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Collaborative Research: A Reaction Kinetics Database for Modeling Biogeochemical Systems

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Cover

Federal Agency and Organization Element to Which Report is Submitted:	4900
Federal Grant or Other Identifying Number Assigned by Agency:	1124093
Project Title:	Collaborative Research: A Reaction Kinetics Database for Modeling Biogeochemical Systems
PD/PI Name:	Amanda A Olsen, Principal Investigator
Recipient Organization:	University of Maine
Project/Grant Period:	09/01/2011 - 08/31/2013
Reporting Period:	09/01/2012 - 08/31/2013
Submitting Official (if other than PD\PI):	Amanda A Olsen Principal Investigator
Submission Date:	02/05/2015
Signature of Submitting Official (signature shall be submitted in accordance with agency specific instructions)	Amanda A Olsen

Accomplishments

* What are the major goals of the project?

The goal of this project was to develop an online geochemical kinetics database called EarthKin. In order to establish an online repository for environmental kinetics data we will do the following:

1. continue to compile legacy data, focusing on mineral dissolution kinetics data
2. add microbial Mn reduction data from Bandstra et al. (2011) to the database
3. begin to compile similar Fe reduction rate data
4. develop rate constants based on analysis of existing experimental data
5. develop an appropriate schema for EarthKin so that the data which is currently stored in Microsoft Excel spreadsheets can be integrated into EarthChem where data is stored in XML format
6. develop the EarthKin database as an Access database and populate it with data
7. build tools to allow users to enter new data into EarthKin
8. place the Access database online at CZEN.org as a preliminary step before migrating it to EarthChem in future work

*** What was accomplished under these goals (you must provide information for at least one of the 4 categories below)?**

Major Activities:

Task 1: Before the beginning of this funding period, graduate students at Penn State University had compiled legacy dissolution kinetics data for a small group of minerals under limited temperatures. As part of this project, we compiled legacy data for a much broader group of minerals, including silicate, carbonate, and sulfide minerals. Additionally, we expanded the data available for the existing minerals over a much wider range of temperatures. Mineral dissolution kinetics data are now included in the database for

- aluminum oxides,
- anthophyllite,
- augite,
- biotite,
- bronzite,
- carbonate group minerals,
- chlorite,
- chrysotile,
- diopside,
- enstatite,
- epidote,
- forsterite,
- fayalite,
- iron oxides,
- hornblende,
- illite,
- kaolinite,
- muscovite,
- orthosilicates,
- phlogopite,
- phosphates,
- rhodonite,
- smectite
- talc,
- tephroite,
- tremolite,
- willemite
- wollastonite,
- glasses and basalts

Dissolution kinetics data were compiled over all available temperature and pH ranges.

Specific Objectives:

Significant Results:

Key outcomes or

Other achievements:

*** What opportunities for training and professional development has the project provided?**

Four students were trained under this grant. Kimberly Negrich (M.S. 2013) and Agnes Taylor (M.S 2014) both worked on Tasks 1, 5, and 6. Taylor attended Goldschmidt in 2012 to meet with scientists interested in data management at an EarthChem meeting. She has also traveled to Penn State to interface with the other PIs. Undergraduate student Jason Lively (B.S. 2015) and high school intern Brittney Nickerson worked on Tasks 1 and 6.

*** How have the results been disseminated to communities of interest?**

We are still working to publish the database at czen.org. We expect it to be available to the community by April 2015.

At that point, we will begin to publicize the database via email and talks. Additionally, Olsen and PI Niu plan to publish a paper in the Journal of Environmental Informatics.

Products**Books****Book Chapters****Conference Papers and Presentations**

K. Negrich, J.L. Baumeister, E.M. Yardley, J.D. MacRae, E.M. Hausrath, and A.A. Olsen (2012). *BIOGEOCHEMICAL WEATHERING OF SERPENTINITE IN FIELD AND LABORATORY STUDIES*. Goldschmidt 2012. Montreal, QC.

Status = PUBLISHED; Acknowledgement of Federal Support = Yes

Amanda Albright Olsen (2012). *EarthKin*. EarthChem Workshop at Goldschmidt 2012. Montreal, QC. Status =

OTHER; Acknowledgement of Federal Support = Yes

AMANDA ALBRIGHT OLSEN, ELISABETH HAUSRATH, EILEEN YARDLEY, MICHAEL BODKIN, JULIE BAUMEISTER, AND KIMBERLY NEGRICH (2012). *Using laboratory-derived mineral dissolution rates to test chemical weathering in the field: A field, lab, and modeling perspective incorporating biology*. Goldschmidt 2012. Montreal, QC. Status = PUBLISHED; Acknowledgement of Federal Support = Yes

Inventions**Journals****Licenses****Other Products****Other Publications****Patents****Technologies or Techniques****Thesis/Dissertations****Websites****Supporting Files****Filename****Description****Uploaded****Uploaded**

		By	On
AOlsen 2012 Goldschmidt abstract 1-30-12.pdf	Abstract for invited talk at Goldschmidt 2012 that utilized EarthKin data	Amanda Olsen	02/04/2015
Goldschmidt2012Abstract_Negrich.pdf	Abstract for poster at Goldschmidt 2012 that utilized EarthKin data	Amanda Olsen	02/04/2015
earthkin Goldschmidt 2012 gs.pdf	PDF of presentation delivered by Olsen at EarthChem workshop at Goldschmidt 2012. Presentation was given to about 50 scientists interested in data management.	Amanda Olsen	02/04/2015

Participants/Organizations

What individuals have worked on the project?

Name	Most Senior Project Role	Nearest Person Month Worked
Olsen, Amanda	PD/PI	2
Taylor, Agnes	Graduate Student (research assistant)	12
Lively, Jason	Undergraduate Student	2
Nickerson, Brittney	High School Student	1

Full details of individuals who have worked on the project:

Amanda A Olsen

Email: amanda.a.olsen@maine.edu

Most Senior Project Role: PD/PI

Nearest Person Month Worked: 2

Contribution to the Project: Olsen oversaw all students working on data acquisition and analysis. Olsen worked with colleagues from PSU to design the database and is currently working with PSU to disseminate the database via czen.org.

Funding Support: NSF provided one month of summer salary for Olsen.

International Collaboration: No

International Travel: Yes, Canada - 0 years, 0 months, 5 days

Agnes Taylor

Email: agnes.taylor@maine.edu

Most Senior Project Role: Graduate Student (research assistant)

Nearest Person Month Worked: 12

Contribution to the Project: Taylor's job was to complete Tasks 1, 5, and 6 for this project. She also oversaw the work of undergraduate and high school students.

Funding Support: NSF

International Collaboration: No

International Travel: No

Jason Lively

Email: jason.lively@maine.edu

Most Senior Project Role: Undergraduate Student

Nearest Person Month Worked: 2

Contribution to the Project: Lively worked under the supervision of Taylor to populate the database with mineral dissolution kinetics data and proof data that had been previously input.

Funding Support: UMaine internal support

International Collaboration: No

International Travel: No

Brittney Nickerson

Email: brittney.nickerson@maine.edu

Most Senior Project Role: High School Student

Nearest Person Month Worked: 1

Contribution to the Project: Nickerson worked under the supervision of Taylor to populate the database with mineral dissolution kinetics data and proof data that had been previously input.

Funding Support: Maine Space Grant Consortium

International Collaboration: No

International Travel: No

What other organizations have been involved as partners?

Nothing to report.

What other collaborators or contacts have been involved?

NO

Impacts

What is the impact on the development of the principal discipline(s) of the project?

We produced an environmental kinetics database (EarthKin) that will be widely available to the scientific community in the very near future. Because the database runs in Microsoft Access, it is usable by anyone with access to Microsoft Office.

What is the impact on other disciplines?

Although we expect the primary users of this database to be members of the earth science community, we expect this database to have wide applicability to users interested in

- soil science
- CO2 sequestration
- climate modeling
- chemical engineering
- biogeochemistry
- reactive transport modeling
- microbiology.

Because many of the users of environmental kinetics data have little background in geochemical kinetics, we have tried to compile the data in such a way that is easy to understand for the average user. We also make the original source of the data clear o users. We hope that this leads to an increase in citations for the papers from which the data were compiled.

What is the impact on the development of human resources?

This project trained two female graduate students, one undergraduate student, and one female high school student. Both graduate students have successfully defended M.S. theses. One has gone on to a job in industry; the other just recently graduated and is on the job market. The undergraduate student who worked on the project, Jay Lively, was recently accepted into an MS program at Western Kentucky University. The high school student has recently started an undergraduate program at the University of Maine.

This grant also contributed to the career of an early career female faculty member.

What is the impact on physical resources that form infrastructure?

Nothing to report.

What is the impact on institutional resources that form infrastructure?

Nothing to report.

What is the impact on information resources that form infrastructure?

The goal of this project was to build an environmental kinetics database. Because of logistical issues, the database is not yet available online. However, we expect the database will be available on czen.org by April 2015.

What is the impact on technology transfer?

Nothing to report.

What is the impact on society beyond science and technology?

Environmental kinetics data are used in diverse fields that have important impacts on society. Perhaps the most obvious is the field of carbon dioxide sequestration. In order to predict the chemical reactions that will occur when CO₂ is injected into the ground, it is crucial to understand the kinetics of the reactions. Relevant dissolution kinetics data are available through EarthKin.

Changes/Problems

Changes in approach and reason for change

Nothing to report.

Actual or Anticipated problems or delays and actions or plans to resolve them

Although the construction of the database is complete, we have had some delays with deploying the database at czen.org. These delays were primarily due to the graduation fo the graduate students funded on the project which left the project unstaffed. PI Olsen is working with PI Niu from PSU, and we expect that the database will be available to

the public by April 2015.

Changes that have a significant impact on expenditures

Nothing to report.

Significant changes in use or care of human subjects

Nothing to report.

Significant changes in use or care of vertebrate animals

Nothing to report.

Significant changes in use or care of biohazards

Nothing to report.

Special Requirements**Responses to any special reporting requirements specified in the award terms and conditions, as well as any award specific reporting requirements.**

Nothing to report.