

**NSF workshop: Expanding the role of Reactive Transport Modeling (RTM)
within the Biogeochemical Sciences**

April 13 – 15, 2014
Embassy Suites Alexandria Hotel, 1900 Diagonal Road, Alexandria, VA 22314
800-228-9290 or 703-684-5900

APRIL 13

- 5:30 – 7 pm: Optional dinner for early arrivals (meet in hotel lobby)
7 – 9 pm: Registration/Icebreaker: Orientation and brief introductory presentation
(Virginia Hall, Hors d'Oeuvres, Cash bar)

APRIL 14

- 7:30 – 8:30 Complementary breakfast outside the lobby area
8:35 – 8:45 Welcome and introduction: Enriqueta Barrera (Salons A/B)
8:45 – 9:00 Outline of workshop, participants introduction, survey results
(Salons A/B)

Session 1: Frontiers in reactive transport modeling (Salons A/B)

- 9:00 – 9:30 Presentation 1: Carl Steefel
9:30 – 10:00 Presentation 2: Eric Sonnenthal
10:00 – 10:20 Coffee Break
10:20 – 11:40 Pop-up presentations (12 @ 5 minutes each)
(Bolton, Zachara, Moore, Tutolo, Lawrence, Li, Kocar, Sullivan, Jin, Maher,
Dietrich, Perdrial)
11:40 – 12:00 Presentation 3: Uli Mayer
12:00 – 1:30 Lunch and group discussion (Virginia Perfunction)
Presentation of current efforts in RTM education (Maher, Li, Sitchler)
Discussion of educational needs and future directions for RTM

Session 2: Advances in data-model integration (Salons A/B)

- 1:30 – 1:50 Presentation 4: Aaron Thompson
1:50 – 2:20 Presentation 5: Susan Brantley
2:20 – 3:15 Pop-up presentations (7 @ 5 minutes each)
(Druhan, Kumar, Bao, Biesman, Sitchler, Meile, Valocchi)
3:00 – 3:20 Coffee Break

Session 3:

- 3:20 – 5:30 Organization and Breakout group discussion
(Carlyle Room, Marymount Room, Salon A, Salon B)

6:30 – 8:30 Dinner (Salon C)

APRIL 15 (Salons A/B except breakout group writing)

- 7:30 – 8:30 Complementary breakfast outside the lobby area
8:30 – 10:00 Report from breakout groups and discussion
10:00 – 10:20 Coffee Break
10:20 – 11:00 Group discussion

- 11:00 – 12:30 Breakout group writing
(Carlyle Room, Marymount Room, Salon A, Salon B)
- 12:30 – 1:30 Lunch and group discussion
Identify main themes and strategies for advancing themes
Discussion of next steps from workshop
- 1:45 – 2:45 Continued writing, follow-up assignments, etc.
- 2:45 – 3:00 Closing remarks

Proposed driving questions for presentations and breakout discussions:

Breakout discussion items: Technical developments and frontiers in reactive transport modeling

1 - What are key outstanding hypotheses that could be addressed with current capabilities?

2 - What are additional modeling capabilities that would expand the scope of scientific hypotheses that can be addressed?

Breakout discussion items: Reactive transport education and support resources

1 - What educational resources are currently available to those who wish to incorporate RTM in their research?

2 - What educational tools are critically needed but are not available, and how should these be developed?

For example:

A - How can we get transport into geochemistry classes to build a strong foundation for RTM for future researchers?

B – What resources and backgrounds do students need to be successful in learning how to apply RTM to (bio)geochemical research?

C - What is the current model of RTM short courses, and are they generating the knowledge and experience necessary to facilitate adoption of RTM approaches? Are there more effective methods for short course learning that promote understanding and long-term engagement?

D - Would diversification of RTM short course topics (additional offerings, more advanced courses) enhance application of RTM by short course students?