Annual Report for Period: 11/2007 - 10/2008 Submitted on: 09/01/2008 Principal Investigator: Duffy, Christopher J. Award ID: NSF EAR 07-25019 Organization: Pennsylvania State University Submitted By: Duffy, Christopher - Principal Investigator Title: The Susquehanna/Shale Hills Critical Zone Observatory

Project Participants

Senior Personnel:

Name: Duffy, Christopher Worked for more than 160 Hours: Yes Contribution to Project: Stable Isotope and Computational Hydrology

Name: Brantley, Susan Worked for more than 160 Hours: Yes Contribution to Project: Geochemistry

Name: Singha, Kamini Worked for more than 160 Hours: Yes Contribution to Project: Hydrogeophysics

Name: Slingerland, Rudy Worked for more than 160 Hours: Yes Contribution to Project: Geomorphology

Name: Toran, Laura Worked for more than 160 Hours: Yes Contribution to Project: Hydrogeophysics

Name: Davis, Kenneth Worked for more than 160 Hours: Yes Contribution to Project: Meteorology

Name: Eissenstat, David Worked for more than 160 Hours: Yes Contribution to Project: Plant Ecology

Name: Kaye, Jason Worked for more than 160 Hours: Yes Contribution to Project: Soil Science

Name: Kirby, Eric Worked for more than 160 Hours: Yes Contribution to Project: Geomorphology Name: Lin, Henry Worked for more than 160 Hours: Yes Contribution to Project: Hydropedology

Name: Miller, Douglas Worked for more than 160 Hours: Yes Contribution to Project: Cyberinfrastructure, Data portal

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: No Contribution to Project: Geochemistry

Name: White, Timothy Worked for more than 160 Hours: Yes Contribution to Project: Soil Science, 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: Tsegaye, Teferi Worked for more than 160 Hours: Yes Contribution to Project: Transect Participant

Name: Santos, Hernan Worked for more than 160 Hours: No

Contribution to Project: Transect Participant

Post-doc:

Name: Jin, Lixin, Earth and Environmental Systems Institute

Graduate Students: (funded or working in parallel efforts at Shale Hills)

Name: Holmes, George, PhD Civil and Environmental Engineering
Name: Andrews, Danielle, PhD Soil Science
Name: Jennifer Williams, PhD Geosciences
Name: Beth Herndon, Geoscience
Name: Yesavage, Tiffany, PhD Geosciences
Name: Cherrey, Kelly, PhD Meteorology
Name: Fuller, Robert, PhD Geosciences
Name: Li, Wenfang, MS Civil and Environmental Engineering
Name: Li, Shuangcai, PhD Civil and Environmental Engineering

Undergraduate Students:

Name: Poonam Giri, Geosciences Molly Holleran, Geosciences

Technician:

Name: Cherrey, Kelly Worked for more than 160 Hours: Yes Contribution to Project: Wireless Field Installations, Power Distribution, Sensor Deployment, Auto-sampler installations for Isotope/Chemistry

Other Senior Participants:

Name: Boyer, Elizabeth Worked for more than 160 Hours: Yes Contribution to Project: Isotope hydrology, precipitation chemistry

Name: Tuttle, Michelle Worked for more than 160 Hours: No Contribution to Project:

Name: Goldhaber, Marty Worked for more than 160 Hours: No Contribution to Project:

Name: Lichtner, Peter Worked for more than 160 Hours: No Contribution to Project: Name: Steefel, Carl Worked for more than 160 Hours: No Contribution to Project:

Name: Wagener, Thorsten Worked for more than 160 Hours: No Contribution to Project: Computational Hydrology

Name: Lehnert, Kirstin Worked for more than 160 Hours: Yes Contribution to Project: Cyberinfrastructure for geochemical data

Research Experience for Undergraduates:

Name: Flemings, John Worked for more than 160 Hours: Yes Contribution to Project: REU at Penn State University as part of the Astrobiology Program, Summer 2008

Name: Melendez-Oyola, Melissa M. Worked for more than 160 Hours: Yes Contribution to Project: University of Puerto Rico, Río Piedras Campus. Environmental Science Program. REU at Penn State University, Horticulture Department, Summer 2008

Name: Duffy, Colin Worked for more than 160 Hours: Yes Contribution to Project: Pennsylvania College of Technology, Electronics and Computer Engineering Technology. REU at Penn State University, Civil and Environmental Engineering, Summer 2008

Partner Organizations

CZEN: The Critical Zone Environmental Network has served as a web-host for the Shale Hills Critical Zone Observatory (www.czen.org/).

GfG Geoinformatics for Geochemistry program, led by Kirstin Lehnert Lamont-Doherty Earth Observatory, Columbia University

CUAHSI: The CUAHSI Hydrologic Information System (HIS) and the Hydrologic Measurement Facility (HMF) teams have been valuable consultants in the development of our data and sensor deployment. The CUAHSI headquarters team has also been helpful through site visits by Rick Hooper and insight on a national strategy.

WATERS: The engineering directorate funded early model development and RTH NET real-time data development and in data mining historical data and information about the Shale Hills site.

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 2way communication and control for all sensors in a high resolution adaptive sensor array. More information on this will be presented next year but seed money has been made available to test the design by the Penn State Institute for CyberScience (ICS) and Penn State Institutes for Energy & the Environment.

Activities and Findings

Research and Education Activities: (See PDF version submitted by PI at the end of the report) See attached work plan

Findings: (See PDF version submitted by PI at the end of the report) See attached

Training and Development:

Outreach Activities:

We have provided press releases, newspaper interviews and are formulating a recurring newsletter to be posted on a project website that is currently offline and under development.

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).

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 environmental education



Creek Environmental National NAEE award for distinguished

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.

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 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 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.

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 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)

Web/Internet Site

CZEN.org is the main site for sharing data within and between the CZO's. The home for the project website is offline and currently under construction. It is expected to be online by October 2008. RTH_NET continues to provide real time hydrologic data at Shale Hills through the CUAHSI-WATERS projects at Penn State.

Other Specific Products

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

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.

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 site visits to CUAHSI, investigators from universities (e.g. University of Pittsburgh, Oregon State) and the field portion of the First International Hydropedology Conference (held at Penn State July 28-31, 2008)

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.

Contributions Beyond Science and Engineering:

The initial year during for the Shale Hills CZO is dedicated to building the necessary infrastructure to support the theoretical and experimental science proposed. This infrastructure (wireless, real time communications, and data streams) will also serve as a

Special Requirements

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

Findings

The following text and diagrams give the status of various activities in the work plan. Refer to the section in the work plan of the same title for a description of activities. Figure 1 illustrates the study site, the digital terrain. A regional road map is at the end of the document.

Geochemistry

Field and Laboratory Soil Analysis:

A 70' boring was drilled at the highest point of the catchment and characterized for chemistry and mineralogy. The un-weathered, deeper portion of the boring is used as parent material in future discussion. Soil cores, from the surface to parent at 10 cm interval, were collected in multiple locations within the catchment, including the ridge top of the catchment (1-D system), three cores along the planar transect (2-D), and three cores along the swale transect (3-D). These samples were analyzed for bulk density, soil chemistry and mineralogy. Comparison between parent and soils suggests dissolution of chlorite and illite followed by precipitation of kaolinite, with vermiculite and hydroxy-interlayered vermiculite as intermediate phases. These mineral transformation reactions are in agreement with soil chemistry, which shows depletion of Mg, Fe, Al and Si to a lesser extent.

Nests of tension lysimeters (soil water sampler) were installed at ridge top, along the planar transect and also along the swale transect. Soil waters and streams were collected weekly for elemental analyses and stable isotope measurements (H and O), as well as different species of nutrients (i.e. C, N and P). Soil gas samplers were installed along the planar transect, and samples were taken monthly for measurements of CO₂, CH₄ and O₂ concentrations. O₂ is an important indicator of the redox conditions in the soil profiles, which is crucial for solubility and transport of redox sensitive elements (e.g., Fe, and Al) and also for reactivity of microbial community.

Neutron techniques were applied to study micro-porosity and micro-structures within the shale chips when rock transforms into soils. Physical breakup at the bedrock-saprolite boundary initiates the soil development and allows chemical dissolution to occur. The fractal dimensions were also investigated by neutron techniques.

South-slope soil cores were analyzed in 2006 and found to exhibit surface Mn enrichment. A north-slope transect was investigated in fall 2007 for comparison. Soil cores were augered at ridge, mid-slope and valley locations. Additionally, shallow pits were dug at three ridge sites to acquire more finely spaced depth samples than obtained by auger. Soil samples were analyzed for particle size distribution, elemental and mineralogical composition, and extractable fractions. North-slope element soil profiles indicate a Mn addition profile similar to that previously observed on the south-slope. Mn is the sole element consistently exhibiting an addition profile in Shale Hills soils. Sequential extractions suggest primarily oxide and amorphous Mn compounds with even distribution between silt- and sand-sized fractions. Preliminary XANES data indicate Mn is present in mixed (+2/+4) oxidation states with an unusual bonding environment. Ongoing work seeks to further elucidate Mn compound characteristics.



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

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.



Root boxes:

Small rhizotrons were installed at ridge, mid-slope, and valley sites in close proximity to south slope cores augered in 2006. Shallow pits (2ft x 2ft x 1ft) were dug and pressure-treated plywood panels were installed against the exposed soil surface. Two of the panels contain transparent acetate windows that allow direct observation of the soil subsurface. The rhizotrons will be used to spatially characterize chemical and biological processes occurring in the root zone.

Microbial:

Microbial community characterization was initiated by summer student John Flemings in the Penn State REU Astrobiology program. Soil samples for microbial analysis were collected from ridge, mid-slope, and valley auger cores using aseptic techniques. Valley samples from four different depths were targeted for heterotrophic and Fe-reduction enrichment cultures. Both direct enumeration and heterotrophic enrichment cultures indicated greatest cell density near the surface that decreased with depth. Consortia grown in Fe-reduction media likewise exhibited greatest growth from near-surface samples; however, enhanced microbial growth was also observed in cultures inoculated from soil near the bedrock interface. This may indicate microbially-mediated Fe redox is occurring at depth. Ensuing microbial and molecular biological work will continue in the coming year. The focus of this work will be to characterize biotic Fe and Mn cycling in order to understand catchment-scale weathering processes.

Model:

A consistent Mn addition profile suggests Mn is input atmospherically. Mass balance models are being developed to quantify atmospheric Mn deposition. Mn input from weathering advance and atmospheric deposition are balanced by chemical and physical weathering out of the system. Atmospheric deposition is evaluated as a function of estimated soil formation and weathering rates. Preliminary calculations suggest a longterm geologic signal best explains the observed magnitude of Mn enrichment. This evaluation will be pursued by examining geographically diverse soil profiles for Mn enrichment. Mn enrichment has also been observed in soils developed on Peoria Loess in the Mississippi River Valley.

CZO Site Instrumentation Infrastructure

Details of individual working group instrumentation can be found in their respective sections. 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 person. Colin Duffy is working on the development of the Adaptive Sensor Array.

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. The 3-tier communication system is shown in Figure 2 below.



Figure 2 Three Tier communication network implemented at Shale Hills: a) microscale communication uses the 802.15.4 ZIGBEE 2.4 ghz radios (Adaptive Sensor Array described below), b) mesoscale range uses Motorola 5.7 ghz network, and c) the world-wide-web is the regional scale.

Adaptive Sensor Array (ASA)

A small prototype adaptive sensor array is currently being tested at Shale Hills for future deployment. The ASA, when fully funded and operational, will provide a new two-way communication capability, where we will be able to examine and control our sensors (soil moisture, groundwater level, met sensors, etc.) 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. Each node in the ASA will have a heterogeneous mix of sensors for atmospheric, subsurface and vegetation measurements. 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 a preliminary design for the ASA once fully implemented. We are currently exploring NSF and other funding sources to advance the prototype to a fully instrumented array. A few characteristics of the ASA technology are listed below.



Figure 3. Three possible "optimal" sensor network configurations for the Shalehills CZO: a) riparian focus, b) two-scale soil moisture focus, and c) stream channel focus. Optimal grids are generated using Delauney Tesselization with constraints (Kumar and Duffy, 2008).

Wireless Ad-Hoc System Characteristics:

- 1) 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.
- 2) Self-organization: The ad hoc network autonomously determines its own configuration parameters including addressing, routing, power control.
- 3) 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.
- 4) 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 the ASA will have up to 40 nodes with up to 8 sensors at each node.

GPS and Laser Site Surveys

GPS site surveys using a laser theodolite have been underway since Fall 2007. The purpose of the survey is to record highly accurate locations of site instrumentation to aid in both model simulations and logistics at the site. The survey is expected to be ongoing as more instrumentation is installed. Joseph Kasprzyk is leading this effort working with Patrick Reed.

Transect site CZO measurements, data management and integration:

An all hands meeting was held for the transect participants on April 27-29, 2008. At the meeting all PIs for the transect sites (see Fig 4) and for the main Penn State site were present to discuss plans for the first year including logistics, instrumentation, and site specific issues. The main result was a field plan for selecting sites for instrumentation and approval of both core activities and instrumentation to be placed at each site along transect.

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





From the meeting it was determined that the first year main focus should be 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.

Geomorphology

Activities for this first year include:

1) Developing a modeling strategy (Fig. 5) for incorporating sediment erosion, transport, and deposition into the Penn State Integrated Hydrologic Model (PIHM). The underlying philosophy, including the mechanics of hillslope and channel sediment transport and their role in the evolution of regolith, were presented at the CUAHSI Biennial Colloquium in July at Boulder, CO.

2) Developing a sampling strategy for isotopic investigation of erosion rates and landscape topography. We are in discussions with Paul Bierman (UVM) as to the details of the sampling, but we expect to begin in Spring 2009. We have also been awaiting the arrival of high-resolution LiDAR digital elevation models of the region (contracted by the State of Pennsylvania). Preliminary data just arrived in the late summer.

3) Recruiting graduate students for the project. A Ph. D. student, Rob Fuller, just matriculated this Fall, 2008 in the Department of Geosciences to work on PIHMSed. A

M.S. student, Poonam Giri, will matriculate in January, 2009 to begin characterization of soil erosion.

PIHMSed: A new strategy for integrated hydrologic and landscape modeling

- 1) Strategy
 - 1) Use GIS tools to decompose study area into a TIN
 - Assemble equations describing hillslope and channel surface processes in each triangular element
 - Use semi-discrete finite volume method to transform any PDEs into ODEs
 - 4) Assemble all ODEs into global system
 - Solve global system by SUNDIALS or PETSc
- 2) Advantages
 - 1) Mass conservation at all elements
 - All major hydrologic and sediment transport processes fully coupled into one ODE system
 - Interactions treated as internal terms on the right hand side of ODE system
 - 4) Flexible model kernel



Siwalik Hills (observed in 30 m DEM and modeled)

Figure. 5 PIHM_SED modeling strategy

Hydrology, Stable Isotope Tracers, and Model Development

Hydrometeorological Instrumentation: In July Kelly Cherrey and team installed a 30 m tower which is used for the meso-scale communication (see Infrastructure section). As of Sept. 2008 an Eddy Covariance system was installed for determining the latent heat flux above the canopy. This will complement 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 started in August 2008 for completing a network of shallow observation wells completed within weathered bedrock, typically at depths ranging from 8 to 15 feet. At this point we have adapted our portable rotary drill rig to drill on hillslopes and have completed several wells. This effort will continue in year 2. All wells will be instrumented for real-time communications (temperature and level). Our 22' drilling trailer is on-site and will remain on-site until late October.

Stable Isotope Instrumentation: In late spring 2008 the Los Gatos Laser Isotope instrument was delivered and set up at PSIEE chemistry laboratory. We have completed testing and paired sample have been sent to a Waterloo Canada lab for comparison. A

groundwater isotope sampling site was installed in late August and Kelly Cherrey has installed the ISCO sampler set to a daily interval. With the help of Beth Boyer we were able to purchase an "event-based" automated isotope and chemistry sampler that will adaptively take precipitation samples during a rainfall event. Figure 6 illustrates this major acquisition. The pad for the auto-sampler has been installed, the instrument has been delivered and will be put in place 22 Sep. 2008. As of Sept. 22 we will have daily



samples of outlet runoff, groundwater, and sampling adaptive precipitation for establishing the isotope record at Shale Hills. This leaves only the soil moisture daily sampler to be completed for our baseline sampling plan. Additional synoptic and event-based experiments are under including design а sapflow isotopic signature studies by Dave Eissenstat.

Figure 6. Automatic Precipitation Sampler Model NSA181 from Birol, Limited, UK.

Computational Hydrology (PIHM): Mukesh Kumar, Gopal Bhatt, and Shuangcai Li are each preparing to defend 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 1000km² 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 (Fall 2008 defense).

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 the mesoscale, 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". We show here several examples where unexpected dynamics emerge and that the predicted phenomenon is hydraulically plausible but will require new experiments to verify. We avoid interpretation of "emergent" or self-organized behavior at this stage since most of what we observe seems to be more simply explained (i.e. principle of "lex parsimoniae"). The simulation was run on an unstructured grid generated with a minimum spatial scale of 0.048 km² for the watershed and 150 m for river while the minimum temporal discretization was set at 10^{-5} min. The spatio-temporal adaptive nature of the solution captures fine- to large scale interactions between processes, topography and landuse/land-cover characteristics. Our focus here is on coupling behavior at event, daily, monthly and seasonal time scales. All of the presented results are for a 2 year simulation period from Nov 1983 to Oct 1985. Figure 8 shows the terrain for the 875 km² Little Juniata watershed (Kumar, Bhatt, and Duffy, 2008). This initial model test area is immediately northwest of Shaver Creek and Shale Hills.





Figure 8. The Little Juniata watershed and initial PIHM testbed is 875 km² and supports a 4th order stream network. The digital elevation model for the watershed is shown here. The watershed is in the transition between the Appalachian Plateau and the Valley and Ridge Physiographic provinces. Although there are many more points in the Kumar and Duffy (2008) paper we demonstrate one finding here.

Evapotranspiration dependence on Topography and Groundwater Spatial variations of each annually-averaged evaporative flux components predicted in PIHM are shown in Fig. 9. Fig. 9a-b shows that transpiration and interception loss closely resembles the vegetation distribution pattern. Regions with Mixed Land Cover (M) have the highest interception and transpiration loss while regions with urban landcover (U) have the smallest losses. The majority of the watershed is covered by deciduous broad leaf vegetation (De BL), which has intermediate evaporative flux values. Evaporation from ground and overland flow has a spatial pattern that bears a resemblance to topography. At higher elevations, the evaporative losses from land appear to be lowest while the highest values are found at lower elevation. By plotting the evaporative flux components along an elevation transect (shown as red band in Fig. 9c) in Fig. 9e, we observe that evapotranspiration has an inverse relationship to average ground water depth. Shallow water table conditions in the valleys (regions along the transect with lower elevations) result in higher evaporative losses since the capillary fringe supplies water to the unsaturated soil above the water table. The relationship is accentuated in regions of large elevation gradient. Thus topography and depth to groundwater add to the complex spatial pattern of evaporative losses which are primarily influenced by the spatial distribution of precipitation, heterogeneity of land cover types and geology.



Fig. 9. Spatial pattern of evaporation from Canopy and Transpiration (shown in (a) and (b)) closely reflect the vegetation pattern. (shown in (d)). Spatial pattern of ground evaporation (shown in (c) strongly depend on the depth of ground water and recharge pattern. Figure (e) shows that the variation in ground evaporation along a transect (shown as a rectangular strip in (c)) across the valley follows an inverse relationship to ground water depth (and elevation). Net ground evaporanspiration is larger for shallow groundwater conditions (at lower elevations) and vice-versa. G4= interception loss, G9=transpiration, G7+G8=net ground evaporanspiration.

Physical Ecology

The plant ecology activities during the first year involved training and constructing of sap flow sensors and associated hardware for deployment in Oct, 2008 to estimate transpiration. All canopy trees in the watershed were inventoried by species and trunk diameter. A total of 2058 upper-canopy trees were located in the watershed. About half of these trees were surveyed over the summer and the remainder will be surveyed in the fall. This will allow effective spatially explicit modeling of tree transpiration based on estimates of sap flow and sapwood area. Beginning analyses of tree species spatial distribution in relation to soil moisture were initiated. A master's level (Jane Wubbels, Horticulture) and Ph.D-level student (Jay Osborne, Ecology) were recruited for the project, matriculating Fall, 2008.

Hydropedology

Understanding complex subsurface heterogeneity and their relations to soil moisture spatial-temporal patterns and preferential flow dynamics are fundamental to hillslope and catchment hydrology. Despite significant progress made in the past decades, our ability to predict preferential flow patterns, thresholds, and pathways in the subsurface across space and time remains limited. The research results from this project would make noticeable impacts on the next generation of hydrologic models.

We have initiated the following work in the 1st year of this project:

- We have completed the initial compilation of soil hydrologic monitoring database collected at the Shale Hills since 2003. This database will soon go online for the community to use after further QA/QC and completion of web service interfaces.
- We have conducted three experiments of combined time-lapsed ground penetrating radar (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 more experiments are planned for the 2nd year.
- We have started close examination of soil moisture response to year-round storm events based on the soil moisture data collected in the past four years using automatic sensors. The objectives to: 1) determine temporal soil moisture states at the Shale Hills Catchment and their related controls on soil moisture distribution and response to storm events; 2) determine whether landform units and soil types can adequately describe soil moisture organization at the Shale Hills; and 3) determine whether systematic changes in the organization of soil moisture are indicative of hydrologic connectivity.
- We have systematically compared manual and automated monitoring systems to study soil water movement in the Shale Hills. Characterization of soil water content and potential distribution and their spatial and temporal variability is central to the understanding of catchment hydrology and biogeochemistry. As such, the need for accurate in situ monitoring of soil hydrologic properties has led to the development of both manual and automated technologies. Both methods of data collection have advantages and disadvantages including cost effectiveness,

spatial and temporal resolutions, time and labor consumption, infrastructure availability, and maintenance needs. More in-depth examinations of the collected datasets and their underlying rationale are being conducted. In addition, how to couple spatially-extensive but temporally-limited manual data with spatially-limited but temporally-intensive automatic data are being explored.

• Collaborative efforts have been established between hydropedology group (Danielle Andrews, Jun Zhang, and Henry Lin) and geochemistry team (Sue Brantley and Lixin Jin), isotope hydrology team (Chris Duffy and Henry Lin), and cyber infrastructure team (Pat Reed, Doug Miller, and Brian Bills) on the common interests of biogeochemical processes, water isotope tracking, combined CZEN.ORG, RTH-Net and HP_Net online web-based data service, and wireless communication at the Shale Hills.

Other tasks accomplished during the 1st year of this project include:

- Two Ph.D students (Danielle Andrews and Jun Zhang) and a MS student (Ken Takagi) have been recruited (using other sources of funding) to conduct their research at the Shale Hills. This significantly strengthens the hydropedology team effort at the Shale Hills. In addition, a new postdoc (Chris Graham) has been identified and will join the CZO team starting in January 15, 2009.
- Lin served as the chair for organizing and hosting the 1st International Conference on Hydropedology held July 28-31, 2008 at Penn State. During this conference, a number of Penn State CZO team members presented their research, and a field trip to the Shale Hills CZO was well received. A total of 145 participants from over 20 countries (covering all continents except Antarctica) participated in this focused interdisciplinary conference, with a large number of leading scientists from diverse fields. The feedbacks that we have received for the conference were overwhelmingly positive.

Lin also served as the lead organizer of a major geoscience program for the International Year of Planet Earth (IYPE) held at the Geoscience World Congress 2008 (33rd IGC) in Oslo, Norway, August 6-15, 2008. The symposium (PES-02) was entitled "*The Earth's Critical Zone and Hydropedology*." During this symposium, the Shale Hills CZO was showcased through Lin's presentation entitled "*Hydropedologic Investigations in the Shale Hills Critical Zone Observatory*", and by Chris Duffy's presentation on the "*Shale Hills/Susquehanna CZO*".

HYDROGEOPHYSICS

Activities Completed

This year, we have drilled four groundwater boreholes, each 16.8 m deep (see Figure 10, Figure 11a). The wells are cased into rock (casing to approximately 2.4 m depth), and open below. The water table has been around 1 m below land surface since the wells have been drilled. The distance between these wells range from approximately 5 to 9 m apart. We have completed a suite of borehole logging in these wells (Figure 2b), including (1) 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

meaures the total dissolved solids in the water column (4) fluid temperature; and (5) optical televiewer, which provides a continuous, oriented, true-color 360° image of the borehole wall. We also attempted to collect heat pulse flowmeter data, which indicate the rate and direction of vertical flow within a borehole, but found that the hydraulic conductivity of the shale was too low to detect flow with this instrument, and the drawdown in the wells was too high to determine the hydraulic conductivity in the more fractured shallow zone. We conducted slug tests to estimate the effective transmissivity of the wells, but have not processed these data completely to do. Overall, these data provide some of the first information and a detailed mapping of the hydrogeology of the subsurface within Shale Hills.



Figure 10. Location of new groundwater wells.

From the drilling and data collected within these 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 (Figure 12) 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. The optical televiewer data have not yet been processed, but when analyzed in conjunction with the drill cuttings should give a clear indication about the geology in situ.



Figure 11a. Terryl Daniels (ungrad, Geosci.) drills wells with the Portadrill Mini air rotary.

Figure 11b. One of many logging tools: the optical televiewer.



Shale Hills Critical Zone Observatory Work Plan, updated August 31, 2008

Topic: Real-Time CZO measurements, data management and integration

Investigator: Chris Duffy, Patrick Reed, Kevin Dressler

Students & research staff: Kelly Cherrey, Colin Duffy

Scope:

Schedule, including field work.

Field infrastructure & support.

Field installations are distributed among the following groups: Geomorphology, Geochemistry, Hydrology, Plant Ecology, Hydropedology, and Hydrogeophysics. Details of their individual group work plans can be found in their respective sections Power and wireless communication will be maintained and operated by the field technician. Testing and application of the adaptive sensor array will be coordinated by Duffy, Reed and Dressler to ensure reliability and integrative qualities to serve the entire project.

Data management. CZO data are archived at CZEN.org and real-time data is stored in a digital library at the Center for Environmental Informatics (CEI). The latter is part of the CUAHSI/WATERS effort by Pat Reed and Michael Piasecki.

Manuscripts in progress & planned. TBD

Topic: Transect measurements, data management and integration

<u>Investigator</u>: Tim White, Kevin Dressler Students & research staff: TBD

Scope:

<u>Schedule, including field work</u>: Plans are being made to offer a fall field trip to the greater Shale Hills CZO group to visit Allenport, Reedsville, Greenwood Furnace SP and a post-glacial solifluction (griz litte) site in Rothrock State Forest. <u>Manuscripts in progress & planned</u>: TBD

Topic: Geomorphology

Investigator: Students & research staff: Scope: Schedule, including field work: Continue PIHM_sed development. Manuscripts in progress & planned: TBD

Topic: Geochemistry

<u>Investigator</u>: Susan Brantley Students & research staff:

Scope:

<u>Schedule, including field work</u>: So far, almost all our activities are on the south slope, which has different vegetation, soil moisture, soil temperature and flow dynamics from the north slope. Collection of soil samples and installation of soil water and soil gas samplers on the north slope of the catchment have been planned for next year. We will also continue neutron scattering studies. In addition to micro-porosity measurements, we will carry out more experiments to explore the connectivity of these pores, which is important for their accessibility to waters.

Manuscripts in progress & planned: TBD

Topic: Hydrology

<u>Investigator</u>: Chris Duffy, Ken Davis, Kevin Dressler, Pat Reed <u>Students & research staff</u>: Colin Duffy, Kelly Cherrey, TBD <u>Scope</u>:

<u>Schedule, including field work</u>: We will install the disdrometer at the weather station. Approximately 12 bedrock observation wells will be installed in 2009 with a depth of 3-7m. A 25 node adaptive sensor array should be completed in 2009 if sufficient funds are found to complete effort. There are 3 sensor packages to be deployed on the sensor array: weather station node (wind set, solar irradiance, atmospheric pressure, relative humidity, temperature); Vegetation (For details see Finding s section. Manuscripts in progress & planned: TBD

Topic: Plant Ecology

Investigator: David Eissenstat Students & research staff: Jane Wubbels, Jay Osborne Scope: Schedule, including field work: Install sap-flow sensor arrays and estimate sapwood area as affected by tree species, trunk diameter, slope and aspect. Assess isotopic signature of water in the stem and compare to that in the soil.

Manuscripts in progress & planned: TBD

Topic: Hydropedology

<u>Investigator</u>: Henry Lin <u>Students & research staff</u>: <u>Scope</u>: <u>Schedule, including field work</u>: Continue instrument deployment, ground penetrating radar, and begin modeling work. <u>Manuscripts in progress & planned</u>: TBD

Topic: Hydrogeophysics

Investigator: Kamini Singha Students & research staff:

Scope:

<u>Schedule, including field work</u>: Terryl Daniels, a Geosciences undergraduate, will be mapping the strike and dip of fractures and bedding features seen in the optical televiewer log and correlating these features with locations mapped as having significant flow within the borehole. Terryl will be identifying transmissive fractures or geologic units open to the boreholes and determining whether there is a particular orientation to these features for his senior thesis.

Brad Kuntz, a new Masters student in Geosciences, will be exploring groundwater transport within the watershed, and whether fracture flow and transport is notable within the shale, or whether transport is largely diffusive. To start, Brad will be conducting column experiments using conservative tracers and hand-cored material. In the spring, will we conduct a series of push-pull tracer tests within the newly drilled wells, concentrating on a fractured zone with measureable flow.

In conjunction with Dr. Patrick Reed, we are working on developing an adaptive experimental framework that couples to a simulation/inversion framework to resolve

Outreach Activities: Starting in June of 2009 and running for the following 4 years, I will be developing and running a three-week integrated hydrogeophysics summer course, the field portion of which will be based at the CZO. Undergraduate researchers will combine field experimentation with in-class instruction to develop hypotheses regarding the processes controlling solute transport under different regimes. They will create numerical models using COMSOL Multiphysics to help analyze and interpret their data. This project is in collaboration with three Historically Black Colleges and Universities partnered with Penn State and the Summer Research Opportunity Program, a summer-long internship that engages students from minority groups and institutions in research at majority institutions of the Committee on Institutional Cooperation (the academic arm of the Big 10 Athletic Conference). Our goals are to test whether 1) flow connectivity varies seasonally and with events, and 2) thresholdlike subsurface stormflow is caused, in part, by the interconnection of lateral preferential flow paths and the development and expansion of transient saturated areas around the stream. While numerous data types can be used to help describe expanding saturation, how to integrate these data, given varying support volumes, to quantify processes occurring at multiple temporal and spatial scales, remains a challenging problem. The question of how well we need to resolve moisture connectivity to quantify both moisture dynamics, as well, is not clear. We propose to develop a framework for bridging observation and prediction through evolving experimental arrays, multiobjective optimization, and sensitivity analyses.

Manuscripts in progress & planned: TBD

Site Map for State College and Shaver Creek Experimental Watershed, site of the Penn State Critical Zone Observatory (see "A" on the map).

