
Contribution ID: **745** Type: **Oral Presentation**

# Effective dispersion coefficients for the upscaling of pore-scale mixing and reaction in heterogeneous porous media

*Friday, 4 June 2021 14:45 (15 minutes)*

We upscale reactive mixing using effective dispersion coefficients to capture the combined effect of pore-scale heterogeneity and molecular diffusion on the evolution of the mixing interface between two initially segregated dissolved species. These effective dispersion coefficients are defined as the average spatial variance of the solute plume that evolves from a pointlike injection (the transport Green function).
We numerically investigate the effective longitudinal dispersion coefficients in two porous media of different structure heterogeneity and through different Péclet number regimes for each medium. We find that, as distance traveled increases (or time spent), the solute experiences the pore-scale velocity field heterogeneity due to advection and transverse diffusion, resulting in an evolution of the dispersion coefficients. They evolve from the value of molecular diffusion at early time, then undergo an advection dominated regime, to finally reach the value of hydrodynamic dispersion at late times. Thus, at times smaller than the diffusion time over a characteristic pore length, the effective dispersion coefficients can be significantly smaller than the hydrodynamic dispersion coefficients. Therefore, mismatches between pore-scale reaction data from experiment or simulations and Darcy scale predictions based on temporally constant hydrodynamic dispersion can be explained through these differences. We use the effective dispersion coefficients to approximate the transport Green function and to quantify the incomplete mixing occurring at the pore-scale. We evaluate the evolution of two initially segregated species via this methodology. The dispersive lamella approach accurately predicts the evolution of the product mass of an instantaneous bimolecular reaction obtained from direct numerical simulations. These results shed some new light on pore-scale mixing, the notion of incomplete mixing, and its prediction and upscaling in terms of an effective mixing model.

## Time Block Preference

Time Block B (14:00-17:00 CET)

## References

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**Session Classification:** MS8

**Track Classification:** (MS8) Mixing, dispersion and reaction processes across scales in heterogeneous and fractured media