MULTI-SCALE COMPUTATIONAL FRAMEWORKS FOR HIERACHICAL POROUS MATERIAL DESIGN

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By virtue of their extensive potential in energy conversion and storage, catalysis, photocatalysis, adsorption, separation and life science applications, significant interest has been devoted to the design and synthesis of hierarchical porous materials. The main factors which determines the performance of hierarchical porous materials for an application include structure (pore size, porosity, tortuosity), materials (scaffold, dopants) and operating conditions. Traditionally, these hierarchical porous materials are synthesised and fabricated through a manual trial and error procedure, which is an expensive and time-consuming approach. However, there have been significant advances in mathematical, computational and engineering tools toward solving and optimising multiscale descriptions of physical phenomena. This motivates a computational-aided framework to tailor the fabrication of hierarchical porous materials to be optimised in performance for their specific application.

In this work, a reactive-transport system in porous media is modelled using computational fluid dynamics. While microscale descriptions are too computationally expensive and macroscale models fail to accurately describe a physical phenomena in specific parts of computational domains, hybrid - or multiscale - algorithms, are used. Using the information provided by the numerical simulation, multiscale model-based design of experiments are developed to optimise the material’s performance on their particular usage. It is proposed that hierarchical multiscale modeling offers a systematic framework for identification of the important scales and parameters where one should focus experimental efforts on.