Journal of Power Sources 304 (2016) 402–408

Contents lists available at ScienceDirect

Journal of Power Sources

journal homepage: www.elsevier.com/locate/jpowsour

The effect of coupled mass transport and internal reforming on modeling of solid oxide fuel cells part II: Benchmarking transient response and dynamic model fidelity assessment

Kevin J. Albrecht, Robert J. Braun *

Department of Mechanical Engineering, College of Engineering and Computational Sciences, Colorado School of Mines, 1610 Illinois Street, Golden, CO 80401, USA

HIGHLIGHTS

- Direct comparison of dynamic 1-D and 'quasi' 2-D SOFC cell-level models.
- 'Quasi' 2-D SOFC model necessary for capturing highly coupled physics.
- Mass transport dynamics impact the transient electrochemical response.
- Delays in fuel and air flow rate exaggerate the importance of mass transport dynamics.

ARTICLE INFO

Article history:
Received 21 February 2015
Received in revised form 8 July 2015
Accepted 27 July 2015

Keywords:
Dynamic
SOFC
Modeling
Mass transfer
Dusty gas model
Internal reforming

ABSTRACT

One- and 'quasi' two-dimensional (2-D) dynamic, interface charge transport models of a solid oxide fuel cell (SOFC) developed previously in a companion paper, are benchmarked against other models and simulated to evaluate the effects of coupled transport and chemistry. Because the reforming reaction can distort the concentration profiles of the species within the anode, a 'quasi' 2-D model that captures porous media mass transport and electrochemistry is required. The impact of a change in concentration at the triple-phase boundary is twofold wherein the local Nernst potential and anode exchange current densities are influenced, thereby altering the current density and temperature distributions of the cell. Thus, the dynamic response of the cell models are compared, and benchmarked against previous channel-level models to gauge the relative importance of capturing in-situ reforming phenomena on cell performance. Simulation results indicate differences in the transient electrochemical response for a step in current density where the 'quasi' 2-D model predicts a slower rise and fall in cell potential due to the additional volume of the porous media and mass transport dynamics. Delays in fuel flow rate are shown to increase the difference observed in the electrochemical response of the cells.

1. Introduction

Solid oxide fuel cells (SOFC) have received continued interest over the past decade due to their high electrical efficiency, fuel flexibility, and high quality waste heat. These benefits suggest that SOFCs are likely to play a role as a distributed energy resource, especially if life cycle cost can be reduced or significant incentives such as a carbon tax are implemented. At the current point in SOFC development, degradation effects severely limit the operational lifetime of SOFCs. The development of models which can determine when harmful operational conditions may be encountered are paramount to commercial success. Although the focus of this paper is not on quantifying degradation effects, they are considered when assessing the level of fidelity necessary for accurately predicting cell performance.

Proper selection of SOFC model fidelity is typically guided by model purpose but is often challenged by a lack of understanding of the implications of various model simplifications that are usually made for the purposes of computational efficiency and the availability of experimental data to support model validation. Dynamic, interface charge transport channel-level modeling requires the implementation of transient species, energy, and momentum balances coupled with additional submodels to capture the porous media mass transport and electrochemistry of the cell. Many channel-level models implement the same modeling

* Corresponding author.
E-mail addresses: kalbrech@mymail.mines.edu (K.J. Albrecht), rbraun@mines.edu (R.J. Braun).

http://dx.doi.org/10.1016/j.jpowsour.2015.07.087
0378-7753/

methodology of considering the diffusion within the porous anode as both a linear reduction in hydrogen and a linear increase in steam concentration, which are proportional to the local current density. This assumption is made to decouple the effects of the reforming reaction on the electrochemical model, allowing for the formulation of a one-dimensional (1-D) model. In cells where internal reforming of methane occurs, this assumption is violated due the diffusion of methane into the porous anode where the steam reforming reaction consumes water and produces hydrogen, which is catalyzed by the nickel surface. The reforming reaction distorts concentration profiles of the species within the anode, where hydrogen concentration at the TPB may be higher or lower than that of the fuel channel depending on the operating conditions and position along the length of the cell. Thus, because of local concentration variations within the cell layers, transport resistances and electrochemical performance may be quite different than in either hydrogen-only supplied SOFCs or during the relatively short time intervals when the cell is responding to dynamic load change. The present work is a companion paper to a prior model development effort [4], which seeks to evaluate model fidelity when simulating the transient response of SOFCs, thereby elucidating the circumstances which justify higher-order modeling efforts intended to support system-level SOFC performance modeling.

Over the past years there have been countless modeling efforts of dynamic SOFCs with system-level simulations in mind [1–3,9,11,13–15,19–21], including both lumped and spatially resolved models. Typically, these models include oversimplifications of the physical processes occurring in the cell such as internal reforming, mass transport, and electrochemical kinetics. The reason behind the simplification is to decouple the effects of electrochemistry and internal reforming, leading to a more computationally efficient model, where the cell is approximated as lumped or over a single dimension. However, neglecting the coupled effects could influence cell behavior and operational envelopes. When the goal of the model is to assess potentially harmful system transient effects on the cell and other balance-of-plant (BOP) components, a model that is physically based and verified against experimental data is paramount.

2. Prior SOFC dynamic modeling & verification

Our previous work [4] has developed and discussed the multi-dimensional, interface charge transfer channel-level models for both steady-state and dynamic operation. Experimental verification of dynamic fuel cell models is quite difficult to accomplish in the laboratory, as it requires fast, time dependent data for cell temperature, voltage, and gas species evolution, including streamwise profiles of locally measured variables. Additionally, labscale verification against a cell within a furnace is not entirely representative of an adiabatic cell within a system. Lacking such data, the approach taken here [20] is to benchmark our results against other models in the extant literature. Thus, this paper focuses specifically on channel-level dynamic models and a direct comparison of the levels of fidelity implemented. Prior to presenting benchmarking results, we first give a brief overview of prior relevant dynamic modeling work.

Dynamic channel-level SOFC models can be divided into varying levels of fidelity, which are dependent on the level of spatial discretization. The simplest dynamic model is a lumped model where no spatial discretization is present, these models are computationally efficient and a good option for model predictive control or where rapid dynamic simulation is of interest [23,17]. The term lumped has also been used to classify the resolution of different layers within a spatially distributed model where the temperature has been lumped transverse to the bulk flow resulting in a model which falls in between the fully lumped model and the 1-D channel-level model [12]. Theses models have merit from a system-level modeling perspective, however, effects of flow configuration and temperature distribution are lost due to the lumped nature.

The 1-D model of intermediate fidelity is highly utilized in dynamic modeling efforts particularly on the system-level where the temperatures for different layers have been resolved transverse to the axial flow, however, the temperature or species gradients within the specific layers have not been resolved transverse to the axial flow [2,3,11]. Transport between the different layers is established based on a resistive network where convection coefficients based on Nusselt number correlations and plug flow have been assumed. This methodology is capable of simulating a counter or co-flow configuration, however, species gradients within the anode and the anode volume contributing to species transients have been neglected.

The ‘quasi’ 2-D model of higher fidelity extends the 1-D methodology and resolves the species profile in a second dimension throughout the depth of the anode [8,9]. However, the channel composition and temperature are still considered to be lumped. This model extends the 1-D dynamics and is able to capture the species transients within the anode, and the effect of the internal reforming on the current density and temperature profile of the cell. The species transients are important to capture in SOFC modeling since prior system-level modeling results have indicated that dynamic load-following ability is limited by anode fuel depletion. Additionally, this model allows for a robust simulation tool where the electrode design can be easily modified to determine the dynamic and steady-state operational benefits.

High fidelity 2-D or 3-D models have been developed as well, where the species and temperature distributions have been fully resolved in space [7,5]. This modeling methodology has been implemented from button cells and simplified geometries to the full cell level models. The dynamics of these model suggest that they would be difficult to implement into a system-level model. However, dynamic system-level models with this level of fidelity still have been developed [18]. These models provide useful results for known geometries or commercial designs, however, system configuration studies or general results would be difficult to obtain where exact geometries are unknown. Simulation of 3-D geometries would require extensive knowledge of the stack/system including sealing, stack manifolding, hardware packaging details which describe both the relative location of the individual system components, and insulation characteristics, and detailed dimensional information of the system – all of which are typically closely guarded as proprietary.

The development of design and simulation tools, which are computationally efficient and capture the coupled effects of parameter changes on the cell performance, are still important to develop. Many dynamic SOFC models have been developed to assess the effects of transient SOFC operation on performance. An in-depth review of these models is provided in our companion paper to the present work [4]. Here we emphasize that one of the main differences between prior efforts and the present work is the assessment of the importance of model fidelity as it pertains to resolving electrode species transport and reaction during steady-state operation. In particular, we establish the importance of detailed reaction and transport modeling (via resolving the anode electrode) on cell-level model-prediction whose primary purpose is implementation in stack and system-level simulation. The remaining sections of this paper will benchmark the dynamic response of the current models against previous modeling efforts, and compare the dynamic operation of the two models developed in the companion paper by the authors [4].