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Mechanistic modeling of electrochemical charge transfer in HT-PEM fuel cells

Anusree Unnikrishnan[a,b], N. Rajalakshmi[b], Vinod M. Janardhanan[a,1,]

[a]*Department of Chemical Engineering, Indian Institute of Technology Hyderabad, Telangana 502 285, India*
[b]*Center for Fuel Cell Technology, ARCI, IITM Research Park, Chennai 600 113, India*

Abstract

An electrochemical model for H_2 oxidation and O_2 reduction in HT-PEM fuel cells derived from multi-step single electron transfer elementary reactions is presented. The exchange current density expressions are free from arbitrary order dependency with respect to the concentration of reactants and products. The reaction mechanism also considers CO adsorption and desorption, which enables the prediction of cell performance drop due to CO poisoning. The electrochemical model is coupled with a quasi two dimensional model of the cell, which resolves the flow channel in the axial direction and the electrodes along its length and thickness. A 3 cm long cell is simulated and the results are compared with experimental measurements. Very good agreement is obtained between the model predictions and experimental measurements for cell operating on pure H_2 and with 1-16% CO in the temperature range of 150 to 200 ^{o}C.

Keywords: Kinetics, CO poisoning, Modeling, HOR, ORR

1. Introduction

High temperature polymer electrolyte fuel cells (HT-PEM) offer several advantages over the low temperature polymer electrolyte membrane fuel cells (LT-PEM) such as i) improved tolerance to impurities, ii) enhanced electrode kinetics, iii) easier heat rejection, and iv) easier water management [1]. Numerical modeling is a powerful tool to understand the thermo-chemical and physico-chemical processes that take place within the gas diffusion layer (GDL) and the catalyst layer (CL) during the cell operation. A number of models, starting from analytical to 3D are reported in the literature that vary widely in their complexity [2–5]. However, none of these models investigate the details of hydrogen oxidation reaction (HOR) or oxygen reduction reaction (ORR) under HT-PEM operating conditions. On the other hand, HOR and ORR are extensively studied in the context of LT-PEM fuel cells [6–11]. Most of the these studies are based on the data obtained from micro electrode (ME) and rotating disc electrode (RDE) experiments performed at room temperature. Nevertheless, there are ambiguities associated with the kinetics of HOR and ORR based on RDE measurements due to the presence of mass transport resistance [12]. It has been generally

Email address: vj@iith.ac.in, Tel: +91 (0) 40 2301 6073, Fax: +91(0) 40 2301 6032 (Vinod M. Janardhanan)