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Lattice Boltzmann Method and Iodide Oxidation in a Porous Anode

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ABSTRACT

Electrochemistry, a field revolving around charge transport, is omnipresent in our every-day life. It is found in batteries, water treatment, medicine, and food processing, to name a few. Porous electrodes are becoming increasingly prevalent in electrochemical systems due to enhanced reaction kinetics and mass transport. The arising complexity of the electrochemical processes at the pore-scale, involving multicomponent reactive flow, poses numerous challenges to the macro-continuum mathematical models. This work is aimed at the development of pore-scale numerical model using the Lattice Boltzmann Method and focuses on anodic iodide oxidation under the aqueous condition. The relationship between concentration, flow rate and potential are investigated in a flow-through porous electrode. Based on the dilute solution theory, with the assumption of excess supporting electrolyte and electroneutrality, the current is described by Ohm's law while migration is assumed to be negligible. Butler-Volmer kinetics are employed at the solid-liquid interface. The consumption of iodide and production of iodine are described via a reaction source/ sink added to the concentration probability distribution function, respectively. The model is initially tested in one dimension and is shown to agree with the finite element results. It is then extended to two-dimensional porous geometry which is randomly generated following Gaussian distribution and separated into active and inactive nodes for interfacial reactions. It was observed that under lower flow regimes reactant concentration was lower corresponding to higher product concentration. Iodine concentration decreased by almost 75 % with increased in Reynolds number (Re) from 0.1 to 5 when porosity was 0.9. Decreasing porosity to 0.7 with Re=1, resulted in 25% iodine production increase.

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