Contribution ID: **23** Type: **Oral Presentation**

Investigating the limits of averaging: a numerical case study employing diffusion-reaction in porous media

Monday, 13 May 2024 13:25 (15 minutes)

Effective descriptions are often utilized to describe mass transfer phenomena in porous media, i.e. in heterogeneous catalysis, filtering or subsurface transport. Besides more than a century of research, the a priori determination of the relevant effective transport parameters has shown to be elusive and is still subject of research. A major challenge is the appropriate mathematical upscaling of the intricate influence of pore-scale phenomena on the Darcy-scale behavior for realistic morphologies. Typically, such upscaling procedures incorporate convenient estimates to determine the significance of the pore scale transport phenomena with respect to the Darcy scale. Often, such estimates are based on the pore space geometry, macroscopic transport properties and external process parameters. A popular example there is the assumption, that the pore side length scale is significantly smaller than the representative dimension of the porous medium.
To gain insight into the applicability of commonly used averaged descriptions with respect to the coarseness of the pore space, direct numerical simulations of diffusion with first order surface reaction in a resolved pore space were employed. There, a 3D resolved model was developed, based on the finite volume approach utilizing a second order implicit immersed boundary method to accommodate the representation of the pore space. The developing transient species profile was monitored and compared with the analytically derived profiles to the complementary averaged problem.
To investigate the limitations of the averaging approach, the numerical model was applied to a variety of model porous media with varying characteristic length scales and particle Thiele moduli. The generated insights concerning the emergence of Darcy scale behavior from pore scale phenomena will be presented and implications discussed.

Acceptance of the Terms & Conditions

Click here to agree

Student Awards

Country

Netherlands

Porous Media & Biology Focused Abstracts

References

Primary author: RIEDER, David (TU Eindhoven)

Co-authors: Dr PETERS, Frank (TU Eindhoven); Prof. KUIPERS, Hans (TU Eindhoven)

Presenter: RIEDER, David (TU Eindhoven)

Session Classification: MS08

Track Classification: (MS08) Mixing, dispersion and reaction processes across scales in heterogeneous and fractured media