

## A flux boundary scheme in the lattice Boltzmann method and its applications in the simulation of membrane desalination

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## ABSTRACT

In membrane desalination processes, such as brackish water and seawater desalination, the concentration polarization (ĈP) and surface fouling are remarkable features affecting the performance of these filtration technologies. In this paper, a flux boundary scheme in the lattice Boltzmann method is proposed to predict the CP and inorganic fouling growth on the membrane surface. The proposed flux boundary scheme can be used to prescribe mass flux directly on the boundary, without the normal derivative calculation nor the boundary neighboring nodes interpolation. The flux boundary scheme is numerically validated with a number of cases including different flux boundary conditions. Successful applications of the proposed flux boundary scheme to large Peclet number convection-diffusion desalination processes reveal the CP and fouling phenomena. Results of the CP and permeate flux prediction are compared with a finite element method (FEM) benchmark in a complete rejection condition. Simulation results show that the CP is reduced with a rejection rate considered, that is, without the complete rejection assumption. A higher membrane rejection rate results in better product water quality, but this is accompanied by a higher CP and lower permeate flux. This conclusion indicates a trade-off between membrane selectivity (salt rejection) and membrane permeability (permeate flux). When applied to the simulation of inorganic fouling growth in membrane desalination, the present flux boundary scheme provides results that agree well with reported results in terms of the crystal size, mass accumulation and concentration distribution. The proposed flux boundary scheme has a first-order accuracy for both straight boundaries and curved boundaries.

*Keywords:* Flux boundary scheme; Mass transport; Membrane filtration; Lattice Boltzmann method; Concentration polarization; Inorganic fouling

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