A Computational Fluid Dynamics Model Development for Solid Oxide Fuel Cells with Direct Internal Reforming based on Electrochemical Effectiveness Concept

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We propose a computational fluid dynamics (CFD) model for solid oxide fuel cells (SOFCs) which can accurately consider both the microscale charge transfer process inside the electrodes and the macroscale heat transfer and fluid flow, by incorporating the numerical framework of the CFD software and the electrochemical effectiveness concept [1]. The electrochemical effectiveness model enables accurate prediction of the current generation in thin active functional layers without performing complicated calculation for the charge transfer process in the electrodes. This new integrated approach is believed to help overcome the limitation of expensive computation cost and low numerical stability involved in the development of CFD models for SOFCs with detailed microscale consideration.

The present CFD model is developed using FLUENT as the calculation platform and applied to two-dimensional simulations of planar, anode-supported SOFCs operated with methane reformate gas. The heat transfer, mass transfer, electronic conduction, chemical reactions and fluid flow are calculated by the validated solution procedure of FLUENT. The electrochemical effectiveness model is responsible for the determination of the current generation rate considering ionic conduction and Butler-Volmer reaction kinetics in thin active functional layers. The effectiveness model is combined with FLUENT using user-defined function (UDF), user-defined scalar (UDS), and user-defined memory (UDM) capabilities. The properties, variables and source terms required for the conservation of mass, species, charge, momentum, and energy are communicated between the macroscale calculation and the effectiveness model via various UDFs, UDSs, and UDMs.

The preliminary study on hydrogen-fueled SOFCs showed excellent agreement between the results of the conventional micro/macro scale model [2] and the present CFD model. In this study, we present the CFD model development for methane-fueled SOFCs with direct internal reforming (DIR) of methane. Three global reaction steps of steam reforming, water-gas shift reaction, and reverse methanation on the nickel catalyst surface are additionally considered. First, the reliability of the present model is demonstrated by comparing the results with those of the conventional micro/macro scale model for methane-fueled SOFCs [3]. Then, the results of several parametric studies are presented, including the effects of electrode microstructural parameters and reformate gas composition.

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References