Transport in Porous Media
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Editorial to the Special Issue: Mixing in Porous Media

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Mixing in porous media is a key process for a wide range of natural and engineered systems in geological, biological and synthetic porous media. It is a multi-scale phenomenon with spatial scales ranging from micrometers (pores and capillaries) to kilometers (aquifers and reservoirs), and temporal scales that range from seconds to years. Mixing in porous media is an interdisciplinary subject with a diversity of scientific and engineering applications that include the understanding of karst formation, groundwater and soil remediation, underground hydrogen storage, geological radioactive waste storage, geothermal energy production, mining, oil and gas production, porous reactors and batteries, as well as drug delivery, and nutrient transport in biological tissue and capillaries.

The quantitative understanding and prediction of mixing is complicated due to the presence of spatial heterogeneity inherent to natural and engineered porous media. Heterogeneity leads to transport, mixing and reaction behaviors that cannot be accounted for using the conventional upscaling paradigm based on constant hydrodynamic dispersion coefficients. In the past two decades, advances in the imaging of porous media structure and processes, and increased computational capabilities (Blunt et al. 2013) have facilitated new experimental, numerical and theoretical approaches (Rolle and Le Borgne 2019) to probe the mechanisms and controls of mixing, and cast them into predictive mathematical models. These developments were discussed at the Lorentz Center workshop on *Mixing in Porous Media* that was held in Leiden, The Netherlands, from 3 to 7 February 2020. There, the idea for this Special Issue originated with the aim to give an account of recent developments in the field of *Mixing in Porous Media*. This special issue consists of twenty-two contributions that cover different aspects of mixing in porous and fractured media at the pore and continuum scales, in single fractures and fracture networks.

Two review papers report on concepts and approaches for mixing in porous media (Dentz et al. 2022) and the dynamical system approach to transport in porous media (Metcalfe et al. 2022). Nine articles focus on hydrodynamic flow, mixing and dispersion processes on the pore scale and their upscaling to the continuum scale. The papers by Sole-Mari et al. (2022) and Oliveira et al. (2022) investigate mixing, reaction and dispersion in the pore space of highly resolved three-dimensional synthetic porous media. The direct numerical

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flow and transport simulations of Sole-Mari et al. (2022) highlight the impact of incomplete mixing on bimolecular chemical reactions. Oliveira et al. (2022) use a continuous-time random walk (CTRW) approach to investigate the impact of spatial heterogeneity on particle displacement distributions and effective dissolution rates. Gouze et al. (2021) study solute dispersion in digital images of three-dimensional heterogeneous rocks of different complexity using direct numerical flow and transport simulations. The large-scale dispersion behavior is related to the Eulerian flow distribution through an upscaled CTRW model. Markale et al. (2022) and Perez et al. (2021) focus on solute mixing and reaction in partially saturated porous media. Markale et al. (2022) study the pore-scale mechanisms of adsorption for different saturations and the impact of pore-scale mixing and preferential flow path. Perez et al. (2021) analyze the impact of different saturation degrees on reactive mixing as quantified by a fast bimolecular reaction. Icardi et al. (2022) present a population balance model for pore-scale particle transport that accounts for breakage, aggregation and surface deposition. Kim et al. (2022) use a combined experimental and numerical approach to quantify the impact of pore-scale flow and transport on transport and mixing in turbulent channel flow. They find that pore-scale flow dominates channel scale solute transport, which is upscaled using a spatial Markov model. Abdolahzadeh et al. (2022) provide a numerical study of the impact of the channel geometry on mixing in active micromixers. Kanavas et al. (2021) use a graph-theoretic approach to relate the spatial distribution of pore-scale flow to the heterogeneity characteristics of porous media. They identify structural constraints for the separation of flow into stagnant and preferential flow regions.

Three papers consider transport and reactive mixing in fracture networks and single fractures. Kong et al. (2022) present an experimental study on the role of high permeability inclusions in a 3D-dimensional fractured porous medium for solute transport and mixing. Their study provides insight into the interplay between network scale and pore-scale transport in the matrix. The article by Sherman et al. (2021) investigates transport, mixing and chemical reactions in three-dimensional discrete fracture networks using direct numerical simulations. These authors find that reactions tend to localize in high-velocity fractures and that the spatial distribution of chemical reactions depends on the Damköhler number. Yoon and Kang (2021) focus on reactive mixing in a rough fracture at different Reynolds and Péclet numbers. They find a spatially nonuniform reactivity distribution, which can be modeled by a velocity-dependent reaction probability.

Four articles focus on hydrodynamic mixing and dispersion at the continuum scale. Neupauer et al. (2021) investigate the reversibility of solute dispersion in Darcy-scale push–pull experiments of radial outward and inward flow. The authors find reversibility of the spreading pattern, which indicates incomplete mixing on the length and timescales of the experiment. The paper by Bonazzi et al. (2022) studies solute mixing in three-dimensional multi-Gaussian hydraulic conductivity fields using high-fidelity numerical flow and random walk particle tracking simulations. These authors propose a mixed-distribution approach to model the distribution of concentration point values. Soler-Sagarra et al. (2022) propose a phase-space approach, termed the multi-advective water mixing approach, to separate solute spreading from mixing. This approach is tested for solute dispersion and mixing in Poiseuille flow. Schmidt et al. (2022) present a numerical study on the optimal time step to simulate diffusive mass transfer between interacting Lagrangian particles, which is tested under different Darcy-scale flow conditions.

Four papers are concerned with the characterization and upscaling of diffusive mass transfer, which is a key process for solute mixing. Fernandez Visentini et al. (2021) investigated the electrical signatures of diffusive mixing in a porous medium using a combination of milli-fluidic tracer experiments and numerical simulations. They find that the electrical data correlate well with the concentration variance and scalar dissipation rate indicating the possibility to characterized mixing from geoelectrical monitoring. Hamada and de Anna (2021) report on a new method to directly measure diffusion coefficient of solutes or suspensions in liquids by optically determining the spatial solute concentration profiles. This method does not rely on a priori knowledge of fluid or tracer properties. Zech and de Winter (2022) study the upscaling of diffusion coefficients in porous media, and the variability of diffusion coefficients measured at scales smaller than the representative elementary volume. These authors propose to represent this variability in terms of probability distribution functions that can be parameterized by porosity. The paper by Aquino et al. (2022) analyzes the dilution of reactive plumes under diffusion and nonlinear reactions. The authors quantify the interaction of these processes on the evolution of probability distribution of concentration point values.

While these contributions do not mean to cover the full breadth of mixing processes in porous in media, they provide an illustration of current research questions, directions and challenges, and reflect conceptual and methodological approaches to characterize and quantify mixing in porous media available today.

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Declarations

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