Goldschmidt 2026 Abstract
https://doi.org/10.46427/gold2026.34504

A novel coupled LBM-IBM-CAM model for simulating pore-scale biofilm growth in porous media

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Biogeochemical reactions have attracted widespread attention due to significant implications for the evolution of ecological environments in recent years. Biofilms served as the primary sites for biogeochemistry reaction and altered pore-scale uniformity and the intrinsic pore structure of porous media in the meanwhile. Traditional continuum models often overlooked pore blockage and spatial heterogeneity of the biodegradation rates, and most pore-scale models assumed initial biomass is uniformly distributed on the surface of the porous medium particles. These simplifications and limitations led to much uncertainty and challenging in simulating biofilms in porous media and their complex geochemical interactions with environment. To address this, a framework based on the hybrid Lattice Boltzmann Method (LBM), Individual-Based Method (IBM) and Cellular Automata Method (CAM) for pore-scale numerical simulations was developed; microorganisms were treated as motile and dividing individuals through IBM to obtain the initial biomass distribution, CAM was used to represent biofilm growth and detachment; and LBM was also used to model the flow field and geochemical field of the involved species. In addition, the pore-scale model simulated the collapse and filling of biofilms, which corresponded respectively to the structural integrity collapse of biofilms after the loss of support and the dense packing characteristic of biofilms under natural conditions in subsurface environment. Two-dimensional porous media geometry was randomly generated, and pore-scale simulations were performed using the geometry as computational domains in this work. The simulation results demonstrated that the growth dynamics of microorganisms within the simulation domain align with the classical Logistic growth curve and bio-clogging formed in the inlet region of the porous medium caused a reduction in the permeability of the media by two orders of magnitude about 92.8%, which was consistent with previously reported experimental research on biofilm clogging. This work is expected to provide a detailed characterization of biofilm growth in porous media, the interactions between biofilms and water flow, and geochemical reactions occurring within the biofilm.

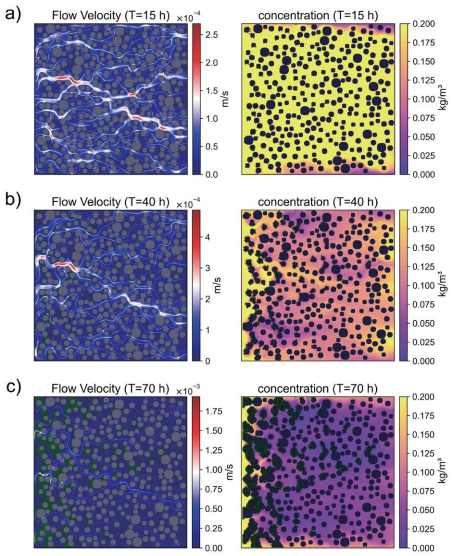

Figure 1. Biofilm distribution, flow field and substrate concentration at different times under hydraulic condition of $u = 0.04$ mm/s and $c = 0.2$ kg/m^3.

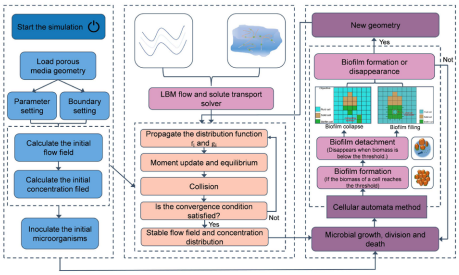

Figure 2. Schematic overview of the modeling framework based on LBM-IBM-CAM.