Development of Solute Transport Data Sets for Benchmarking Pore-Scale Numerical Simulators

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Introduction. Developing predictive models of multiphase flow and reactive transport at the pore scale is a challenge common to diverse science areas. Increasingly, it has become more important in subsurface research due to its relevance to contaminant and colloidal transport, non-aqueous phase liquid dissolution, and deep sequestration of CO2. Currently, several independent research groups are developing numerical simulations of multiphase flow and reactive transport at the pore scale without experimental data sets to test, verify, and validate the models. To our knowledge, only Willingham et al. (2008; 2010) have reported efforts to simulate a limited set of micromodel solute transport experiments. Despite the numerous numerical pore-scale studies evaluating solute mixing available in the literature, there has only been limited testing against experimental data, primarily due to measurement limitations (Werth et al., 2010). These numerical models use a variety of computational approaches, and each has strengths in areas such as accuracy, computational speed, or scalability. Because of different numerical approaches, there is a strong benefit in benchmarking these models against common experimental data sets. Such a benchmark challenge would highlight relative strengths of each approach and serve to accelerate progress in the field.

At the Pore-scale Modeling Challenge/Workshop held at the EMSL on August 9 and 10, 2011, attendants indicated that a benchmarking effort should include definition of “learning sets” of mutually beneficial pore-scale experimental studies to calibrate numerical models and “challenge sets” designed to numerically predict results without knowing the experimental results. Micromodels would be fabricated using EMSL’s new microfabrication capability and flow experiments conducted using EMSL’s state-of-the-art microfluidics subsurface flow and transport capabilities. Based on the recommendations of the workshop participants, a total of five micromodel experimental sets have been designed to develop the necessary data to test and verify simulators in their ability to model pore-scale transverse mixing.