Contribution ID: **609** Type: **Oral Presentation**

The effect of upscaling the reaction rate on predictive modeling in subsurface processes

Monday, 22 May 2023 15:00 (15 minutes)

Reactive transport is a multi-scale and multi-disciplinary process used to study various environmental and subsurface applications including geothermal utilization, carbon dioxide storage, well acidizing, and contaminant remediation. Much research has been conducted to simulate reactive transport using the Eulerian approach, Lagrangian particle tracking models, and various pore-scale models. To simulate the process on larger scales, continuum models have been used due to their fewer resources demanding nature compared to other approaches.

Eulerian (continuum) models are usually expressed with a PDE describing the transport and the interconnected reaction in the form of the Advection-dispersion-reaction equation (ADRE). In cases with homogeneous reactions, which is the purpose of this study, using the reaction constant derived from the well-mixed batch reaction results in the over-prediction of the product formation in continuum models. The reactants segregation, incomplete mixing, non-Fickian transport, and the fact that ADRE is limited in considering the effect of the local fluctuations and heterogeneity of the transport and the reaction at the pore level, have been introduced as the underlying reasons for the differences.

This discrepancy has been tackled by considering a time-dependent effective rate coefficient, a smaller dispersion coefficient different from the conservative experiment, as well as non-Fickian diffusion in time or space, using an effective constant reaction rate, and considering beta distribution for the mixing ratios within the representative elementary volume (REV). Continuum models usually need more than one calibration parameter to match the experimental results which may lead to inconsistencies if the initial or boundary conditions change which undermines the generality of these models. Instead, using pore-scale models that are capable of replicating realistic variations of velocity and reaction at the pore level is of great importance. In this manner, direct numerical simulations such as Lattice Boltzmann Method (LBM) or Pore Network Modeling (PNM) are viable tools to carry out the pore-scale simulations.

The upscaled reaction rate extracted from the pore-scale simulation by volume averaging, which reflects the effect of structural heterogeneity, and preferential flow pathways, can be utilized as an input to continuum models to amplify the reliability of the Darcy-scale, and field-scale predictions. In such a way, one can include the pore-scale chemical reactions and fluctuations in the large-scale transport in subsurface heterogeneous porous structures.

This study leverages pore network modeling for pore-scale simulations due to its fast and accurate enough computation of reactive transport phenomenon, and much less computationally demanding nature compared to direct methods. The pore-scale model incorporates incomplete mixing at the pore level by the relationship between the effective reaction constant (Keff) and the Peclet number, validated by experimental results. PNM simulations were executed on a network with a size of a REV. Upscaled reaction rates were derived by performing volume averaging on the pore-scale reaction rates and were used in the continuum model to predict the experimental results. Furthermore, the capability of this upscaling method in predicting the reactive process in a 2D heterogeneous porous medium was inspected.

Participation

In-Person

References

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Session Classification: MS18

Track Classification: (MS18) Innovative Methods for Characterization, Monitoring, and In-Situ Remediation of Contaminated Soils and Aquifers