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Evaluating the uncertainty of upscaled reaction rates in a structured fluvial aquifer using an ensemble mass transfer particle tracking framework

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Mixing limited reactions are highly influenced by the architecture of the geological deposits they flow through because the structured nature of the material can severely limit the ability of the reactants to mix. The complex patterns created by meandering and braided rivers result in sharp interfaces that interrupt correlation lengths and directions that are below the typical resolution of simulation grids for field scale problems. How to accurately upscale their effects without explicitly resolving these sedimentary contacts is unclear, meaning that predictions of reactive transport behaviors in such systems remain highly uncertain. This work investigates how these small scale (<1m) sedimentary structures affect local and global mass transformation rates for a mixing limited reaction system. A hybrid Lagrangian method, termed mass transfer particle tracking (MTPT), was used to resolve the small-scale mixing processes as realistically as possible at the centimeter-scale representative elementary volume size for these deposits. An ensemble of over 250 highly conditioned realizations of the hydrogeology of a 16m by 4m by 3.5m study site along the Rio Grande in Albuquerque, New Mexico were used along with the MTPT framework to quantify the uncertainty in the reaction rates over time. The ensemble results were then compared to the amount of mass that would be produced if each domain were homogenized instead. Using the average resulted in higher times more mass production than the ensemble and the variance of homogenized simulations exhibited a much larger range of rates. Accounting for this difference could allow more robust representations of reaction rates in models that do not explicitly include the small-scale geological contacts, so several upscaled models for doing based on the geological structure are considered for steady-state and transient reactive transport scenarios. We show that reactant covariance- or colocation-based models are highly accurate as descriptive tools and present evidence that they show strong potential as predictive tools as well.

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References

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