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Homogenized Lattice Boltzmann Model for Simulating Multi-Phase Flows in Heterogeneous Porous Media

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Abstract: Lithium-ion (Li-ion) batteries play a major role in the electrification of many business sectors as well as public and private transportation. Although being a mature battery technology, the manufacturing of Li-ion batteries has still room for optimization. A relevant example is the process step of electrolyte filling that comes with unwanted pore-scale effects such as gas entrapment. However, the underlying physics can be hardly studied using experiments, leading to the necessity of enhancing mesoscopic modeling and simulation methods.
In this context, the lattice Boltzmann method has recently gained importance for studying flow in complex porous media. It comes however at the cost of large computational expenses, especially when simultaneously simulating flow in structurally resolved pores at different length scales. Therefore, homogenization methods have been developed to circumvent the explicit modelling of pores at the smallest length scale, but describe the flow by a Darcy-Brinkman-type approach instead where only the mean permeability of the medium is considered.
In this work, we present such a homogenized lattice Boltzmann method (HLBM) that combines a grayscale approach with the multi-component Shan-Chen model. It enables simulations of multi-phase flow in heterogenous porous media by physically modelling fluid-fluid and fluid-solid interactions even at sub-resolution scales. The HLBM presented here shows special advantages: the interfacial tension and wetting conditions are not affected by the homogenization and physical properties are continuous across interfaces between different porous media.
The model was validated using different test cases for single- and two-phase fluid flow. The results are in excellent agreement with the corresponding analytical solutions where available. In addition, the HLBM was applied to electrolyte filling of Li-ion batteries. On the one hand, it was used to study the influence of the nanoporous and partially permeable carbon-binder domain on the electrolyte flow. On the other hand, it was used to study flow in a fully homogenized separator microstructure with local heterogeneities.
All in all, it is shown that the HLBM can be applied to study multi-phase flow in porous media from which the pore sizes differ by orders of magnitude, without fully resolving the microstructure. This speeds up simulation times significantly. Thus, the HLBM is an efficient approach that can be applied to energy storage materials, but is not limited to it.

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Keywords: Lattice Boltzmann method, porous media, Li-ion batteries, electrolyte filling

Participation

In-Person

References

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