Modeling of Ammonia-fed Solid Oxide Cells in COMSOL Multiphysics®

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Abstract

The high temperature of solid oxide fuel cells (SOFCs) allow for a wide range of possible fuels. While pure hydrogen remains the ideal choice, problems abound regarding its production, storage, and transport. Methane/natural gas has also been investigated for potential use in SOFCs, however hydrocarbons still result in greenhouse emissions. Recently ammonia has been proposed as an alternative fuel for fuel cells. Ammonia stores hydrogen in its bonds, is carbon free, and has a well-established global distribution network.

Very few models of ammonia-fed SOFCs have been reported. Those already published are mostly thermodynamic/electrochemical 0D or 1D models. Only two computational fluid dynamics (CFD) based models have been reported to date. Both are of high temperature SOFCs, and based on the Tamura Ldt. model of ammonia decomposition, where the rate of decomposition is dependent on ammonia concentration only. This work presents a 2D CFD model of an intermediate temperature (proton conducting) ammonia-fed SOFC. At these intermediate temperatures, hydrogen inhibits the rate of ammonia decomposition, a phenomenon characterized by the Temkin-Pyzhev model of ammonia decomposition. The present model accounts for fluid flow, internal ammonia decomposition with hydrogen inhibition, fuel cell electrochemical reactions, chemical species transport using the Dusty Gas Model, and heat transfers.

The fully coupled model is implemented in COMSOL Multiphysics®. It utilizes the Navier-Stokes equations with Darcy's law source terms, heat transfer in porous media, and the transport of concentrated chemical species modules. Moreover, COMSOL does not contain a built-in module to facilitate the Dusty Gas Model, which is widely regarded as the most accurate model for the transport of chemical species in porous media. Instead, a modification of Fick's law is used, which closely approximates the Dusty Gas Model.

Reference

[1] Cheddie D. Ammonia as a Hydrogen Source for Fuel Cells: A Review. In: Minic D, ed. Hydrogen Energy – Challenges and Perspectives. Rijeka, Croatia: InTech; 2012.

[2] Ni M. Thermo-electrochemical modeling of ammonia-fueled solid oxide fuel cells considering ammonia thermal decomposition in the anode. International Journal of Hydrogen Energy. 2011;36:3153-3166.

[3] Cheddie D. Modelling of Ammonia-Fed SOFCs. In: A. Mendez-Vilas (Ed.), "Materials and Processes for Energy: Communicating Current Research and Technological Developments", Formatex Research Center (2013), Badajoz, Spain, in press.

[4] Tamaru K. A "new" general mechanism of ammonia synthesis and decomposition on transition metals. Accounts of Chemical Research, 1988;21:88-94.

[5] Kong W, Zhu H, Fei Z, Lin Z. A modified dusty gas model in the form of Fick's model for the prediction of multicomponent mass transport in a solid oxide fuel cell anode. Journal of Power Sources, 2012;206:171-178.

Figures used in the abstract

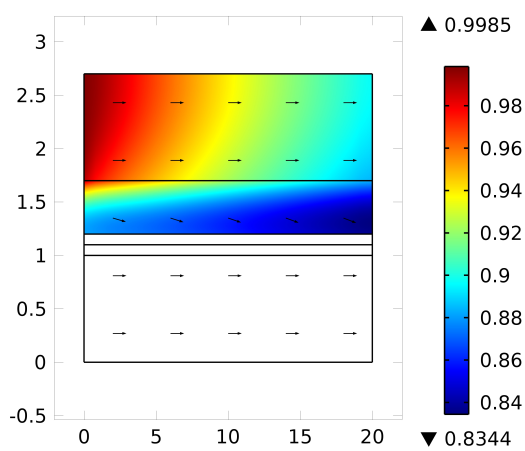

Figure 1: Ammonia Mole Fraction.

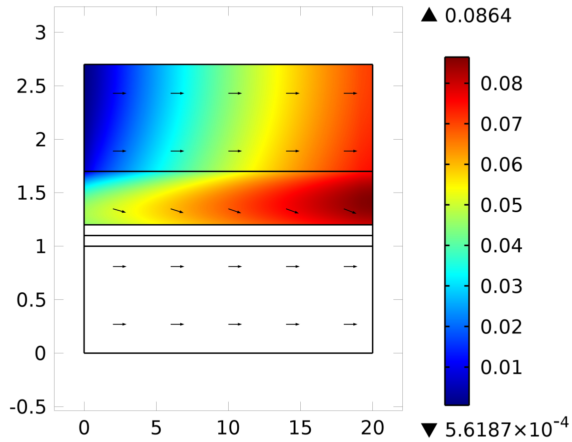

Figure 2: Hydrogen Mole Fraction.

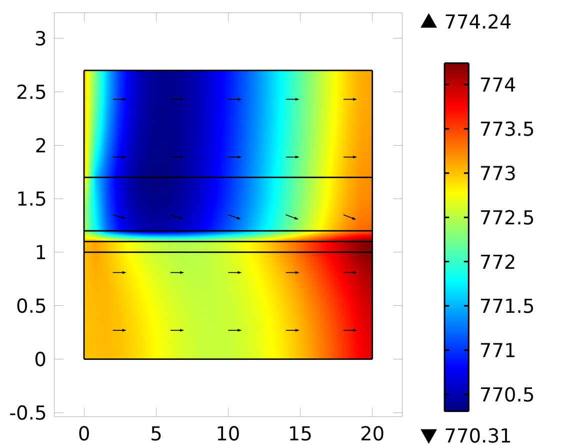

Figure 3: Temperature (K).