Zone Observatory. Earth and Planetary Science Letters.

Mizsei, D., 2010. Rates and Mechanisms of Soil Carbon Sequestration at the Shale Hills Critical Zone Observatory Undergraduate Thesis, Pennsylvania State University, University Park, 51 pp.

#### Visit to Stockholm and Sheffield: Bryn Kimball

I visited scientists at Stockholm University and the Royal Institute of Technology (KTH) in Stockholm, Sweden and the University of Sheffield in Sheffield, UK. The purpose of this visit was to share and learn information about current and recent research projects, and to collect published mineral dissolution rates to be included in the EarthKin database.

#### Stockholm-November 23-27, 2009

#### Royal Institue of Technology

My primary hostess in Stockholm was Dr. Maria Malmström (malmstro@kth.se) at KTH. Her past publications on biotite and sulfide mineral dissolution were what attracted us to contact her initially. With Maria I discussed the Salmon and Malmström (2006) publication. I included the kinetic data from this publication in a chalcopyrite dissolution compilation that was part of my dissertation and that will eventually be included in the EarthKin database. I found that chalcopyrite dissolution rates from this publication were orders of magnitude different from other rates determined under similar conditions, so I wanted to discuss why that may be with her. We concluded that the most likely reason for the rate discrepancy was because chalcopyrite made up a small amount (0.2 - 1 wt. %) of the solids used in the leach experiments. This was a useful discussion for me because it furthered my understanding of whole rock dissolution and what minerals are likely to contribute most to element release.

At KTH I also met with recent graduate Dr. Åsa Zazzi (aasaz@kth.se) and her primary advisor Dr. Susana Wold (wold@kth.se). Dr. Zazzi (previously Åsa Gustafsson) recentley defended her doctoral dissertation, which contains chlorite dissolution rate data. Some of her data has been published before (Gustafsson and Puigdomenech, 2003), and Dr. Joel Moore has included this data in his compilation of clay dissolution rates. Dr. Zazzi mentioned that in a review by Alekseyev (2007), this previous work was presented incorrectly, and that most people interpret her rates incorrectly. In her abstract Dr. Zazzi gave rates of Si release as a function of pH, and Alekseyev interpreted that work as rates of chlorite dissolution as a function of pH. Dr. Moore made the same mistake, but has been able to fix it since my meeting with Dr. Zazzi. Dr. Zazzi has more chlorite dissolution data that is in preparation for publication. This data likely will not be included in Dr. Moore's compilation, but can be included in the EarthKin database in the future. Dr. Wold also mentioned that one of her past students has kinetic data for uraninite dissolution.

I formally presented my chalcopyrite dissolution compilation project to Dr. Malmström and Dr. Wold on November 26, 2009. The discussion that followed focused on how such compilations would be better facilitated by growth of the EarthKin database. Both Dr. Malmström and Dr. Wold were excited about contributing data to the EarthKin database and utilizing the database for future research.

I also had the pleasure of meeting Dr. Jon Petter Gustafsson (gustafjp@kth.se)\_and one of his PhD students at KTH. Dr. Gustafsson developed Visual Minteq, which is a chemical equilibrium model for the calculation of metal speciation, solubility equilibria, etc. for natural waters. The default database for Visual Minteq is based on that for MINTEQA2 ver 4.0, but contains more thermodynamic data for organic material. As a result, this program is particularly useful for those studying soil chemistry.

# Stockholm University

At Stockholm University I met with Dr. Sara Holmström (sara.holmstrom@geo.su.se) and her PhD student Frida Edberg (frida.edberg@itm.su.se). Frida is researching the microbial community structure and chemical profile of a stratified lake. She has not focused on kinetic data in her research so far. Dr. Holmström experimented with dissolution of olivine and biotite under abiotic conditions or in the presence of ligands, including siderophores, in her PhD research. These data are published. She has also experimented with dissolution of biogenic Mn-oxides and Mn-substituted goethite. I believe this data is published as well. For more Fe oxide dissolution data, Dr. Holmström recommended publications by Dr. Owen Duckworth (owen\_duckworth@ncsu.edu).

Frida Edburg is co-advised by Dr. Birgitta Kalinowski who works for SKB (Svensk Kärnbränslehantering AB)— a Swedish nuclear fuel and waste management company. SKB funds a large scale research project near Oskarshamn, Sweden called The Åspö Hard Rock Laboratory. At Åspö scientists from many countries experiment with the future storage of spent nuclear fuel. This is a field scale pilot project that precedes the actual storage of spent fuel elsewhere, and tests such factors as the strength of storage containers under varying underground conditions, the diffusion of groundwater through nominally impermeable rock, the influence of microorganisms on corrosion of storage containers, and much more. Dr. Kalinowski and I were taken on a tour of most of the 3,600 meter long tunnel that spirals to 460 meters depth, and stopped to learn about experiments taking place along the length of the tunnel.

# Sheffield—November 30-December 4, 2009

# University of Sheffield

I visited Dr. Steven Banwart at the University of Sheffield. He is on the advisory committee for the EarthKin database project. Dr. Banwart gave me the doctoral dissertation of his previous student Stephanie Croxford. This dissertation contains rate data for the dissolution of whole rocks from a coalbearing sequence in Wales. Dr. Croxford chose a career in industry and did not choose to publish her dissertation work. Dr. Banwart granted me permission to cull kinetic data from Dr. Croxford's dissertation to be included in the EarthKin database. I spent my week in Sheffield collecting rate data from Dr. Croxford's dissertation and calculating dissolution rates for pyrite and illite. Rate data for other minerals, such as kaolinite, albite, and quartz, is available in this dissertation but is less reliable given the low proportion of these minerals in the dissolving solid and/or the unstable element release rates. I plan to provide recalculated pyrite and illite dissolution rates based on the data in this dissertation. These rates may be included in the EarthKin database.

#### REFERENCES

- Alekseyev, V. A. (2007) Equations for the dissolution reaction rates of montmorillonite, illite and chlorite. *Geochemistry International* **45**, 770-788.
- Gustafsson, A. B. and Puigdomenech, I. (2003) The effect of pH on chlorite dissolution rates at 25°C. Materials Research Society Symposium.
- Salmon, S. U. and Malmström, M. E. (2006) Quantification of mineral dissolution rates and applicability of rate laws: Laboratory studies of mill tailings. *Applied Geochemistry* **21**, 269-288.

# Shale Transect Team (Tim White, Susan Brantley, Ashlee Dere)

To be added.