

Center for Environmental Kinetics Analysis Proposal

1. *Name of existing center:* Center for Environmental Kinetics Analysis

2. *Director:* Susan Brantley. Please see Appendix A for partial Vitae.

3. *Participants:*

CEKA Faculty

William Burgos, Environmental
Engineering
Susan Brantley, Geosciences
Peter Heaney, Geosciences
James Kubicki, Geosciences
Bruce Logan, Environmental
Engineering
Carmen Enid Martinez, Crop and Soil
Science

Karl Mueller, Chemistry
Kwadwo Osseo-Asare, Materials
Science and Engineering
Ming Tien, Biochemistry and Molecular
Biology
Ryan Mathur, Geology Department,
Juniata College
Ken Merz, Chemistry Department,
University of Florida

CEKA Postdoctoral Scholars and Staff

Chuck Anderson, Outreach and
Visualization Specialist
Joel Bandstra, Kinetics Synthesis,
Postdoctoral Scholar
Lixin Jin, Field Research Specialist
Matthew Karasek, Administrative
Assistant

Lachlan MacLean, Postdoctoral Scholar
Alexander Mitin, Computational
Chemist
Jochen Nuester, Postdoctoral Scholar
Amanda Olsen, Kinetics Synthesis,
Postdoctoral Scholar

CEKA Funded Graduate Students

Biochemistry and Molecular Biology

Dan Ross
Camille Stephen
Yufeng Qian

Chemistry

Michael Davis
Rebecca Sanders
Nancy Washton (Ph.D., 2007)

Environmental Engineering

Melanie Lucas

Env Eng(con't)

Charles McDonough (M.S., 2006)
Fenglong Sun
Daniel Tai
Hui Tan
Charles Winslow
Rachel Wagner

Geosciences

R. Kramer Campen (Ph.D., 2007)
Timothy Fischer

Geosc(con't)

Beth Herndon
Daniel Hummer
Christina Lopano (Ph.D., 2006)
Joel Moore
Alexis Navarre-Sitchler
Kristina Peterson
Brendan Puls
Aaron Regberg

Andrew Wall
Jennifer Williams

Materials Science

Stephen Ajayi

Soil Science

Katya Bazilevskaya

CEKA DOE Personnel

Young-Shin Jun, Lawrence Berkeley
National Laboratory
Qinjun Kang, Los Alamos National
Laboratory
Li Li, Lawrence Berkeley National
Laboratory
Peter Lichtner, Los Alamos National
Laboratory
Tetyana Pereyathko, Pacific Northwest
National Laboratory

Carl Steefel, Lawrence Berkeley
National Laboratory
Glenn Waychunas, Lawrence Berkeley
National Laboratory
Li Yang, Lawrence Berkeley National
Laboratory
John Zachara, Pacific Northwest
National Laboratory

CEKA Advisory Committee

James A. Dyer, DuPont Engineering
Research and Technology
Clare Grey, SUNY Stony Brook
Hubert E. King, Jr., ExxonMobil
Research and Engineering Co.
Philip M. Jardine, Oak Ridge National
Laboratory
Eric E. Roden, University of Wisconsin

4. Rationale and Activities:

CEKA is an initiative to catalyze a deeper understanding of molecular issues related to environmental chemical kinetics with respect to understanding how these kinetics cross scale. We focus on geochemical cycling of elements, fate and transport of contaminants, and carbon sequestration within the critical zone. CEKA researchers have identified important questions that need to be addressed in these areas and have grouped them into a set of 14 “consensus projects” that cross disciplines and scales. Some of the activities run by CEKA are summarized below.

Geowall:

Explaining complex multidimensional datasets is always a challenge, but becomes even more difficult with untrained audiences such as beginning students or nonscientists. The Center for Environmental Kinetic Analysis (CEKA) is employing the GeoWall, an affordable and portable 3D data visualization system using off the shelf components, to meet this challenge in its outreach and educational activities. By using the GeoWall to present true 3D visualizations of molecular dynamics modeling, groundwater flow, contaminant transport, and the chemistry and kinetics of weathering, CEKA personnel can convey concepts that would otherwise be inaccessible to their audience. CEKA outreach and educational efforts employ one GeoWall permanently installed in the Earth and Mineral Sciences Museum at Penn State and a second portable GeoWall that is used for outreach visits and in classrooms. Chuck Anderson leads the effort on the construction and implementation of the GeoWall.

Summer Research Experience for Undergraduates (REU):

We have identified significant questions related to environmental kinetics that could be uniquely addressed using our expertise to guide students in pioneering work. The summer undergrad program offers the opportunity for independent research under the guidance of CEKA faculty. Undergrad participants experience the type of relationship that exists between grad students and their advisors. Students are expected to work 40 hours per week on their research. Both faculty advisors and grad students are available to the students to provide insight and guidance.

Interaction within Penn State’s Environmental Community:

To promote the sharing of information and research, CEKA hosts a monthly “30 Slides” talk by a member of the CEKA community. This community includes not only the funded research and students, but also anyone with an interest in environmental kinetics.

5. Funding Opportunities:

CEKA is funded both by the National Science Foundation Chemistry/EAR and by the Dept of Energy Office of Basic Environmental Research. A small amount of EESI money has been used as match for CEKA. CEKA helped Karl Mueller to get \$2.5 m in funding to create a cyberinfrastructure for environmental chemistry. This development involves Brantley and Kubicki and will probably develop into future funding. CEKA also began working at the Shale Hills watershed: this work was instrumental toward the Penn State Critical Zone Observatory proposal that was recently funded for \$4m (Chris Duffy, EESI Affiliate, was PI). CEKA has therefore been responsible for at least \$6.5m in funding that has come into Penn State and that is benefiting PSU students. We are currently seeking a way to keep CEKA funding into the future.

6. Center Needs

The Center does not request specific funds. Office space for the staff running CEKA is needed; occasionally, we will nominate students for EESI Environmental Scholarships.

7. Management Structure

Director Susan L. Brantley and Assistant Director James D. Kubicki are responsible for all aspects of CEKA management in coordination with a Steering Committee of faculty drawn from three colleges. In addition, Dr. Kubicki manages the CEKA computational facility as a part of the Environmental Computational Facility within the Earth and Environmental Systems Institute. The *Administrative Assistant*, Matthew Karasek assists with all budgetary and paperwork activities, as well as with promoting interaction for CEKA participants at monthly mini-retreats.

The *Kinetics Synthesis Specialists*, **Joel Bandstra and Amanda Olsen**, are in charge of fitting all compiled kinetic data to kinetic rate equations and compiling the rate constants into user-friendly formats for publication. The specialists produce, in concert with the overall group, two kinetics data bases describing rates of mineral-water reactions: one that compiles kinetic measurements, and one that compiles rate models. These databases will be peer-reviewed publications and will be placed on the web.

The *Field Research Coordinator*, **Lixin Jin**, conducts her own individual environmental kinetic research and is also in charge of coordinating, with the administrative assistant, all educational and research activities for graduate and post-doctoral students.

The *Visualization and Outreach Specialist*, **Charles D. Anderson**, coordinates all outreach activities through interaction with the director of Penn State's Space Grant Consortium (Lisa Brown) and the director of the College of Earth and Mineral Science Mineral Museum (Russ Graham).

Two committees within CEKA promote communication and governance: a *Steering Committee* and an *External Advisory Committee*.

The *Steering Committee* consists of the Director (Brantley), Assistant Director (Kubicki), the Kinetic Synthesis Specialist, the Research and Education Coordinator, the Visualization Specialist and the three Interest Group (IG) leaders: Karl Mueller, Dissolution Interest Group (DIG); Peter Heaney, Precipitation Interest Group (PIG); and Ming Tien, Bioreaction Interest Group (BIG). Nominations for CEKA graduate students are presented to the Steering Committee which then selects those students who most fulfill the mission of CEKA and who balance the disciplinary cross section of CEKA from among the nominees. Decisions regarding allocation of funds are made by the Director in consultation with the Steering Committee.

The *External Advisory Committee* typically includes four members: two drawn from academia, one from industry, and one from government. The External Advisory Committee reviews all aspects of CEKA work, including research, education, and outreach.

8. Past Budgets and Work.

NSF CEKA Funding and Budget summaries:

In the 04/05 year, the total NSF CEKA budget was \$448,118.

In the 05/06 year, the total NSF CEKA budget was \$769,973

In the 06/07 year, the total NSF CEKA budget was \$ 1,115,904

In the current year to date (07/08), the total NSF CEKA Budget is \$678,593.

Total NSF funds to date \$3,012,588

PSU Match Funds Spent*:

\$177,158 04/05

\$74,767 05/06

\$65,243 06/07

\$55,294 07/08 to date

\$372,462 Total to date

**This figure includes only costs captured in cost center and does not reflect match support from Geosciences.*

9. Support Letters.

See Attached letters.

Appendix A.

CURRICULUM VITA

Susan L. Brantley

Earth and Environmental Systems Institute, Director

Pennsylvania State University
2217 Earth & Engineering Science
Building
University Park, PA 16802

Phone: 814-865-1619
Fax: 814-865-3191
brantley@eesi.psu.edu

Birthdate: August 11, 1958

Degrees:

- 1980 - B.A., Chemistry, Princeton University, Magna cum Laude

- 1983 - M.A., Geological and Geophysical Sciences, Princeton University
- 1987 - Ph.D., Geological and Geophysical Sciences, Princeton University

Professional Experience

- 8/80-8/81 Fulbright Scholar in Peru
- /81-9/86 Teaching and Research Assistant in Dept. of Geological and Geophysical Sciences, Princeton University
- 9/86-6/91 Assistant Professor of Geosciences, Penn State
- 6/91-7/97 Associate Professor of Geosciences, Penn State
- 1/95-7/95 Visiting Scientist, U.S. Geological Survey Menlo Center
- 1/95-7/95 Visiting Scientist, Stanford University
- 7/97-present Full Professor of Geosciences, Penn State
- 7/98-04/03 Director, Center for Environmental Chemistry and Geochemistry, Penn State
- 8/99-1/03 Director, Biogeochemical Research Initiative for Education, Penn State
- 1/03-7/03 Visiting Scientist, U.S. Geological Survey Menlo Center
- 4/03-present Director of Earth & Environmental Systems Institute, College of Earth and Mineral Sciences, Penn State
- 1/04-1/06 Vice-President, Geochemical Society
- 9/04-present Director, Center for Environmental Kinetics Analysis, Penn State
- 1/06-present President, Geochemical Society
- 2006 Fellow, American Geophysical Union

Honors and Awards

- 1982-1985 NSF Graduate Student Fellowship
- 1981-1982 IBM Fellowship, Princeton University
- 1987-1992 NSF Presidential Young Investigator Award
- 1988-1993 David and Lucile Packard Fellowship
- 1996 Wilson Research Award, College of Earth and Mineral Sciences, Penn State
- 2001 Pardee Lecturer, Geological Society of America National Meeting
- 2002 Ingerson Lecturer of the Geochemical Society, Geol. Society of America National Meeting
- 2003 Wilson Faculty Mentoring Award, College of Earth and Mineral Sciences, Penn State
- 2006 Pardee Lecturer, Geological Society of America National Meeting 2007 Elected AGU Fellow
- 2007 Wilson Award for Outstanding Service, College of Earth and Mineral Sciences, Penn State

Brantley has published more than 100 papers in peer-reviewed journals.

A complete vita is available upon request.



April 28, 2008

James D. Kubicki
Dept. of Geosciences
The Pennsylvania State University
University Park, PA 16802

To whom it may concern:

I am writing in support of the Center for Environmental Kinetics Analysis proposal to the Earth & Environmental Systems Institute. The request is for minimal support in the form of office space for CEKA personnel. CEKA has been successful in bringing together scientists from many disciplines and in training students in an interdisciplinary environment. CEKA has expanded its influence beyond the original set of investigators at PSU and has gathered interest from a number of scientists outside of PSU. New grants have been obtained that have affiliation with CEKA, so EESI support of CEKA is a cost-effective use of institute resources.

Yours truly,

James D. Kubicki

Date: April 24, 2008
To: The EESI Judging Committee
From: Ming Tien
re: center support

To the EESI Judging Committee:

I am writing in support of continuation for the Center for Environmental Kinetics Analysis (CEKA). CEKA is an NSF-funded Environmental Molecular Science Institute that has brought together researchers with diverse scientific disciplines working on environmental sciences. It has provided a great platform for interdisciplinary graduate student and postdoctorate training. CEKA has also facilitated collaborating faculty to garner funding to study environmental kinetics at different scales. CEKA brings together chemists, geochemists, biochemists, soil scientists, materials scientists and engineers with the focus on measuring and synthesizing kinetic data for environmental systems and on modeling the temporal evolution of such systems. As CEKA winds down on its funding, many advances have been made which could possibly lead to future projects and associated funding.

My involvement with CEKA is as a participating scientist, the leader of the Bioreactions Interest Group (BIG) and an active member of the CEKA Steering Committee. As a participating scientist, I have co-advised five CEKA students since 2005 with two other CEKA investigators. CEKA granted many of these students the opportunity to work with faculty outside of their own program. As the leader of BIG, I witness these interactions on a monthly basis during our interest group meeting. Beyond the BIG interest group (there are a total of three interest groups in CEKA), all of CEKA meets once a month also in our "30 slides" meeting. CEKA has also allowed the postdoctorate associates, the faculty and the student to visit DOE laboratories, not only for conferences but also for research. Thus through a number of different mechanisms, CEKA has lowered the walls between different departments and colleges within Penn State thereby facilitating interdisciplinary education and research. It has also expanded the culture of students and postdoctorate associated through a number of collaborations outside of the Penn State community.

I fully support the continuation of CEKA as a center in EESI. Please do not hesitate to contact me if you have any questions.