Numerical Modeling of the Sulfur Poisoning Effect on the Ni-YSZ Porous Anode of SOFCs

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Presence of H_2S in the fuel can have adverse effect on the performance of Solid oxide fuel cells (SOFCs) because it can poison the Ni-based anodes. Poisoning occurs by sulfur adsorption on the electrochemically active sites on Ni. This study is aimed at predicting the effect of the sulfur poisoning on the performance of SOFC with porous Ni- YSZ anode.

Our work includes two parts: (i) Modification of the kinetic expression for hydrogen electro-oxidation reaction at anode, and (ii) Implementation of the new kinetic formulation to an existing along-channel two-dimensional porous Ni-YSZ half-cell model.

Following the approach of Goodwin and co-workers [1], a Butler-Volmer like kinetic expression for hydrogen electro-oxidation was derived. In this approach, the final expression is obtained by considering one of the charge-transfer reactions to be the rate-limiting step in the elementary reaction scheme. The H_2S effect is introduced as H_2S dissociative adsorption reaction. The resulting kinetic formulation shows that the extent of electrochemical depression by introducing H_2S is a function of two ratios: ratio of partial pressures (P_{H2S}/P_{H2}) and ratio of equilibrium constant for the H_2S and H_2 adsorption reactions (K_2/K_1). The equilibrium constants of H_2S and H_2 adsorption reactions can be obtained form the thermodynamics of the reactions but not readily available.

The new kinetic formulation was implemented in an existing along-the-channel two-dimensional (2D) porous Ni-YSZ anode half-cell model. This 2D multiphysics model considers the following phenomena:

- Multicomponent species transport in the gas channel and porous anode media
- Momentum transport in the gas channel and porous anode.
- Ionic and electronic Charge transport in porous anode and electrolyte.

The model is employed to evaluate the loss in the half-cell performance for various H_2S concentrations in the inlet to the fuel stream.

Figure 1 shows the schematic of the 2D half-cell model and the polarization curve with H_2S inlet molar fraction of 1E-10.
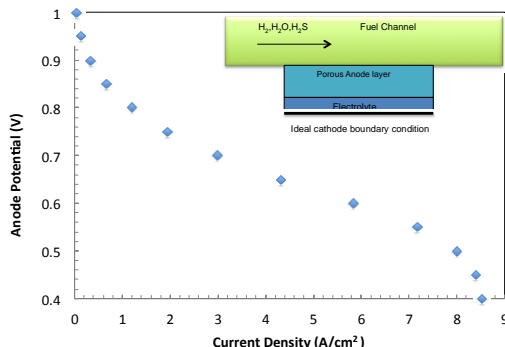

Figure 1. Polarization behaviour of the porous anode. Anode potential refers to the nominal overpotential of the anode. Simulation conditions: xH_2=0.97, xH_2O=0.03, xH_2S=1E-10, T=973K. (Inset: Schematic representation of the 2D geometry.)

Figure 2 shows the current density as a function of K_2 at H_2S inlet molar fractions of 1 and 0.1 ppm, and anode potential of 0.6 (V).
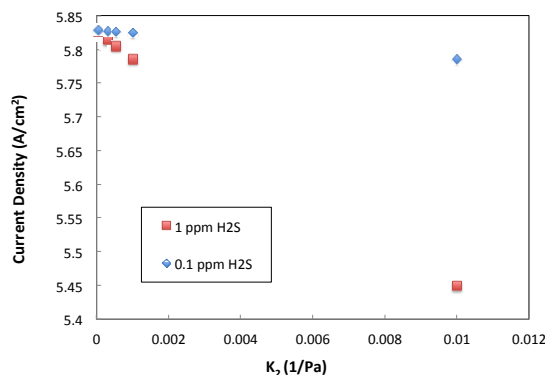

Figure 2. Current density vs. K_2 at 1 and 0.1 ppm of inlet H_2S concentrations. Simulation conditions: xH2=0.97, xH2O=0.03, V_a=0.6(V), T=973K.

Increase of the H_2S concentration results in a loss in current density. Maximum loss in current density is observed at K_2=0.01.

References:

1. Huayang Zhu, Robert J. Kee, Vinod M. Janardhanan, Olaf Deutschmann, and David G. Goodwin. *Journal of The Electrochemical Society*, 152 (12) A2427-A2440 (2005)
2. Monder, and K.Karan. *ECS Transactions*, 35 (1) 977-985 (2011)