Fractional Dispersion, Mixing and Chemical Reactions

D Bolster[1], D.A Benson[2], P de Anna[3], T Le Borgne[3], A Tartakovsky[4] and M Dentz[5]

[1]*University of Notre Dame, Notre Dame, IN, USA*
[2]*Colorado School of Mines, Golden, CO, USA*
[3] *Geosciences Rennes, UMR 6118, CNRS, Universite de Rennes 1, Rennes, France*
[4] *Pacific Northwestern national Lab, WA, USA*
[5] *Institute of Environmental Analysis and Water Studies (IDAEA), CSIC, Barcelona, Spain*

ABSTRACT:

The space fractional advection-dispersion equation (fADE) describes the temporal change of solute concentration due to mass transfer from locations that can be distant from the observation volume. Such long-range mass transfer changes the character of mixing. By using a variety of common mixing metrics we study how mixing behaves in a system where transport is governed by the fADE. In particular, when contrasted to classical Fickian dispersion, we demonstrate that space fractional dispersion causes where and how quickly mixing occurs in the system to change.

Our interest in mixing comes from the fact that it is a fundamental driver of many chemical reactions. To this end we study the influence that transport by the fADE has on chemical reactions. We focus on two types of bimolecular reactions: (i) instantaneous equilibrium precipitation reactions and (ii) kinetic irreversible reactions. We compare and contrast fractional dispersion systems to classical Fickian ones. For reaction type (i) we demonstrate that in systems with fractional dispersion, reaction products would be found in places precluded by Fickian dispersion. For reaction type (ii) we focus on incomplete mixing as a suppressant of reactions and demonstrate that space fractional dispersion typically weakens incomplete mixing effects.