

**Multi-scale modeling of water and thermal management for
proton exchange membrane fuel cells**

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Abstract Content:

Revealing the multi-physics heat and mass transfer coupled with electrochemical reaction mechanism in the proton exchange membrane fuel cell (PEMFC) is of primary importance for its commercialization development, which is a typical multi-scale problem and can be roughly clarified into component-, cell-, stack-, and system-levels. At component level, we developed a series coupled gas/liquid transport-electrochemical reaction model based on real electrode structure to regulate the water and thermal states inside electrodes, including the gas diffusion layer (GDL) and catalyst layer (CL). Besides, the conventional three-dimensional (3D) cell-level model was extended to commercial-scale fuel cells ($\sim 360 \text{ cm}^2$) for fuel cell vehicle (FCV) applications, which includes full cell structure morphology, and a topology-optimized algorithm was implemented in the design and optimization of coolant channel structure. Moreover, a 3D stack model was developed for the air-cooled fuel cell stack, and the temperature distribution inside the stack and polarization curve were validated against the experimental data simultaneously. And a high-precision and fast-response stack design software was developed by combining a 1D PEMFC model and an artificial neural network (ANN) model predicting the distribution characteristics in the manifold of the stack. A system-level fast simulation software including detailed BOP components was introduced to provide guidance for control algorithms and efficient operation of systems. The modeling and simulation works at these four levels are believed to play a vital role in the R&D of PEMFC.