

Research Project #20

Connecting Microstructural Evolution to the Effective Properties of Materials Using Lattice-Boltzmann Simulations and Machine Learning (IFN-2 & JSC)

Many engineering and energy applications, including fuel cells and batteries, heterogeneous catalysis, subsurface hydrogen extraction, and nuclear waste disposal systems, require a comprehensive understanding of porous microstructural evolution under coupled multiphase flow and chemical reactions [1,2,3]. The evolution of these microstructures critically influences the thermal, flow, and chemical properties of the system, thereby determining the overall system's performance and reliability.

However, establishing quantitative relationships between the evolving topological features of these complex microstructures and their corresponding effective properties remains a significant numerical challenge. Classical correlations, such as the Kozeny-Carman, Archie's, and Quirk-Millington equations, often fail to describe systems undergoing dynamic-topological, multiphase-flow, and chemical transformations, where assumptions of homogeneity, isotropy, and steady-state transport no longer hold. In these evolving microstructures, topological changes arising from processes such as precipitation or dissolution and interaction among different phases lead to nonlinear and time-dependent variations in transport pathways that cannot be captured by classical relationships.

High-fidelity numerical simulations, including using Lattice-Boltzmann methods, have advanced our ability to resolve these processes at the micro scale [2]. Nevertheless, there is currently no efficient Lattice-Boltzmann solver capable of handling coupled multiphase flow and chemical reactions, especially of treating the triple-point problem, i.e., locations, where solid, fluid, and gaseous media meet, in a numerically stable manner. Existing solvers often adopt simplified representation of chemical reactions, which may lead to inaccurate predictions of topological changes [4]. Moreover, while Lattice-Boltzmann simulations can provide valuable insights, relying solely on high-fidelity computations is prohibitive for exploring large parameter spaces.

To overcome these limitations, this project aims to develop an efficient reactive multiphase Lattice-Boltzmann solver at microscale, and a machine-learning based framework to extend correlation between various topologies and effective properties. We also plan to provide an open-source implementation of the framework for the broader scientific community. The approach will be validated using our recent microfluidic experimental data [3].

Tasks of the PhD project are:

- **WP-1:** Development of a parallel, reactive multiphase flow solver that combines a scalable multi-species Lattice-Boltzmann solver (e.g., from the m-AIA framework [preferred] [2,5], Palabos) and a thermodynamics-based chemical solver (e.g., Reaktoro [preferred] [6], PhreeqC).
- **WP-2:** Development of a machine-learning based framework to correlate microstructural topologies with their effective properties, incorporating generative AI approaches.

Once established, this framework will allow the design of porous microstructures to enhance fuel cell and battery performance, control chemical reactions in subsurface systems for optimized hydrogen production and ensure safety in nuclear waste disposal.

We offer:

- An interdisciplinary research team, consisting of computational science and engineering, geoscience, and geochemistry experts, embedded into an international environment
- Excellent scientific instrumentation, including exascale high-performance computing infrastructure and a cutting-edge radioactive-enabled microscopy laboratory
- Opportunities to attend national and international conferences, and to interact with international collaborators

- Payment and social benefits based on the labor agreement for the public sector employment (TVöD)

Location of the HiTEC Fellow	Forschungszentrum Jülich, Institute of Fusion Energy and Nuclear Waste Management - Nuclear Waste Management (INF-2), Director: Prof. Dr. Dirk Bosbach, Reactive Transport group, Head: Dr. Jenna Poonoosamy https://www.fz-juelich.de/en/ifn/ifn-2
Partners of the HiTEC Project	Forschungszentrum Jülich, Jülich Supercomputing Centre (JSC), Directors: Prof. Dr. Dr. Thomas Lippert and Prof. Dr. Kristel Michielsen, Simulation and Data Lab "Fluids & Solids Engineering", Head: Dr. Andreas Lintermann https://www.fz-juelich.de/en/jsc
Specific requirements	MSc in computational science and engineering, computational geoscience, physics, mathematics, or related discipline with a focus on computational flow in porous media with chemical reactions
For project specific questions please contact	Dr. Ryan Santoso, IFN-2, r.santoso@fz-juelich.de Dr. Jenna Poonoosamy, IFN-2, j.poonoosamy@fz-juelich.de Dr. Andreas Lintermann, JSC, a.lintermann@fz-juelich.de

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- [6] Leal, A. M. (2015). Reaktoro: An open-source unified framework for modeling chemically reactive systems. URL: <https://reaktoro.org>.