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Lattice Boltzmann modeling of the interfacial mass transport and heterogeneous chemical reaction in the multiphase system: numerical models and applications

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Multiphase reactive transport in porous media is widely encountered in natural and engineering processes. Pore-scale modeling is an effective means to understand the mechanism of the multiphase reactive transport, but the related models still need development. In the present work, we proposed a multiphase mass transport numerical model based on the lattice Boltzmann (LB) method, referred to as the CST-LB model. This model involved continuum species transport (CST) term into the mass transport LB model to simulate interfacial species transport within the multiphase system, which is compatible with different multiphase LB models. We combined the CST-LB model with the multicomponent multiphase pseudopotential model to simulate multiphase mass transport with a large solvent's density ratio and different solute's Henry coefficient. The boundary schemes were also proposed to simulate heterogeneous chemical reactions in the multiphase system. For the CST-LB model, a lattice-interface-tracking scheme of the heterogeneous chemical reaction boundary was provided. Meanwhile, the local-average virtual density boundary scheme for the multicomponent pseudopotential model was formulated to avoid the unphysical mass transport layer caused by traditional wetting boundary treatments. The solid structure evolution during the multiphase reactive flow was also concerned and the numerical implementation of multiphase flow, interfacial mass transport, and heterogeneous chemical reaction was coupled. A series of benchmark cases have been carried on to validate the accuracy of the present models, which showed excellent numerical performance. Finally, we applied the proposed models to simulate complicated processes of methane hydrate dissociation in the sediment and discussed the role of mass transport on the dissociation behavior. Different dissociation patterns were identified under various water saturation and fluid velocities. The limitation effect of mass transport on the dissociation rate was quantified and upscaling parameters such as permeability curves were obtained. The proposed numerical models provided the solution to investigate multiphase reactive transport in porous media, which can also be applied for numerous engineering scenarios.

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References

Time Block Preference

Time Block A (09:00-12:00 CET)

Participation

Online

Primary author: Mr YANG, Junyu (Tsinghua University)

Co-authors: Dr XU, Qianghui (Tsinghua University); Mr LIU, Zhiying (Tsinghua University); Prof. SHI, Lin (Tsinghua University)

Presenter: Mr YANG, Junyu (Tsinghua University)

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