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A Brief History of Reactive Transport —Sue Brantley Enters Stage Left

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In my first presentation A Brief History of Reactive Transport, I explored the early days where geochemists and former physicists developed the first models for multi-component geochemistry-aware transport. It became clear, however, that to arrive at any kind of recognized role for reactive transport in the geosciences, the community needed to demonstrate the usefulness and generality of the approach. This effort “got legs” in part through its ability to assimilate comprehensive thermodynamic databases, in most cases originating in the code SUPCRT from Helgeson and co-workers and packaged in the LLNL database. Another push came from the surge in interest in geochemical kinetics, the importance of which was highlighted when transport processes were involved. Some of this work was presented relatively early, including the first kinetic reactive transport treatment of chemical weathering in Steefel and Van Cappellen (1990). The following years saw mostly incremental and creeping progress in gaining the acceptance of reactive transport modeling as a discipline and approach, but the situation started to turn around in the early 2000s through the (divine?) intercession of Dr. Susan Brantley. Arguably the real breakthrough came with Sue Brantley’s successful organization of a joint NSF-DOE Biological and Environmental Research project CEKA, that included such luminaries as John Zachara and Peter Lichtner, and which allowed modelers to come together with experimentalists and field geoscientists on both environmental issues and chemical weathering. A noteworthy study here led by Alexis Navarre-Sitchler et al (2009; 2011) presented a new threshold diffusion model that captured the coherence of diffusion-controlled reaction fronts, the location of which was determined by reaction-induced porosity change. The new model was able to reproduce the progress of the reaction front over 350,000 years. A second study involved the kinetic modeling of perhaps the world’s first (and lowest cost) pore scale reactive transport experiment in the geosciences (Li, Steefel, Yang, 2009), reproducing experimental results without any adjustment of laboratory-determined rate coefficients. From here, the pace at which reactive transport was accepted in the geosciences accelerated, a result that is traceable to Sue Brantley’s vision for the integration of experimentation and modeling in the critical zone.