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## A three-dimensional numerical simulation of vanadium redox flow battery

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In this work, we have successfully developed realistic three-dimensional numerical model for the vanadium redox flow battery which includes the electrochemical reactions, fluid dynamics and heat generation. We analyze theoretically the effects of the electrochemical loss in full-scale vanadium redox flow battery during discharge. For a 3-D geometry of the cell, the distribution of pressure, electrolyte flow rate, vanadium concentration, battery voltage, activation loss, concentration loss, Ohmic loss, and heat generation are calculated. The three-dimensional model well captures the trend of experimental data for battery voltage. The effect of voltage loss (activation loss, concentration loss and Ohmic loss) affecting the battery voltage has been numerically investigated with longitudinal and trough-plane direction. The simulated redox flow battery is composed of electrolyte flow passage, membrane (25 $cm^2$ of active area), vanadium solutions, and positive and negative electrodes. The overpotential is higher at the negative electrode than at the positive electrode. And the overpotential decreases from the inlet to the outlet. Due to the transfer coefficient, the change in vanadium ion concentration is higher at the positive electrode than negative electrode. Because of this, the concentration loss is higher at the positive electrode than negative electrode. The presented work has shown the three-dimensional numerical model based on the comprehensive conservation law and chemical species conservation law. The usefulness of the model is to precisely analyze the losses of the vanadium redox flow battery during the discharge process.

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