Annual Report for Period: 11/2008 - 10/2009 Principal Investigator: Duffy, Christopher J. Organization: Penn State University Submitted By: Duffy, Christopher - Principal Investigator Title: Susquehanna/Shale Hills Critical Zone Observatory

#### **Senior Personnel**

#### **Project Participants**

Name: Duffy, Christopher	
Worked for more than 160 Hours:	Yes
Contribution to Project:	
Stable Isotope and Computational Hyd	rology
Name: Slingerland, Rudy	
Worked for more than 160 Hours:	Yes
<b>Contribution to Project:</b>	
Geomorphology	
Name: Brantley, Susan	
Worked for more than 160 Hours:	Yes
<b>Contribution to Project:</b>	
Geochemistry	
Name: Toran, Laura	
Worked for more than 160 Hours:	Yes
<b>Contribution to Project:</b>	
Hydrogeophysics	
Name: Singha, Kamini	
Worked for more than 160 Hours:	Yes
<b>Contribution to Project:</b>	
Hydrogeophysics	
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
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	

**Submitted on:** 09/08/2009 **Award ID:** 0725019 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

	<b>Contribution to Project:</b> Transect Participant		
	Name: Boyer, Elizabeth Worked for more than 160 Hours: Contribution to Project:	Yes	
	Name: Tuttle, Michelle Worked for more than 160 Hours: Contribution to Project: USGS Scientist	No	
	Name: Lichtner, Peter Worked for more than 160 Hours: Contribution to Project: Los Alamos National Lab Scientist	No	
	Name: Goldhaber, Marty Worked for more than 160 Hours: Contribution to Project: Geochemistry	No	
	Name: Steefel, Carl Worked for more than 160 Hours: Contribution to Project: USGS scientist	No	
	Name: Lehnert, Kirsten Worked for more than 160 Hours: Contribution to Project: Geochemistry Informatics	No	
Post-doc			
	Name: Jin, Lixin Worked for more than 160 Hours: Contribution to Project: Leads geochemistry field experiment	Yes	
	Name: Graham, Chris Worked for more than 160 Hours: Contribution to Project: Leads Hydropedology field experiment	Yes	
Graduate Student see Activites Section			
Undergraduate Student see Activities Section			
Technician, Programmer			
Other Participant Instrument Engineer Name: Cherrey, Kelly			

Worked for more than 160 Hours: Yes

#### **Contribution to Project:**

In charge of installing sensors and communications

#### **Research Experience for Undergraduates See Activities**

#### **Organizational Partners**

**CZEN:** The Critical Zone Environmental Network

CUAHSI: The Consortium of Universities for Advancing Hydrologic Science

**GfG Geoinformatics for Geochemistry** 

Waters Network

#### **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 below

**Findings: (See PDF version submitted by PI at the end of the report)** see below

Training and Development:

see below

**Outreach Activities:** 

see below

#### **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,

Jin, L., Ravella, R., Ketchum, B., Heaney, P, and Brantley, S.L., "Mineral Weathering and Elemental Transport during Hillslope Evolution: Regolith Formation on Shale at Shale Hills Critical Zone Observatory", Geochimica et Cosmochimica Acta, p., vol., (2009). Submitted,

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,

Kumar, M. C. J. Duffy,, "Object Oriented Shared Data Model for GIS and Distributed Hydrologic Models", Journal of International Journal 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, "Earth???s Critical Zone and Hydropedology: Concepts, Characteristics, and Advances", Hydrology and Earth System Science, 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,

#### **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 and Decision Making

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

#### Web/Internet Site

#### URL(s):

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

#### **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 Critical Zone Exploration Network (CZEN) is a network of people, sites, tools, and ideas to investigate processes within the Critical Zone.

#### **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:see below

Sharing Information: see below Sharing Information: Available from Prof Henry Lin

Contributions

Contributions within Discipline: see below

see attached file

## **Contributions to Other Disciplines:**

see below

**Contributions to Human Resource Development:** see below

**Contributions to Resources for Research and Education:** see below

**Contributions Beyond Science and Engineering:** see below

**Special Requirements** 

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

Categories for which nothing is reported:

## **Report of Activities, Findings, Contribution, Plans**

The following is a description of Activities and Findings organized by research themes. Figure 1 illustrates the study site, the digital terrain model for the surrounding region.



Shaver Creek digital image (above) lies within the Valley and Ridge physiographic province. Winter image at Shale Hills CZO watershed (right).

Susquehanna/Shale Hills Critical Zone Observatory lies within the Penn State Experimental Forest. The site and region support earth science research and long term hydrologic datasets making Shale Hills and the larger region an ideal site to focus on CZO research for hydrologic geochemical, geomorphological, ecological, soil, and isotopic studies. The Shale Hills CZO is investigating rates and mechanisms of soil/regolith formation on a simple but ubiquitous bedrock lithology. The hydrologic function of the watershed is being investigated by intensive measurements and instrumentation along with the next generation of integrated modeling tools.



Figure 1. Shaver Creek Watershed & Susquehanna/Shale Hills CZO

#### **Research and Education Activities**

#### **Training and Education:**

#### 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: Cherrey, Kelly, PhD Meteorology
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: 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

## **Undergraduate Students:**

Name: 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

## **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

#### Contribution to Project: 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 doublemajoring 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)

#### **Outreach Activities:**

**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 3<sup>rd</sup>, 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) O<sub>18</sub> and H<sub>2</sub> 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  $21^{st}$  – 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.

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.

**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.

**8.** 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).

**9.** 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.



Shaver's Creek Environmental Center: National NAEE award for distinguished environmental education

# Journal Publications

2008 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.

2007 Brantley, S.L., Goldhaber, M.B., and Ragnarsdottir, V. Crossing disciplines and scales to understand the Critical Zone. Elements 3, 307-314.

2007 Brantley, S. L., White, T. S., Ragnarsdottir, K. C. (eds.) The Critical Zone: Where Rock Meets Life, Elements, v 3.

2007 Brantley, S.L., Goldhaber, M.B., and Ragnarsdottir, V. Crossing disciplines and scales to understand the Critical Zone. Elements 3, 307-314.

2008 Brantley, S. L. Understanding Soil Time. Science 321, 1454-1455.

2009 Brantley, S.L. and White, A.F. Approaches to Modeling Weathered Regolith *in* <u>Thermodynamics and Kinetics of Water-Rock Interaction</u>, E.H. Oelkers and J. Schott, (eds), Reviews in Mineralogy and Geochemistry, V. 70, p. 435-484.

2009 Jin, L., Ravella, R., Ketchum, B., Heaney, P, and Brantley, S.L. Mineral Weathering and Elemental Transport during Hillslope Evolution: Regolith Formation on Shale at Shale Hills Critical Zone Observatory. Submitted to <u>Geochimica et</u> <u>Cosmochimica Acta</u>

2008 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, in press.

2009 Kumar, M. C. J. Duffy, Object Oriented Shared Data Model for GIS and Distributed Hydrologic Models, Journal of International Journal Geographical Information Science, in press.

2008 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* 59:34–49.

2009 Lin, H.S., H.J. Vogel, and J. Seibert (Editors). Hydropedology and the Earth's Critical Zone. *Hydrology and Earth System Science* special issue. (In progress)

2010 Lin, H.S., H. Flühler, W. Otten, and H.J. Vogel (Editors). Soil Architecture and Preferential Flow across Scales. *Journal of Hydrology* special issue. (In progress)

2009 Lin, H.S. Comments on Energy-based Pedogenic Models by Field and Minasny (2008) and Rasmussen (2008). *Soil Science Society of America Journal*. (In press)

2009 Lin, H.S. Earth's Critical Zone and Hydropedology: Concepts, Characteristics, and Advances. *Hydrology and Earth System Science Dis.* 6:3417-3481.

2009 Lin, H.S. Hydropedology and the Earth's Critical Zone. *In* Ratten Lal (Editor-in-Chief) *Encyclopedia of Soil Science*. Taylor and Francis Group. (In process)

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

2008 Lin, H.S., K. Singha, D. Chittleborough, H.-J. Vogel, and S. Mooney. Advancing the Emerging Field of Hydropedology, *Eos Trans. AGU*, 89(48), 490, doi:10.1029/2008EO480009.

2008 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. *IUSS Bulletin* 113:51-54.

2007 Qu Y., C. J. Duffy, A semi-discrete finite volume formulation for multiprocess watershed simulation, Water Resour. Res., 43, W08419, doi:10.1029/2006WR005752.

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

2007 Brantley, S. L., White, T. S., Ragnarsdottir, K. C. (eds.) The Critical Zone: Where Rock Meets Life, Elements, v 3.

2008 Jin, L. and Brantley, S.L., Using Water Chemistry to Characterize Chemical Weathering in the Critical Zone Observatory: Shale Hills Catchment (Central Pennsylvania, USA). American Geophysical Union fall meeting, San Francisco, CA.

2009 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.

2009 Herndon E.M., Jin L., and Brantley S.L., Mn enrichment in surface soils: a signal for dust? American Geophysical Union fall meeting, San Francisco, CA, 2008. 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.

2008 Lin, H.S., E. Brook, P. McDaniel, and J. Boll. Hydropedology and Surface/Subsurface Runoff Processes. *In* M. G. Anderson (Editor-in-Chief) *Encyclopedia of Hydrologic Sciences*. John Wiley & Sons, Ltd. (In press)

2008 Bhatt, G. M. Kumar, and C.J. Duffy, Bridging the Gap between Geohydrologic Data and Distributed Hydrologic Modeling. Proceedings iEMSs 2008: International Congress on Environmental Modelling and Software: Integrating Sciences and Information Technology for Environmental Assessment and Decision, M. Sànchez-Marrè, J. Béjar, J. Comas, A. Rizzoli and G. Guariso (Eds.)

2008 Kumar, M. and C.J. Duffy, Shared Data Model to Support Environment Sensor Network Data in Hydrologic Models. Proceedings iEMSs 2008: International Congress on Environmental Modelling and Software: Integrating Sciences and Information Technology for Environmental Assessment and Decision M. Sànchez-Marrè, J. Béjar, J. Comas, A. Rizzoli and G. Guariso (Eds.)

2008 A set of 3 DVD for The 1<sup>st</sup> International Conference on Hydropedology held July 28-31, at Penn State Univ. in University Park, PA.

2008 Lin, H.S., J. Zhang, D. Andrews, K. Takagi, and J. Doolittle. Hydropedologic investigations in the Shale Hills catchment. GEOCHIMICA ET COSMOCHIMICA ACTA. 72 (12):A552.

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

2008 Lin, H.S., J. Zhang, D. Andrews, K. Takagi, and J. Doolittle. Hydropedologic investigations in the Shale Hills catchment. The 1st International Conference on Hydropedology, July 28-31, 2008, Penn State, University Park, PA.

2008 Andrews, D., L. Li, H.S. Lin, and S. Brantley. Nutrient Dynamics along a Planar Hillslope in a Small, Forested Catchment, Central Pennsylvania. Joint annual meetings of GSA and SSSA in October 5-9, Houston, TX.

2008 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. The 1st International Conference on Hydropedology, July 28-31, 2008, Penn State, University Park, PA.

2008 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.

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

# Web/Internet Site

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. <u>http://www.czo.psu.edu/</u>

CZEN.org continues to be a site for sharing data within the CZEN-CZO community: <u>http://www.czen.org</u>

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. <u>http://www.rthnet.psu.edu/</u>

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. <u>http://cataract01.cee.psu.edu/czo/sap/</u>

LPM is a our new disdrometer or Laser Precipitation Monitor. The data is available at: <u>http://cataract01.cee.psu.edu/czo/lpm/</u>

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. The data on the server is in a SQL database format <u>http://cataract01.cee.psu.edu/czo/eko/</u>

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. This includes the disdrometer data for precipitation <u>http://cataract01.cee.psu.edu/czo/lpm</u> and will eventually include the eddy flux data, although the eddy-flux won't be provided in real time due to the extensive processing necessary.

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. The ISO\_NET data is available at <a href="http://cataract01.cee.psu.edu/czo/iso">http://cataract01.cee.psu.edu/czo/iso</a>.

# **Other Specific Products**

## **General 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.

The CZO data (time series, geospatial, open source modeling) are being provided to the community through SourceForge <u>http://sourceforge.net/projects/pihmgis/</u> and <u>http://sourceforge.net/projects/pihmgis/</u>.

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.

## **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 left figure shows the hypsometric curve for Little Juniata Watershed. Delaunay Triangulation is used to tile the watershed while using hypsometric function as a constraint. In regions of higher topographic extremes/gradient, concentration of meshes is higher. Note the formation of smaller triangles besides the streams. Similar divisional constraints can be used for vegetation and climate regimes. The figure below illustrates the user interface for PIHM\_GIS.



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: <u>http://csdms.colorado.edu/wiki/Models</u>

#### **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.

#### **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 we offer (see above).

#### **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.

#### **Special Requirements**

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

## **CZO Site Infrastructure**

## **Activities and Findings**

This section details progress on power, communications and sensor array infrastructure that cut across the research groups. Kelley Cherrey is the full-time instrumentation and sensor engineer. Colin Duffy is working on the development of eKo.NET adaptive sensor array. Kevin Dressler led the drilling program with help from Chris Graham and other CZO scientists and students.

## Power

A 15 amp, 120 volt service was extended to the Shale Hills site and 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 will be installed as time permits.

## Wireless Communication Network

We have installed a 5.7 GHz Motorola multipoint access wireless system at Shale Hills which will serve Shale Hills and the larger Penn State Forest with web communication. This will provide a meso-scale link from the watershed to the university and ultimately to regional web services. This backbone is installed on the eddy flux/wireless communication tower with resources from 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. A ground system of 900MHz antennas and radios connects the distributed measurement arrays to the backbone.

## Adaptive Sensor Network (eKo.NET)

A 25 node adaptive sensor network was installed at Shale Hills this year for monitoring snow depth and subsurface conditions. Each node in eKo.NET monitors: soil moisture, 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 two-way communication capability with each node, and the ability to examine and control our sensors from any browser. The system is intended to advance predictive understanding of the energy-water-carbon system by fusion of the sensing of state variables with our physical models and information system. The nodes or "motes" are based on Crossbow data acquisition and radio technology (www.xbow.com/eko/). Wireless ad-hoc networks are packet based, multi-hop, radio networks consisting of mobile wireless nodes communicating over a shared wireless channel. The Figure below illustrates the design for eKo.NET once fully implemented. We are currently exploring NSF and other funding sources to advance the prototype to a fully instrumented array. Characteristics of our eKo.NET technology is shown in the figure below.

## Wireless Ad-Hoc System Characteristics:

- 1) Energy Conservation: The ad-hoc network has a limited power supply and limited capacity to generate its own power. Thus, the nodes in such a network utilize minimum energy for longevity. In our case the nodes use solar power or D cells.
- 2) Scalability: An environmental ad hoc network can theoretically grow to hundreds of nodes. For wireless network infrastructures, scalability is achieved by a hierarchical construction. However, in the forest canopy we have found that ~ 1 node per acre is optimal for communication. We expect that each eKo.NET node can additional sensors with up to 8 sensors at each node.
- 3) Multi-hopping: A multi-hopping network is one in which the path from a source to a destination traverses several other nodes. Environmental changes as well as changes in the density of foliage render a highly variable radio propagation path. Thus, whenever a direct path is unavailable from a source to a destination, ad-hoc networks have the capability to route the data via other nodes increasing reliability.
- 4) Self-organization: The ad hoc network autonomously determines its own configuration parameters including addressing, routing, power control.



Figure: eKo.NET configuration showing the multi-tiered wireless sensor nodes operating at 2.4 GHZ and the 5.2 GHZ Motorola Multipoint radio for connecting to the Penn State backbone. The long term goal is to build a portable or relocatable array that would be used to "scale up" the CZO observing system to other sites within the Juniata River basin.

## Geochemistry

E Herndon (grad), L Jin (postdoc), L Ma (postdoc), J Morales (undergrad REU, Univ. of Puerto Rico, also participated in SROP program), T Yesavage (grad), X Yuan (faculty visitor, Hohai University, Nanjing, China), S Williams (Univ. of West Alabama)—here as an REU and participated in the SROP program.

## **Activities and Findings**

- 1) Small-angle neutron scattering experiments on shale chips from SSHO were carried out and results showed that the porosity, specific surface areas and fractal dimensions vary as shale weathering progresses, in response to clay dissolution.
- 2) Mn enrichment observed in SSHO soils was quantified using mass balance models and determined to be the product of aeolian deposition from industrial sources, indicating anthropogenic influence on soil chemistry.
- 3) U disequilibrium isotopes were measured in SSHO soils and used to calculate regolith residence time and production rates, showing that at SSHO, regolith formation occurred prior to the peri-glacial period and regolith production rates vary inversely with soil thickness.
- 4) The abundance of dissimilatory iron-reducing bacteria is directly related to soil moisture levels in the Shale Hills watershed (see photo).



Enrichments of iron-reducing bacteria from the valley floor of the watershed. Photo by T Yesavage.

5) The activity of four hydrolytic enzymes associated with plant roots (acid phosphatase, amino-peptidase, chitinase, and B-glucosidase) were visualized and localized within the root community, utilizing root boxes in place at Shale Hills. Acid phosphatase activity was highest in the primary root, with less in the soil, and even less in the secondary root. While some of the enzyme activity was correlated to actual roots, some was also attributed to microorganisms and fungi growing around the roots.

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.

## Contribution

1) Lixin Jin will install suction lysimeters on the northern swale at ridge top, mid-slope and valley floor sites.

2) Lixin Jin and Danielle Andrews will place O2 sensors and redox probes on the valley floor of both the south planar hillslope and swale. They will be placed at 3 depths for each site and hooked up to a datalogger through multiplexers.

3) Lin Ma and Lixin Jin will collect riverine sediments at stream beds for geochemical analysis (major, trace and U/Th isotopes).

4) Nick Kaiser, Danielle Andrews and Lixin Jin installed soil gas samplers at the ridge top, mid-slope, and valley floor along the south swale (July 13th).

5) Weekly collection of ISCO samples (stream and groundwater) by Danielle Andrews and Maya Bhatt.

6) Weekly collection of soil water samples by Danielle Andrews and Maya Bhatt.

7) Multiple soil cores within Shale Hills for soil particle size distribution analysis by Lin Ma (locations to be determined).

8) Possible collection of soils and stream sediments for cosmogenic nuclide analysis by Lin Ma and Eric Kirby.

9) Ongoing modeling of geochemistry, mineralogy, and hydrology.

10) Weekly to monthly collection of soil gas samples along the south planar and swale transects by Lixin Jin and Daniel Mizsei.

11) Lixin Jin will carry out small neutron scattering experiments at National Institute of Standards and Technology to study weathering of shale. This will allow us to construct a generalized model of pore development and initiation of soil formation.



Figure 1. Variation of fractal dimension (A), porosity (B), and surface area (C) as a function of depth of samples from Susquehanna Shale Hills Observatory. A shift from mass fractal to surface fractal is observed as weathering intensifies and mineral surfaces become smoother. Porosity increases towards the surface, from 4% in unweathered bedrock to about 15% at 10 cm below ground. Surface area increases to 300  $m^2/g$  but decreases again due to loss of clay minerals and exposure of quartz.

Brantley had five invited talks:

"Reading the Clues in Chemical and Textural Depth Profiles in Critical Zone Systems." Keynote, Goldschmidt, Davos, Switzerland. June 21-26, 2009.

"Controls on weathering rates at the Susquehanna Shale Hills Critical Zone Observatory." European Geosciences Union General Assembly 2009, Vienna, Austria. April 19-24, 2009. Lin Ma gave the talk.

"Observations Emerging from a Network of Critical Zone Observatories: Shale Weathering at the Susquehanna Shale Hills Observatory." Pardee Symposium, Geological Society of America, Houston, Texas. October 5-9, 2009.

"CZEN Observatories—the U.S. Experience." European SoilCritZone Workshop 3, Crete, Greece. September 5-9, 2008.

"Probing the Interface of Bedrock Weathering using Neutron Scattering Analysis', at the International Confernce on Neutron Scattering, Knoxville TN, Spring 09 Susan L. Brantley, Lixin Jin, David Cole, Gernot Rother, Alexis Navarre-Sitchler. This work was also highlighted in the 2009 annual report of National Institute of Standards and Technology Center for Neutron Research.

Lixin Jin had two invited talks:

"Characterizing weathering fronts of shales by small-angle neutron scattering: Pores and interconnectivity". ExxonMobile Research and Engineering Company, Clinton, New Jersey. Dec-2008.

"Fate of agricultural liming: CO<sub>2</sub> sink or source?" Global Soil Change Workshop at Duke University: International Network of Long-term Soil Experiments, June 8-11, 2009.

**Objectives and Scope** (if different from original proposal): Unchanged...We are measuring the rates and mechanisms of regolith formation at Shale Hills.

# Geomorphology

Rudy Slingerland and Eric Kirby

## **Activities and Findings**

1) Continuing work on incorporating sediment erosion, transport, and deposition into the Penn State Integrated Hydrologic Model (PIHM). Efforts were mainly directed towards development of a hillslope sediment flux model incorporating tree-throw and freeze-thaw creep. Appendix I contains some of this work.

2) Continuing work on defining how the processes and products of the SHO regolith mill have changed in response to past climatic, base level, and land-use perturbations.

Our results show that Pennsylvania landscapes are still adjusting to past climatic and base level conditions. Analysis of high-resolution LiDAR digital elevation models of the region shows numerous periglacial features (Figs. 1 & 2). Therefore the extent to which the SHO regolith thickness and processes are palimpsest is the subject of intensified on-going investigation. Appendix II contains a pdf of my recent SHO summer seminar. 3) Recruiting graduate students for the project.

## Work Plan

Incorporate the new hillslope flux laws into PIHM\_Sed, improve the overland and channel flow formulations to simulate unsteady non-uniform flows, and conduct validation experiments against SHO data, particularly lidar and regolith thickness data.

## Contributions

APPENDIX I. <u>Hyperlink to RLS pdf document</u> APPENDIX II. <u>Hyperlink to RLS pps of summer seminar</u>



Kilometers

Figure 1. Shaded Relief map of PAMAP lidar with SHO indicated in very light blue near center of figure. Note the relict braided stream upstream of Lake Perez with alluvial terraces, interpreted to have been

formed during earlier periglacial conditions from increased sediment yields of coarser grain sizes. Adjustments in this truck stream are suspected to have changed the base level in the SHO catchment.



Figure 2. (A) Shaded relief image from PAMAP lidar data showing solifluction lobes on the SE side of Thickhead Mountain, 16 km ENE of SHO; and (B) topographic profile along line of section in A. Undulation heights lie between 5 and 12 ft, with a wavelength about 320 ft. Features are probably the cause of "brown over red" soils noted in soil surveys, indicating significant downslope creep during earlier LGM permafrost conditions.

## Hydrology, Stable Isotope Tracers, and Model Development

## **Activities and Findings**

*Hydrometeorological Instrumentation*: Last October Kelly Cherrey installed the Eddy Flux on our 30 m tower for determining the latent heat and CO2 flux above the canopy. This complements our weather station at the site which includes, a Kipp and Zonen 4 component radiation sensor, Ott Pluvio load cell-type precipitation gauge, R. M. Young wind set, Theis disdrometer, and acoustic snow depth sensor.

A bedrock observation well drilling program was carried out from October 2008 to August 2009 (Dressler, Duffy, Duffy and Graham) and we installed a network of shallow observation wells completed within the weathered shale bedrock, typically at depths ranging from 8 to 15 feet. At this point we have completed all wells. Each well location is being instrumented for real-time communications as described earlier under the eKo.net section in Site Infrastructure.

*Stable Isotope Network*: In 2008 the Los Gatos Laser Isotope instrument was delivered and set up at PSIEE laboratory. Two continuous groundwater isotope sampling sites with ISCO samplers have been installed set to a daily sampling interval. With the help of Beth Boyer we were able to purchase and install an "event-based" automated isotope and chemistry sampler adaptively takes precipitation samples for 4-hour intervals during a rainfall event. Presently we have continuous daily samples of outlet runoff, groundwater, and adaptive precipitation sampling for establishing the isotope record at Shale Hills. We are taking synoptic soil moisture sampler on a weekly basis, as well as 15 new observation wells in the weathered shale for weekly samples and sapflow and leaf

isotopic signature studies by Dave Eissenstat. The completes our baseline sampling plan for stable isotopes.

# Contributions

**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. The 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 13 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 1, and the location of the instruments is shown in figure 2. The comprehensive sampling of the network is possible because of the DLT-100 liquid water stable isotope analyzer from Los Gatos Research, with a reproducibility of  $\pm 0.2\%_0$  for oxygen-18 and  $\pm 1.0\%_0$  for deuterium, and the capability to run approximately 30 samples per day.



Figure 1. Examples of the instruments used to sample the isotopes at the Shale Hills CZO: a. Eigenbrodt NSA-181S 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 f. Vegetation sites for synoptic isotope sampling.

The goal of the research is to identify flow paths and time scales of water from precipitation input to the watershed through\_stream flow output. Although results are preliminary stream water, groundwater and soil water all show a departure from the local meteoric water line(figure 3). Time series analysis and spatial principal component analysis is used to "classify" dominant modes and processes affecting stable isotope dynamics in the watershed. 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 mean age and residence time of the water in the watershed.



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



*Figure 3. Local meteoric water line for Shale Hills, including the equation and R2 value for the correlation line* 

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*Computational Hydrology (PIHM):* Mukesh Kumar, and Shuangcai Li completed and defended their PhD dissertations in the Fall 2008. They have provided the core of the modeling team up to this point and have unselfishly helped the new PhD students George Holmes and Wenfang Li get started on their graduate research. PIHM (The Penn State Integrated Hydrologic Model) along with the new PIHM\_GIS tool has made major progress this year. Specific findings and accomplishments are:

1). The model PIHM (Penn State Integrated Hydrologic Model) initially developed by Qu and Duffy (2007), has been extended to include new strategies for domain decomposition using unstructured grids, a new river module, and overland flow-infiltration scheme. PIHM is available as an open-source project on Source Forge and we welcome the larger community to participate in advancing the modeling system (http://sourceforge.net/projects/pihmmodel/).

2) A data model has been developed which tightly couples the physical model and apriori digital data with an open-source GIS tool referred to as PIHM\_GIS. The model is forced by standard digital data sets and has been tested on a 1000km<sup>2</sup> watershed in PA. The open source GIS is also available on Source Forge <u>http://sourceforge.net/projects/pihmgis/</u>. Details of the shared data model are found in Kumar, Bhatt, and Duffy (2008).

3) A parallel HPC version of the model, necessary for large-scale simulations, is nearing completion and is being tested on a site in the Susquehanna River basin as part of M. Kumar's PhD dissertation.

4) An extension to the data model has been developed which tightly couples sensor networks to the GIS and the physical modeling system. This extension of our research to include the sensor networks was found to be extremely important and necessary to take advantage of the a-priori data for optimal parameter estimation and model calibration, and for ultimate assimilation of multivariate parameters and forcing within the physical model (Kumar, Bhatt, and Duffy, 2008).

*Simulating Multi-Scale Hydrologic Behavior* The goal of this component of our research has been to explore whether fully coupled processes and a-priori data form a practical basis for application of integrated models at multiple scales, and to further see if this model-data coupling strategy leads to any new or interesting results that might not be obvious from weakly coupled or uncoupled modeling approaches. Recall that our model strategy is based on a direct or natural coupling of the equations within a finite volume or "kernel". Now that all sensor instrumentation is installed including a network of observation wells into the permanent water table we are prepared to begin the modeling pahse of the study. The figure below illustrates the multi-scale strategy we are working on. High resolution data at the process scale (Shale Hills), scaled up to meso-scale simulations for Shavers Creek (175 km<sup>2</sup>), and the entire Juniata river basin.



## **Plan for Next Year**

The modeling research will accelerate to include assessing the role of groundwater on land surface energy budgets, incorporation of sediment and solute transport in PIHM.

# **Physiological Ecology**

## **Activities and Findings**

During the second year, the following work was accomplished:

1) A complete survey of all canopy trees greater than 8" in diameter at breast height (DBH), begun in summer 2008, was completed. Distribution maps of species were generated from this data (**Figs. 1-3**). Species distribution patterns were identified and compared with soil depth and soil moisture data from Henry Lin's group to hypothesize factors controlling distribution.

2) A congeneric contrast of 6 species in 3 genera was developed to study water uptake and transport in trees. Species included *Carya glabra* (Pignut hickory), *C. tomentosa* (Mockernut hickory), *Pinus strobus* (White pine), *P. virginiana* (Virginia pine), *Quercus alba* (White oak), and *Q. prinus* (Chestnut oak). Four sites throughout the watershed were chosen for sampling to represent wet and dry conditions and control for environmental variation (**Fig. 4**). Masters student Jane Wubbels (Horticulture Department) and REU Rebekah Zimmerer (Gordon College) trained with arborist Jim Savage (PSU Horticulture Department) to learn to climb trees (**Images 1-2**). They collected leaf and branch samples from 30 trees twice during the summer. Jane Wubbels will continue with another round of sampling this summer and a final round in September.

- Midday leaf water potential was measured on site with 3-5 replicates per tree. Results so far show that trees have not been experiencing water stress.
- Small branch samples were collected for isotopic (<sup>18</sup>O and <sup>2</sup>H) analysis. These samples will be taken to the Stable Isotope Laboratory at Cornell University this fall to have the xylem sap water extracted. The extracted water will then be analyzed using the Los Gatos Laser Isotope instrument at PSIEE at Penn State. Because of the wet conditions this summer and because past research has shown that trees will use the most readily available water source, we do not expect to be able to discern species-level differences in water usage from our samples thus far.
- More branch samples were collected to measure specific hydraulic conductivity, capacitance, and xylem vulnerability. Preliminary results show large differences between genera for xylem vulnerability and specific conductivity. Further analysis is needed to determine the significance of species-level variation.
- Leaves were collected from these branches and scanned to obtain leaf area. Some leaves were dried and ground for <sup>13</sup>C analysis to determine water use efficiency. These samples will be processed this fall. Other leaves were shared with the geochemistry group for chemical analysis.
- REU Rebekah Zimmerer (Gordon College) measured predawn and midday water potential (Images 3-4), specific conductivity, and xylem vulnerability on 4 of the same species (*P. strobus, P. virginiana, Q. alba,* and *Q. rubra*) at the common garden at the Russell E. Larson Agriculture Research Farm at Rock Springs. The common garden set up controls for age and environmental factors more than is possible in a natural site. Controlling as many environmental factors as possible helps to discern whether variation we see at Shale Hills is the result of genetics or an individual's plasticity.

## Contributions

We have also been involved in constructing a sap flow network at the Shale Hills CZO. This project is led by David Eissenstat and Fredrick Meinzer (Research Ecologist and Research Team Leader, USDA Forest Service, Pacific Northwest Research Station) with assistance from Postdoctoral fellow, Kate McCulloh (Oregon State University). Technical assistance has been provided by Matt Peoples, Tom Adams and Kelly Cherrey. Sap flow sensors (heat dissipation probes) have been installed in three locations in the watershed including two on the north facing slope and one on the ridge line of the south facing slope (Figure 5). A total of 28 trees of 7 tree species are being measured for sap flux using a total of 66 sap flow sensors installed at multiples depths in the tree. Data are being continuously logged and transmitted to the web. As shown in Fig. 6, strong diurnal patterns of high water flux during the day (heated thermocouple exhibiting a smaller difference in temperature to that of the control, unheated thermocouple) and little flux at night (large difference in temperature between heated and unheated thermocouples) are evident.







*Figure 5. Location of various research activities at Shale Hills Critical Zone Observatory.*


Fig. 6. Example output of sap flow sensors for Liriodendron tulipfera at 3 depths in the tree (blue: 1.5 cm; red: 3 cm: green: 5 cm). Note how flux at 5 cm depth is less than closer to the bark.

# Aug 5, 11:20am to Aug 17, 12:40pm



Image 1. Graduate student Jane

Wubbels climbing a Virginia pine (Pinus virginiana).



Image 2. Graduate student Jane Wubbels sampling from a

Chestnut oak (Quercus prinus).



predawn water potentials at the common garden.



Image 3. REU Rebekah Zimmerer taking

Image 4. Common garden at sunrise.

## Hydropedology

#### **Activities and Findings**

Ground Penetrate Radar (GPR) provides a non-invasive way to reveal the subsurface complexity. We have demonstrated that GPR is suitable to identify subsurface structure in the Shale Hill CZO. However, static radargram only provides a qualitative description of subsurface characteristics. In this study, we have innovatively developed time-lapsed GPR with soil water sensors to identify subsurface flow patterns in real time. A 3 by 4 meter grid was established along several hillslopes. In each grid, multiple ECH<sub>2</sub>O-TE probes were installed at different depths (5, 10 and 30 cm) and the probes were connected to CR1000 datalogger to record the soil water dynamics at 2-minutes interval. We have conducted several experiments of combined time-lapsed GPR and real-time soil moisture monitoring, aiming at identifying subsurface flow pathways and patterns while quantifying soil moisture distribution. The results are encouraging and two manuscripts are currently in preparation. Key findings include: 1) quick lateral flow through fractured shale, and 2) the timing is important in terms of suitable soil moisture condition for obtaining best GPR results. Some photos and GPR images are shown below:



Graduate student Jun Zhang and NRCS collaborator Jim Doolittle were working on GPR scanning of a hillslope at the Shale Hills Catchment.



Experimental setup of time-lapsed GPR scanning and real-time soil moisture monitoring with introduced water infiltration in a hillslope at the Shale Hills Catchment.



A: Time lapse GPR image before and after infiltration. Red arrow indicates the location of infiltration intake. Dash line is the two way travel time to the apex of

hyperbola, which indicates the depth of buried metal plate used for GPR image calibration.

# **B:** Difference between radargrams before infiltration and after 0, 15, 30 minutes infiltration, respectively (from top to bottom)

We have collected some soil columns from the Shale Hills CZO and conducted highresolution computed tomography (CT) analysis. The results revealed the heterogeneity and spatial organization of soil pore space and rock fragments (see an image below). Such results have implications in many areas, such as weathering, flow and transport, and chemical reactions. Our 3-D visualization of the pore network and solute tracer distributions over time showed that both the pore network and the flow pattern varied considerably with soil depth, in part due to the soil horizonation and different macropores involved. Our results revealed a sequential initialization of the transport process from the macropore domain to the matrix domain and a decreased degree of interaction between the two domains with soil depth. This study illustrates that preferential flow pathways in intact structured soils consist of a complex network of micropores in the soil matrix and macropores created by rock fragments, animal burrows, root channels, and soil aggregates. Modeling of this flow network and its impacts on chemical kinetics, weathering front, nutrient cycling, and contaminant transport would require a new approach different from the classical continuum-based approach.



CT Image of Weathered Shale Fragments in the Shale Hills CZO Soil

REU student Kristen N. Jurinko completed a research project in summer 2009 on "*Quantitative relationships between soil moisture, geology, tree distribution, and topography in the Shale Hills catchment.*" In her 35-page report, she explored the quantitative relationships between (1) soil moisture distribution at the Shale Hills catchment with (2) depth to bedrock, (3) tree distribution, and (4) topography. She found that topography, depth to bedrock, soil moisture, and tree distribution play a role in one another. For example, depth to bedrock in the valley floor and swale is deep, leading to higher soil moisture (especially deeper in the profile) and characteristic trees such as eastern hemlock, maple, white pine, and white oak trees. Conversely, depth to bedrock is much shallow in the ridge or steep hillslopes, leading to generally drier soils and tree species of chestnut oak, red oak, hickory, and Virginia pine. The soil moisture data and distribution maps help improve the understanding of annual hydrological processes in the whole catchment. We are currently working on revising this report to see how we may translate that into a publishable manuscript. Below are some of this REU student's research results:



Soil moisture storage correlation with function of depth in different landscape units at the Shale Hill CZO.

**Error! Reference source not found.** 

(a) 1093 Oak trees, (b) chestnut oak, (c) red oak, and (d) white oak tree distributions over the 20 cm soil moisture storage content for all the measured days (n=22 days).



REU student Kristen Jurinko working in Henry Lin's lab in summer 2009.

Ken Takagi successfully defended his Master thesis on "Static and Dynamic Controls of Soil Moisture Spatial-Temporal Variability in the Shale Hills Catchment." Currently, two manuscripts are being developed for journal publications. This study utilized a fourvear database consisting of soil moisture monitoring at 106 locations from the surface down to 1.1-m depth within a 7.8-ha Shale Hills CZO. The objectives were to 1) examine the controls of horizontal and vertical variability within three dominant soil series-landform units (SLUs) in the catchment; 2) utilize temporal stability analysis to identify locations that represent catchment-wide mean soil moisture and assess the uncertainty in using single locations to represent mean soil moisture; and 3) investigate temporal changes in the correlation between soil-terrain attributes and soil moisture to assess the best predictors of soil moisture. The results showed that both horizontal and vertical variability increased exponentially with increasing mean catchment-wide soil moisture ( $\mathbb{R}^2 = 0.863$  and 0.748, respectively, p < 0.05). The valley SLU exhibited the highest horizontal and vertical variability while the concave hillslope exhibited the lowest horizontal variability and the planar hillslope had the lowest vertical variability. Hydrologic processes active during high soil moisture that occurred in limited areas of the catchment (e.g., concentrated lateral flow and groundwater-soil water interaction) increased overall catchment-wide soil moisture variability, while processes operating

across the catchment during period of low soil moisture (e.g., evapotranspiration) decreased overall catchment-wide soil moisture variability. Individually, topographic wetness index, depth to bedrock, and percent rock fragments in the soil had the highest mean Spearman correlation coefficient with depth-weighted mean soil moisture ( $\mathbf{R}^2$  = 0.508, 0.496, and 0.450, respectively, p < 0.05), and such corrections were statistically significant over all measurement days over the four years from 2004 to 2008 regardless The linear regression  $R^2$  between soil moisture and elevation of year or season. decreased with an increase in catchment-wide soil moisture, while such  $R^2$  between soil moisture and curvature, upslope contributing area, topographic wetness index, and depth to bedrock increased with increasing catchment-wide soil moisture, suggesting the dominance of subsurface lateral flow as the catchment becomes wetter. Thus, as the catchment gets wetter, the tightly coupled soil thickness and topography play an increasing role in predicting soil moisture distribution in this catchment. Among the 11 soil-terrain attributes examined for predicting soil moisture, slope and percentage rock fragments were included in >95% of the optimal regression equations. The adjusted  $R^2$ for the optimal regression equations increased with increasing watershed wetness, with a mean value of 0.659 and a maximum of 0.785. This study sheds light on the complex and dynamic relationship between catchment wetness state, hydrologic processes, and soil moisture variability. This will help determine appropriate soil-terrain attributes for predicting soil moisture during different times of the year using both static and dynamic controls of soil moisture. Some of the results are highlighted below:





We have constructed and installed redox probes at multiple depths in selected 8 sites, as well as additional water table sensors at 10 sites. We have also worked with Chris Duffy's group to design and install 25 wireless EKO nodes throughout the Shale Hills CZO.

We have collected and analyzed over 500 DOC samples, and continue weekly field data collections of soil hydrology and water chemistry.

## Work Plan

- We will continue systematic soil moisture monitoring, along with water table, redox, soil water chemistry, and others. We will also continue to closely examine soil moisture response to year-round storm events based on the soil moisture data collected in the past years. We plan to develop a suite of hydropedograph analysis tools for extracting information out of real-time automatic soil moisture monitoring.
- We will start to develop a network-based model for subsurface preferential flow at the Shale Hills.

- A new graduate student Doug Baldwin will start his Master research focusing on soil water potential data and their relationships to flow dynamics and tree distribution at the Shale Hills CZO.
- We plan to conduct more CT and GPR related work on Shale Hills soils, and plan to develop more scientific visualization modules for showing the complex and dynamic hydropedologic processes in the Shale Hills subsurface.

## Contributions

- Subsurface lateral flow in the catchment has been observed to contribute substantially to direct runoff. But understanding the occurrence and intensity of subsurface lateral flow is difficult because of the subsurface complexity and the lack of appropriate tools to identify this complexity. In this study, we innovatively used time-lapsed GPR in combination with real-time soil water monitoring to identify subsurface flow regime in different hillslopes and soil types at the Shale Hills Catchment. The results of this study have significant implications for developing a next generation of hydrologic models that explicitly consider flow pathways, patterns, and flow configuration evolution.
- We have developed many 3D (X, Y, Z; or X, Y, and time) and 4D (X, Y, Z, and time) animations of subsurface preferential flow at the pedon and hillslope scales based on the database collected from this project, which benefits classroom teaching and public education via "seeing is believing." For example, one of such animations is viewable and downloadable at <a href="http://hydropedology.psu.edu/">http://hydropedology.psu.edu/</a>.
- Soil hydrology often triggers "hot spots" and "hot moments" of biogeochemical processes and nutrient dynamics, hence subsurface flow pathways and their network also become a frontier for effective coupling of soil hydrology and biogeochemistry. The dearth of effective and compelling visualizations of heterogeneous world underfoot has long limited students and the general public's interest and understanding of complex soil and water interactions, thus the scientific visualizations produced in this project will contribute to revitalizing the education and outreach of integrated natural resources management and environmental protection.

## HYDROGEOPHYSICS

**Participants:** Kamini Singha, Brad Kuntz (PSU MS Student), Terryl Daniels (PSU BSc student). REU field students: Valentina Prado Mitchell Johnson, Tamika Shannon, Maurice Dukes, Nate Wysocki, Nathan Barber, Ahmad Yusof, Erica Folio

## **Activities and Findings**

We drilled four 17-m 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 subsurface at this site. We also collected surface ground-penetrating radar and electrical resistivity data. Overall, these data provide some of the first information and a detailed mapping of the hydrogeology of the subsurface within Shale Hills.

We have also been conducting tracer tests in soil core. 10 cm diameter soil columns have been retrieved from the field site and have been fitted to a peristaltic pump to flow water vertically from the base of the column. In recent tests, a pore volume of sodium bromide has been injected into the soil column and the effluent monitored with an electrical conductivity sensor. Rose Hill Shale cores have been retrieved and prepared to load in a triaxial compression chamber to conduct similar experiments. These data will be compared to results of a field-scale tracer test conducted this month, as will a significant number of numerical tracer tests.

From the drilling and data collected within the new wells, we can make the following exploratory conclusions: that there is a hard rock zone around 6-7 m below land surface, beneath which is blue-grey shale. The wireline logs indicate that there is substantial variability in the quality of the shale above this hard-drilling zone, 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, but a zone of interest at 5.8 m below land surface looks ideal for the injection of this summer's tracer test. While there is some concern about the injection of tracer impacting the surface water on site, from hydraulic gradient data it appears that the stream may be perched in some areas of the watershed for much of the year.

Soil core concentrations from the conservative NaBr tracer do not entirely fit classical advective-dispersive behavior, which is not unexpected given the heterogeneity of the soil and the possibility of dual porosity transport. A numerical model of the soil column and this particular tracer test are under construction, and this experiment will be followed up with the injection of strontium bromide to explore non-conservative behavior in the soil, and similar tests in the shale material.

## Contributions

We have found that soil core concentrations from conservative tracers do not fit classical advective-dispersive behavior, adding to the literature on this phenomena. We will greatly expand on this work by linking our current experimental work with field and numerical work in the upcoming year.

In conjunction with Dr. Patrick Reed, I am currently working on developing an adaptive experimental framework for bridging observation and prediction through evolving experimental arrays, multiobjective optimization, and sensitivity analyses for tracer tests at the Shale Hills CZO.

#### Transect site CZO measurements, data management and integration:

An all hands meeting was held for the transect participants last year and a 2<sup>nd</sup> 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 plan selecting field for 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.



Figure 4. Location of Mid-Atlantic Transect

From the meeting it was determined that the first year main focus should be 1) development of the regional shale transect; and 2) assessment of parent material heterogeneity as a control on soil type. Both are ongoing.

1) <u>Shale transect development</u> 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.

2) 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.

## **Ontology-Based Search Engine for CZO DATA**

Personnel: Doug Miller, Brian Bills, Kean Hout Soon, Jennifer Williams and Blake Ketchum

## Findings and Activities

Previously, Critical Zone scientists created a spider diagram to depict concepts used for identification and quantification of processes occurring within the Critical Zone. From this ontology, we seek to develop a user-friendly interface from web ontology language (OWL). This language indentifies related concepts within the ontology thus facilitating successful searches of Critical Zone Observatory data. In January, Kean Hout Soon and Jennifer Williams attended a conference in Philadelphia to discuss the current state of database and metadata use across scientific disciplines. We met with principle investigators from both geochemical and hydrological disciplines. The development of a ontology driven metadata search engine with database capabilities was determined feasible and warranted for the Critical Zone Observatory data.

Initially, the flow path or hierarchy of the ontology was refined to fit the structure where sub-concepts, properties, and sub-properties follow the "is a" relation to the overarching concept of Critical Zone. An equality of various concepts and properties was defined through the definition of "synonym" and "see also" relations. The structured framework of Protégé OWL allows for the challenges of scientific semantics to be overcome when domain specific terms are identified and related to all associated terms through sibling relationships. Knowledge transfer within the working group has resulted in the ability for several members to maintain and edit the platform which supports this interface.

Following the creation of numerous synthetic and several accurate metadata files corresponding to previous, current or proposed research at the Susquehanna Shale Hills Observatory (SSHO), algorithms were written and tested to determine the functional relevance of the search engine capacity. Search capabilities were formatted to correspond with meta-data file creation, utilizing either the ontology specifically or free-string vocabularies. Through product introduction and usage to a subset of SSHO investigators, the interface was validated as user-friendly, yet identified later stage developmental needs (i.e. data management, user registration, public vs private data sharing). A step-by-step user guide was created for the interface to assist users in metadata file creation, file search and file edit functions. At this time, we are eager to share the product with the larger SSHO community to further validation and identify modifications which will facilitate future use.

Figure 1. Graphical representation of critical zone ontology concepts. For illustration purposes, detailed properties of concepts are not shown; please refer to the full ontology in the appendix.



# Figure 2. Example metadata record entry.

Metadata Population Metadata Search Metadata Edit					
	Please enter the following information for your dataset and click the Submit button at the bottom of the page				
Posting Date	2009 🗸 07 🗸 01 🗸				
Title	Soil chemistry data from Shale Hills planar transect				
Author	Lixin Jin				
Online Link	)://www.czen.org/content/susquehanna-shale-hills-critical-zone-observatory				
Abstract	We report here soil chemistry data from three sites (ridge top, mid-slope, and valley floor) along a planar transects, at Susquehanna/Shale Hills observatory. Major elements and some trace elements (Ti, and Zr) were <u>tablized</u> as a function of depth at each soil core. The observatory is entirely developed on a Rose Hill shale Formation.				
	Concepts	Corresponding Properties			
Keyword(s)	lithology regolith bedrock water ground_water evapotranspiration surface_water vadose_zone	hydraulic_conductivity chemistry organic_matter trace_elements isotopes extracted minor_elements major_elements stream_or_reservoir_sediments depositional_history mineralogy age colluvium alluvium loess soil soil soil_horizons morphology physical_properties taxonomy			
	Selected Keywords chemistry (regolith), minor elements (regolith),				
	major_elements (regolith)				
Site	Shale Hills 💌				
Progress	Complete V				
Time Period of Content	1950 💙 to 1950 🌱				
Use Constraints					
Point of Contact	Lixin Jin				
	Submit				

#### Figure 3. Example search with ontology keyword assistance.

Metadata Population Metadata Search Metadata Edit Metadata Search Options Term 1 soil (regolith) (required) Term 2 che (optional) Ontology (in graphics) chemistry You can click on the ontology link to chemistry (bedrock) chemistry (dry\_deposition) see the vocabularies that we use. To facilitate your search with the chemistry (flora) chemistry (ground\_water) ontology, we recommend you to use the concepts and subconcepts from the chemistry (precipitation) ontology. chemistry (regolith) 2 chemistry (surface\_water) chemistry (vadose\_zone)

Field(s) to be searched:

⊠Keywords □Title □Abstract

Time Period of Dataset:

anytime 💌 to 🛛 anytime 💌

Region of Dataset:

Shale Hills 🛛 👻

search

# Figure 4. Results of search from parameters defined in Figure 1.

#### Metadata Population Metadata Search Metadata Edit

Search Results :[9] for soil (regolith) and chemistry (regolith). The ranking is based on "Keywords"

Record	Title	Abstract	Keywords	Metadata
1	Vertical distribution of heavy metals in soils as a function of landscape position in the Shale Hills Catchment	[] Heavy metals in Holocene soils accumulate as a function of clay content and mineralogy. []	chemistry (regolith), mineralogy (regolith), soil (regolith), soil_horizons (regolith), physical_properties	<u>Detail</u>
2	lj Soil chemistry data from Shale Hills planar transect	[] If We report here soil chemistry data from three sites (ridge top, mid-slope, and valley floor) along a planar transects, at Susquehanna/Shale Hills observatory. Major elements and some trace elements (Ti, and Zr) were tablized as a function of depth at each soil core. The observatory is entirely developed on a Rose Hill shale Formation. []	chemistry (regolith), minor_elements (regolith), major_elements (regolith), soil (regolith)	<u>Detail</u>
3	Soil Survey Geographic (SSURGO) database for Huntingdon County, Pennsylvania	[] This data set is a digital soil survey and generally is the most detailed level of soil geographic data developed by the National Cooperative Soil Survey. The information was prepared by digitizing maps, by compiling information onto a planimetric correct base and digitizing, or by revising digitized maps using remotely sensed and other information. This data set consists of georeferenced digital map data and computerized attribute data. The map data are in a soil survey area extent format and include a detailed, field verified inventory of soils and miscellaneous areas that normally occur in a repeatable pattern on the landscape and that can be cartographically shown at the scale mapped. A special soil features layer (point and line features) is optional. This layer displays the location of features too small to delineate at the mapping scale, but they are large enough and contrasting enough to significantly influence use and management. The soil map units are linked to attributes in the National Soil Information System relational database, which gives the proportionate extent of the component soils and their properties. SSURGO depicts information about the kinds and distribution of soils on the landscape. The soil map and data used in the SSURGO product were prepared by soil scientists as part of the National Cooperative Soil Survey. []	soil_horizons (regolith), physical_properties (regolith), taxonomy (regolith), morphology (regolith), chemistry	Detail
4	Mineral weathering and hillslope evolution at Shale Hills catchment: a Critical Zone Observatory in central Pennsylvania, USA	[] 1D, 2D, and 3D transects were sampled []	<b>regolith</b> ), <b>soil (regolith</b> ), bulk_density ( <b>regolith</b> ), latitude_or_longitude (location_and_topography	<u>Detail</u>
5	Manganese additions: natural or anthropogenic	[] small catchment in comparison to global additions []	bedrock), major_elements ( <b>regolith</b> ), sedimentary (bedrock), mineralogy (bedrock), mineralogy ( <b>regolith</b> ), <b>soil</b> ( <b>regolith</b> )	<u>Detail</u>
6	lj Organic matter contents in Shale Hills soils	[] Ij We measured total organic carbon and nitrogen contents in three sites along a planar transect (ridge top, mid-slope and valley floor) at Susquehanna/Shale Hills observatory (SSHO), as a function of depth at 10 cm interval. []	organic_matter (regolith), soil (regolith)	<u>Detail</u>
7	Hillslope dynamcis: exposure age and erosion rates	[] cosmogenic nuclides are interpreted and applied to landscape models to calculate soil residence time in a small forested catchment. []	regolith), soil (regolith), aspect (location_and_topography), latitude_or_longitude (location_and_topography	<u>Detail</u>
8	2 Weathering rates and soil formation: insights from landscape position	[] 1D, 2D, and 3D transects were sampled []	, major_elements (regolith), minor_elements (regolith), mineralogy (regolith), soil (regolith)	<u>Detail</u>
9	U and Pb concentrations in surface soils and bedrock: new analytical techniques	[] new analytical techniques for quantifying U, Th, and Pb are applied to a small catchment. []	), stream_or_reservoir_sediments ( <b>regolith</b> ), <b>soil</b> ( <b>regolith</b> ), radiogenic_nuclides (location_and_topography)	<u>Detail</u>

Appendix I (see RLS pdf document)

Appendix II. (see RLS pps of summer seminar)

## **Appendix III: Critical Zone Ontology**

Superconcept = Critical Zone

Concept = Atmosphere

Subconcept = Precipitation

Property = throughfall, stemflow, actual

Sub-property = chemistry

Sub-sub-property = Isotopes

Sub-sub-sub-property =  ${}^{1}$ H,  ${}^{2}$ H,  ${}^{3}$ H,  ${}^{12}$ C,  ${}^{13}$ C,  ${}^{14}$ N,  ${}^{15}$ N,  ${}^{16}$ O,  ${}^{17}$ O,  ${}^{18}$ O,  ${}^{32}$ S,  ${}^{33}$ S,  ${}^{34}$ S,  ${}^{36}$ S,  ${}^{190}$ Pt- ${}^{186}$ Os,  ${}^{147}$ Sm- ${}^{143}$ Nd,  ${}^{87}$ Rb- ${}^{87}$ Sr,  ${}^{187}$ Re- ${}^{187}$ Os,  ${}^{176}$ Lu- ${}^{176}$ Hf,  ${}^{232}$ Th- ${}^{208}$ Pb,

<sup>40</sup>K-<sup>40</sup>Ar, <sup>238</sup>U-<sup>206</sup>Pb, <sup>40</sup>K-<sup>40</sup>Ca, <sup>235</sup>U-<sup>207</sup>Pb,

<sup>129</sup>I-<sup>129</sup>Xe, <sup>10</sup>Be-<sup>10</sup>B, <sup>26</sup>Al-<sup>26</sup>Mg, <sup>36</sup>Cl-<sup>36</sup>Ar/S,

<sup>234</sup>U-<sup>230</sup>Th, <sup>230</sup>Th-<sup>226</sup>Ra, <sup>231</sup>Pa-<sup>227</sup>Ac, <sup>14</sup>C-<sup>14</sup>N,

<sup>226</sup>Ra-<sup>222</sup>Rn, <sup>10</sup>Be, <sup>14</sup>C, <sup>26</sup>Al, <sup>36</sup>Cl, <sup>41</sup>Ca and <sup>129</sup>I

Sub-sub-property = Major elements

Sub-sub-property = Ca, Mg, Na, K, P, HCO<sub>3</sub>, SO<sub>4</sub>, Cl, SiO<sub>2</sub>, Al, Fe, F, NO<sub>3</sub>, NH<sub>4</sub>, pH, DOC, DIC

Sub-sub-property = Minor elements

Sub-sub-sub-property = Rb, Sr, Y, Zr, Nb, Ba, Zn, Ag, Ce, Co, Cs, Cu, Dy, Er, Eu, Ga, Gd, Hf, Ho, La, Lu, Mo, Nd, Ni, Pr, Sm, Sn, Ta, Tb, Th, Tl, Tm, U, V, W, Yb

Property = liquid, frozen, snow

Sub-property = seasonal amount, water equivalence, depth

Subconcept = Heat Flux

Property = sensible, latent

Subconcept = Winds

Property = direction, fetch, velocity

Subconcept = Air Temperature

Property = dew point, wet bulb, dry bulb

Subconcept = Humidity

Property = relative, absolute

Subconcept = Pressure

Property = barometric, water vapor

Subconcept = Radiation

Property = terrestrial

Sub-property = upward, downward

Property = solar

Sub-property = reflected, incident, net, photosynthetic

Subconcept = Dry Deposition

Property = chemistry

Sub-property = Isotopes

Sub-sub-property = <sup>1</sup>H, <sup>2</sup>H, <sup>3</sup>H, <sup>12</sup>C, <sup>13</sup>C, <sup>14</sup>N, <sup>15</sup>N, <sup>16</sup>O, <sup>17</sup>O, <sup>18</sup>O, <sup>32</sup>S, <sup>33</sup>S, <sup>34</sup>S, <sup>36</sup>S, <sup>190</sup>Pt-<sup>186</sup>Os, <sup>147</sup>Sm-<sup>143</sup>Nd, <sup>87</sup>Rb-<sup>87</sup>Sr, <sup>187</sup>Re-<sup>187</sup>Os, <sup>176</sup>Lu-<sup>176</sup>Hf, <sup>232</sup>Th-<sup>208</sup>Pb, <sup>40</sup>K-<sup>40</sup>Ar, <sup>238</sup>U-<sup>206</sup>Pb, <sup>40</sup>K-<sup>40</sup>Ca, <sup>235</sup>U-<sup>207</sup>Pb, <sup>129</sup>I-<sup>129</sup>Xe, <sup>10</sup>Be-<sup>10</sup>B, <sup>26</sup>Al-<sup>26</sup>Mg, <sup>36</sup>Cl-<sup>36</sup>Ar/S, <sup>234</sup>U-<sup>230</sup>Th, <sup>230</sup>Th-<sup>226</sup>Ra, <sup>231</sup>Pa-<sup>227</sup>Ac, <sup>14</sup>C-<sup>14</sup>N, <sup>226</sup>Ra-<sup>222</sup>Rn, <sup>10</sup>Be, <sup>14</sup>C, <sup>26</sup>Al, <sup>36</sup>Cl, <sup>41</sup>Ca and <sup>129</sup>I

Sub-property = Major elements

Sub-sub-property = Ca, Mg, Na, K, P, HCO<sub>3</sub>, SO<sub>4</sub>, Cl, SiO<sub>2</sub>, Al, Fe, F, NO<sub>3</sub>, NH<sub>4</sub>, pH, DOC, DIC

Sub-property = Minor elements

Sub-sub-property = Rb, Sr, Y, Zr, Nb, Ba, Zn, Ag, Ce, Co, Cs, Cu, Dy, Er, Eu, Ga, Gd, Hf, Ho, La, Lu, Mo, Nd, Ni, Pr, Sm, Sn, Ta, Tb, Th, Tl, Tm, U, V, W, Yb

Property = volume

#### Concept = Water

Subconcept = Surface Water

Property = level, stage, flow, gauge height, flow, evaporation, alkalinity, temperature, specific conductance, total dissolved solids

Property = chemistry

Sub-property = Isotopes

Sub-sub-property = <sup>1</sup>H, <sup>2</sup>H, <sup>3</sup>H, <sup>12</sup>C, <sup>13</sup>C, <sup>14</sup>N, <sup>15</sup>N, <sup>16</sup>O, <sup>17</sup>O, <sup>18</sup>O, <sup>32</sup>S, <sup>33</sup>S, <sup>34</sup>S, <sup>36</sup>S, <sup>190</sup>Pt-<sup>186</sup>Os, <sup>147</sup>Sm-<sup>143</sup>Nd, <sup>87</sup>Rb-<sup>87</sup>Sr, <sup>187</sup>Re-<sup>187</sup>Os, <sup>176</sup>Lu-<sup>176</sup>Hf, <sup>232</sup>Th-<sup>208</sup>Pb, <sup>40</sup>K-<sup>40</sup>Ar, <sup>238</sup>U-<sup>206</sup>Pb, <sup>40</sup>K-<sup>40</sup>Ca, <sup>235</sup>U-<sup>207</sup>Pb, <sup>129</sup>I-<sup>129</sup>Xe, <sup>10</sup>Be-<sup>10</sup>B, <sup>26</sup>Al-<sup>26</sup>Mg, <sup>36</sup>Cl-<sup>36</sup>Ar/S, <sup>234</sup>U-<sup>230</sup>Th, <sup>230</sup>Th-<sup>226</sup>Ra, <sup>231</sup>Pa-<sup>227</sup>Ac, <sup>14</sup>C-<sup>14</sup>N, <sup>226</sup>Ra-<sup>222</sup>Rn, <sup>10</sup>Be, <sup>14</sup>C, <sup>26</sup>Al, <sup>36</sup>Cl, <sup>41</sup>Ca and <sup>129</sup>I

Sub-property = Major elements

Sub-sub-property = Ca, Mg, Na, K, P, HCO<sub>3</sub>, SO<sub>4</sub>, Cl, SiO<sub>2</sub>, Al, Fe, F, NO<sub>3</sub>, NH<sub>4</sub>, pH, DOC, DIC

Sub-property = Minor elements

Sub-sub-property = Rb, Sr, Y, Zr, Nb, Ba, Zn, Ag, Ce, Co, Cs, Cu, Dy, Er, Eu, Ga, Gd, Hf, Ho, La, Lu, Mo, Nd, Ni, Pr, Sm, Sn, Ta, Tb, Th, Tl, Tm, U, V, W, Yb

Subconcept = Ground Water

Properties = level, flow, alkalinity, temperature, hydraulic head, hydraulic conductivity, resistance, electrical resistivity, specific conductance, total dissolved solids

**Properties** = chemistry

Sub-property = Isotopes

Sub-sub-property = <sup>1</sup>H, <sup>2</sup>H, <sup>3</sup>H, <sup>12</sup>C, <sup>13</sup>C, <sup>14</sup>N, <sup>15</sup>N, <sup>16</sup>O, <sup>17</sup>O, <sup>18</sup>O, <sup>32</sup>S, <sup>33</sup>S, <sup>34</sup>S, <sup>36</sup>S, <sup>190</sup>Pt-<sup>186</sup>Os, <sup>147</sup>Sm-<sup>143</sup>Nd, <sup>87</sup>Rb-<sup>87</sup>Sr, <sup>187</sup>Re-<sup>187</sup>Os, <sup>176</sup>Lu-<sup>176</sup>Hf, <sup>232</sup>Th-<sup>208</sup>Pb, <sup>40</sup>K-<sup>40</sup>Ar, <sup>238</sup>U-<sup>206</sup>Pb, <sup>40</sup>K-<sup>40</sup>Ca, <sup>235</sup>U-<sup>207</sup>Pb, <sup>129</sup>I-<sup>129</sup>Xe, <sup>10</sup>Be-<sup>10</sup>B, <sup>26</sup>Al-<sup>26</sup>Mg, <sup>36</sup>Cl-<sup>36</sup>Ar/S, <sup>234</sup>U-<sup>230</sup>Th, <sup>230</sup>Th-<sup>226</sup>Ra, <sup>231</sup>Pa-<sup>227</sup>Ac, <sup>14</sup>C-<sup>14</sup>N, <sup>226</sup>Ra-<sup>222</sup>Rn, <sup>10</sup>Be, <sup>14</sup>C, <sup>26</sup>Al, <sup>36</sup>Cl, <sup>41</sup>Ca and <sup>129</sup>I

Sub-property = Major elements

Sub-sub-property = Ca, Mg, Na, K, P, HCO<sub>3</sub>, SO<sub>4</sub>, Cl, SiO<sub>2</sub>, Al, Fe, F, NO<sub>3</sub>, NH<sub>4</sub>, pH, DOC, DIC

Sub-property = Minor elements

Sub-sub-property = Rb, Sr, Y, Zr, Nb, Ba, Zn, Ag, Ce, Co, Cs, Cu, Dy, Er, Eu, Ga, Gd, Hf, Ho, La, Lu, Mo, Nd, Ni, Pr, Sm, Sn, Ta, Tb, Th, Tl, Tm, U, V, W, Yb

Subconcept = Vadose Zone

Properties = soil moisture, matrix potential, alkalinity, temperature, resistance, electrical resistivity, hydraulic conductivity, specific conductance, total dissolved solids

Property = chemistry

Sub-property = soil gas

Sub-sub-property =  $CH_4$ ,  $CO_2$ ,  $O_2$ ,  $NO_2$ 

Sub-sub-property = Isotopes

Sub-sub-property =  ${}^{12}C$ ,  ${}^{13}C$ ,  ${}^{14}N$ ,  ${}^{15}N$ ,  ${}^{16}O$ ,  ${}^{17}O$ ,

Sub-property = pore water

Sub-sub-property = Isotopes

Sub-sub-sub-property =  ${}^{1}$ H,  ${}^{2}$ H,  ${}^{3}$ H,  ${}^{12}$ C,  ${}^{13}$ C,  ${}^{14}$ N,  ${}^{15}$ N,  ${}^{16}$ O,  ${}^{17}$ O,  ${}^{18}$ O,  ${}^{32}$ S,  ${}^{33}$ S,  ${}^{34}$ S,  ${}^{36}$ S,  ${}^{190}$ Pt- ${}^{186}$ Os,  ${}^{147}$ Sm- ${}^{143}$ Nd,  ${}^{87}$ Rb- ${}^{87}$ Sr,  ${}^{187}$ Re- ${}^{187}$ Os,  ${}^{176}$ Lu- ${}^{176}$ Hf,  ${}^{232}$ Th- ${}^{208}$ Pb,  ${}^{40}$ K- ${}^{40}$ Ar,  ${}^{238}$ U- ${}^{206}$ Pb,  ${}^{40}$ K- ${}^{40}$ Ca,  ${}^{235}$ U-  ${}^{207}$ Pb,  ${}^{129}$ I- ${}^{129}$ Xe,  ${}^{10}$ Be- ${}^{10}$ B,  ${}^{26}$ Al- ${}^{26}$ Mg,  ${}^{36}$ Cl- ${}^{36}$ Ar/S,  ${}^{234}$ U- ${}^{230}$ Th,  ${}^{230}$ Th- ${}^{226}$ Ra,  ${}^{231}$ Pa- ${}^{227}$ Ac,  ${}^{14}$ C- ${}^{14}$ N,  ${}^{226}$ Ra- ${}^{222}$ Rn,  ${}^{10}$ Be,  ${}^{14}$ C,  ${}^{26}$ Al,  ${}^{36}$ Cl,  ${}^{41}$ Ca and  ${}^{129}$ I

Sub-sub-property = Major elements

Sub-sub-property = Ca, Mg, Na, K, P, HCO<sub>3</sub>, SO<sub>4</sub>, Cl, SiO<sub>2</sub>, Al, Fe, F, NO<sub>3</sub>, NH<sub>4</sub>, pH, DOC, DIC

Sub-sub-property = Minor elements

Sub-sub-property = Rb, Sr, Y, Zr, Nb, Ba, Zn, Ag, Ce, Co, Cs, Cu, Dy, Er, Eu, Ga, Gd, Hf, Ho, La, Lu, Mo, Nd, Ni, Pr, Sm, Sn, Ta, Tb, Th, Tl, Tm, U, V, W, Yb

Subconcept = Evapotranspiration

Properties= actual, potential

Concept = Lithology

Subconcept = Bedrock

Properties = igneous, metamorphic, sedimentary

Sub-property = age, mineralogy, depositional history, hydraulic conductivity

Sub-property = chemistry

Sub-sub-property = Isotopes

Sub-sub-sub-property =  ${}^{1}$ H,  ${}^{2}$ H,  ${}^{3}$ H,  ${}^{12}$ C,  ${}^{13}$ C,  ${}^{14}$ N,  ${}^{15}$ N,  ${}^{16}$ O,  ${}^{17}$ O,  ${}^{18}$ O,  ${}^{32}$ S,  ${}^{33}$ S,  ${}^{34}$ S,  ${}^{36}$ S,  ${}^{190}$ Pt- ${}^{186}$ Os, <sup>147</sup>Sm-<sup>143</sup>Nd, <sup>87</sup>Rb-<sup>87</sup>Sr, <sup>187</sup>Re-<sup>187</sup>Os, <sup>176</sup>Lu-<sup>176</sup>Hf,
<sup>232</sup>Th-<sup>208</sup>Pb, <sup>40</sup>K-<sup>40</sup>Ar, <sup>238</sup>U-<sup>206</sup>Pb, <sup>40</sup>K-<sup>40</sup>Ca, <sup>235</sup>U-<sup>207</sup>Pb, <sup>129</sup>I-<sup>129</sup>Xe, <sup>10</sup>Be-<sup>10</sup>B, <sup>26</sup>Al-<sup>26</sup>Mg, <sup>36</sup>Cl-<sup>36</sup>Ar/S,
<sup>234</sup>U-<sup>230</sup>Th, <sup>230</sup>Th-<sup>226</sup>Ra, <sup>231</sup>Pa-<sup>227</sup>Ac, <sup>14</sup>C-<sup>14</sup>N,
<sup>226</sup>Ra-<sup>222</sup>Rn, <sup>10</sup>Be, <sup>14</sup>C, <sup>26</sup>Al, <sup>36</sup>Cl, <sup>41</sup>Ca and <sup>129</sup>I

Sub-sub-property = Major elements

Sub-sub-property =  $SiO_2$ ,  $Al_2O_3$ , CaO, MgO,  $Na_2O$ ,  $K_2O$ ,  $Fe_2O_3$ , MnO,  $TiO_2$ ,  $P_2O_5$ ,  $Cr_2O_3$ , LOI

Sub-sub-property = Minor elements

Sub-sub-sub-property = Rb, Sr, Y, Zr, Nb, Ba, Zn, Ag, Ce, Co, Cs, Cu, Dy, Er, Eu, Ga, Gd, Hf, Ho, La, Lu, Mo, Nd, Ni, Pr, Sm, Sn, Ta, Tb, Th, Tl, Tm, U, V, W, Yb

Sub-sub-property = Extracted

Sub-sub-property = pH, exchangeable acidity, CEC, base saturation, Fe-oxides, Al-oxides

Subconcept = Regolith

Properties = alluvium, colluvium, loess, stream/reservoir sediments

Sub-properties = age, depositional history, mineralogy, hydraulic conductivity

Sub-properties = chemistry

Sub-sub-property = Isotopes

Sub-sub-sub-property =  ${}^{1}$ H,  ${}^{2}$ H,  ${}^{3}$ H,  ${}^{12}$ C,  ${}^{13}$ C,  ${}^{14}$ N,  ${}^{15}$ N,  ${}^{16}$ O,  ${}^{17}$ O,  ${}^{18}$ O,  ${}^{32}$ S,  ${}^{33}$ S,  ${}^{34}$ S,  ${}^{36}$ S,  ${}^{190}$ Pt- ${}^{186}$ Os,  ${}^{147}$ Sm- ${}^{143}$ Nd,  ${}^{87}$ Rb- ${}^{87}$ Sr,  ${}^{187}$ Re- ${}^{187}$ Os,  ${}^{176}$ Lu- ${}^{176}$ Hf,  ${}^{232}$ Th- ${}^{208}$ Pb,  ${}^{40}$ K- ${}^{40}$ Ar,  ${}^{238}$ U- ${}^{206}$ Pb,  ${}^{40}$ K- ${}^{40}$ Ca,  ${}^{235}$ U-  ${}^{207}$ Pb,  ${}^{129}$ I- ${}^{129}$ Xe,  ${}^{10}$ Be- ${}^{10}$ B,  ${}^{26}$ Al- ${}^{26}$ Mg,  ${}^{36}$ Cl- ${}^{36}$ Ar/S,  ${}^{234}$ U- ${}^{230}$ Th,  ${}^{230}$ Th- ${}^{226}$ Ra,  ${}^{231}$ Pa- ${}^{227}$ Ac,  ${}^{14}$ C- ${}^{14}$ N,  ${}^{226}$ Ra- ${}^{222}$ Rn,  ${}^{10}$ Be,  ${}^{14}$ C,  ${}^{26}$ Al,  ${}^{36}$ Cl,  ${}^{41}$ Ca and  ${}^{129}$ I

Sub-sub-property = Major elements

Sub-sub-property = SiO<sub>2</sub>, Al<sub>2</sub>O<sub>3</sub>, CaO, MgO, Na<sub>2</sub>O, K<sub>2</sub>O, Fe<sub>2</sub>O<sub>3</sub>, MnO, TiO<sub>2</sub>, P<sub>2</sub>O<sub>5</sub>, Cr<sub>2</sub>O<sub>3</sub>

Sub-sub-property = Minor elements

Sub-sub-sub-property = Rb, Sr, Y, Zr, Nb, Ba, Zn, Ag, Ce, Co, Cs, Cu, Dy, Er, Eu, Ga, Gd, Hf, Ho, La, Lu, Mo, Nd, Ni, Pr, Sm, Sn, Ta, Tb, Th, Tl, Tm, U, V, W, Yb

Sub-sub-property = Extracted

Sub-sub-property = pH, exchangeable acidity, CEC, base saturation, Fe-oxides, Al-oxides

Properties = Soil

Sub-properties = taxonomy, morphology, mineralogy, hydraulic conductivity

Sub-properties = physical properties

Sub-sub-property = grain size distribution, bulk density, specific grain density, BET surface area

Sub-properties = soil horizons

Sub-sub-property = O, A, E, B, C, R, W, AE, EA, EB, BE, BC, AC

Sub-properties = chemistry

Sub-sub-property = Isotopes

Sub-sub-sub-property =  ${}^{1}$ H,  ${}^{2}$ H,  ${}^{3}$ H,  ${}^{12}$ C,  ${}^{13}$ C,  ${}^{14}$ N,  ${}^{15}$ N,  ${}^{16}$ O,  ${}^{17}$ O,  ${}^{18}$ O,  ${}^{32}$ S,  ${}^{33}$ S,  ${}^{34}$ S,  ${}^{36}$ S,  ${}^{190}$ Pt- ${}^{186}$ Os,  ${}^{147}$ Sm- ${}^{143}$ Nd,  ${}^{87}$ Rb- ${}^{87}$ Sr,  ${}^{187}$ Re- ${}^{187}$ Os,  ${}^{176}$ Lu- ${}^{176}$ Hf,  ${}^{232}$ Th- ${}^{208}$ Pb,  ${}^{40}$ K- ${}^{40}$ Ar,  ${}^{238}$ U- ${}^{206}$ Pb,  ${}^{40}$ K- ${}^{40}$ Ca,  ${}^{235}$ U-  ${}^{207}$ Pb,  ${}^{129}$ I- ${}^{129}$ Xe,  ${}^{10}$ Be- ${}^{10}$ B,  ${}^{26}$ Al- ${}^{26}$ Mg,  ${}^{36}$ Cl- ${}^{36}$ Ar/S,  ${}^{234}$ U- ${}^{230}$ Th,  ${}^{230}$ Th- ${}^{226}$ Ra,  ${}^{231}$ Pa- ${}^{227}$ Ac,  ${}^{14}$ C- ${}^{14}$ N,  ${}^{226}$ Ra- ${}^{222}$ Rn,  ${}^{10}$ Be,  ${}^{14}$ C,  ${}^{26}$ Al,  ${}^{36}$ Cl,  ${}^{41}$ Ca and  ${}^{129}$ I

Sub-sub-property = Major elements

Sub-sub-property =  $SiO_2$ ,  $Al_2O_3$ , CaO, MgO,  $Na_2O$ ,  $K_2O$ ,  $Fe_2O_3$ , MnO,  $TiO_2$ ,  $P_2O_5$ ,  $Cr_2O_3$ 

Sub-sub-property = Minor elements

Sub-sub-property = Rb, Sr, Y, Zr, Nb, Ba, Zn, Ag, Ce, Co, Cs, Cu, Dy, Er, Eu, Ga, Gd, Hf, Ho, La, Lu, Mo, Nd, Ni, Pr, Sm, Sn, Ta, Tb, Th, Tl, Tm, U, V, W, Yb

Sub-sub-property = Extracted

Sub-sub-property = pH, exchangeable acidity, CEC, base saturation, Fe-oxides, Al-oxides

Sub-sub-property = organic matter

Sub=sub-sub-property = SOC, SON, <sup>1</sup>H, <sup>2</sup>H, <sup>3</sup>H, <sup>12</sup>C, <sup>13</sup>C, <sup>14</sup>N, <sup>15</sup>N, <sup>16</sup>O, <sup>17</sup>O, <sup>18</sup>O, <sup>32</sup>S, <sup>33</sup>S, <sup>34</sup>S, <sup>36</sup>S, <sup>190</sup>Pt-<sup>186</sup>Os, <sup>147</sup>Sm-<sup>143</sup>Nd, <sup>87</sup>Rb-<sup>87</sup>Sr, <sup>187</sup>Re-<sup>187</sup>Os, <sup>176</sup>Lu-<sup>176</sup>Hf, <sup>232</sup>Th-<sup>208</sup>Pb, <sup>40</sup>K-<sup>40</sup>Ar, <sup>238</sup>U-<sup>206</sup>Pb, <sup>40</sup>K-<sup>40</sup>Ca, <sup>235</sup>U-<sup>207</sup>Pb, <sup>129</sup>I-<sup>129</sup>Xe, <sup>10</sup>Be-<sup>10</sup>B, <sup>26</sup>Al-<sup>26</sup>Mg, <sup>36</sup>Cl-<sup>36</sup>Ar/S, <sup>234</sup>U-<sup>230</sup>Th, <sup>230</sup>Th-<sup>226</sup>Ra, <sup>231</sup>Pa-<sup>227</sup>Ac, <sup>14</sup>C-<sup>14</sup>N, <sup>226</sup>Ra-<sup>222</sup>Rn, <sup>10</sup>Be, <sup>14</sup>C, <sup>26</sup>Al, <sup>36</sup>Cl, <sup>41</sup>Ca and <sup>129</sup>I

Concept = Land Surface

Subconcept = Location & topography

Properties = aspect, latitude/longitude, elevation, relief,

Properties = slope

Sub-property = concave, convex

Properties = surface area, erosion rates

Sub-property = radiogenic nuclides

Sub-sub-property =  ${}^{14}C$ ,  ${}^{137}Cs$ ,  ${}^{210}Pb$ 

Sub-property = cosmogenic nuclides

Sub-sub-property =  ${}^{10}$ Be,  ${}^{14}$ C,  ${}^{26}$ Al,  ${}^{36}$ Cl,  ${}^{39}$ Ar

Sub-property = geological constraints

Subconcept = Watershed

Property = catchment area

Property = stream order

Sub-property = Horton, Strahler

Property = stream segment

Sub-property = profile, cross-section, drainage area

Concept = Biology

Subconcept = Flora

Properties = classification (species), location, leaf specific hydraulic conductivity, stem water potential, hydraulic vulnerability, hydraulic capacitance, productivity, sap flow, transpiration, biomass, litter, root distribution and subsurface biomass

Properties = chemistry

Sub-property = Isotopes

$$\begin{split} & \text{Sub-sub-property} = {}^{1}\text{H}, {}^{2}\text{H}, {}^{3}\text{H}, {}^{12}\text{C}, {}^{13}\text{C}, {}^{14}\text{N}, {}^{15}\text{N}, {}^{16}\text{O}, {}^{17}\text{O}, \\ {}^{18}\text{O}, {}^{32}\text{S}, {}^{33}\text{S}, {}^{34}\text{S}, {}^{36}\text{S}, {}^{190}\text{Pt} {}^{-186}\text{Os}, {}^{147}\text{Sm} {}^{143}\text{Nd}, {}^{87}\text{Rb} {}^{-87}\text{Sr}, \\ {}^{187}\text{Re} {}^{-187}\text{Os}, {}^{176}\text{Lu} {}^{176}\text{Hf}, {}^{232}\text{Th} {}^{-208}\text{Pb}, {}^{40}\text{K} {}^{-40}\text{Ar}, {}^{238}\text{U} {}^{-206}\text{Pb}, \\ {}^{40}\text{K} {}^{-40}\text{Ca}, {}^{235}\text{U} {}^{-207}\text{Pb}, {}^{129}\text{I} {}^{-129}\text{Xe}, {}^{10}\text{Be} {}^{-10}\text{B}, {}^{26}\text{Al} {}^{-26}\text{Mg}, {}^{36}\text{Cl} {}^{-36}\text{Ar/S}, {}^{234}\text{U} {}^{-230}\text{Th}, {}^{230}\text{Th} {}^{-226}\text{Ra}, {}^{231}\text{Pa} {}^{-227}\text{Ac}, {}^{14}\text{C} {}^{-14}\text{N}, \end{split}$$

<sup>226</sup>Ra-<sup>222</sup>Rn, <sup>10</sup>Be, <sup>14</sup>C, <sup>26</sup>Al, <sup>36</sup>Cl, <sup>41</sup>Ca and <sup>129</sup>I

Sub-property = Major elements

Sub-sub-property = Ca, Mg, Na, K, P, HCO<sub>3</sub>, SO<sub>4</sub>, Cl, SiO<sub>2</sub>, Al, Fe, F, NO<sub>3</sub>, NH<sub>4</sub>, pH, DOC, DIC

Sub-property = Minor elements

Sub-sub-property = Rb, Sr, Y, Zr, Nb, Ba, Zn, Ag, Ce, Co, Cs, Cu, Dy, Er, Eu, Ga, Gd, Hf, Ho, La, Lu, Mo, Nd, Ni, Pr, Sm, Sn, Ta, Tb, Th, Tl, Tm, U, V, W, Yb

Subconcept = Fauna

Properties = community composition

Sub-property = DNA, RNA, phospholipid fatty acid

# Properties = microbial biomass

Sub-property = chloroform-fumigated extraction, substrate induced respiration