TUESDAY, AUGUST 23, 2005, P.M.

SESSION 22B: INTERNATIONAL SYMPOSIUM ON FUEL CELL AND HYDROGEN TECHNOLOGIES

MODELLING II - SOFC

Sponsor(s): Materials Science and Engineering Section, The Metallurgical Society of CIM
Room: Imperial Ballroom 5
Chairman: X. LI, University of Waterloo, Canada

PAPER 22B.1 — 15:40

DYNAMIC MODELLING AND CONTROL OF A SOLID OXIDE FUEL CELL.

A. CHAISANTIKULWAT and E. S. MEADOWS, University of Alberta, Canada

Most solid-oxide fuel cell (SOFC) Modelling emphasizes steady state cell operation. However, understanding the dynamic behaviour is essential to predict the performance and limitations of SOFC power systems.

In this work, we demonstrate a dynamic model of a SOFC, and we simulate a feedback control scheme that can maintain output voltage despite load changes. Dynamic response is determined as the solution of coupled partial differential equations derived from conservation laws for energy, mass and electric charge. From such a model, the step responses to system input variables can be determined. Low order dynamic models that are sufficient for feedback control design can be derived from the step responses. The development of the partial differential equation model is outlined, and the limitations of the control system are discussed.

PAPER 22B.2 — 16:00

EXPLORING THE GAS DIFFUSION INDUCED DYNAMIC BEHAVIOUR OF SOLID OXIDE FUEL CELLS.

B. HUANG, Y. QI and K.T. CHUANG, University of Alberta, Canada

With the aim of dynamic simulation and control, a dynamic model of solid oxide fuel cell (SOFC) with a focus on the diffusion process at cell-level is derived in this work. The species dynamics is built in the form of the state-space model. Dynamic properties of SOFC are shown through simulations. It demonstrates that diffusion processes in porous layers play an important role in the dynamic behaviour of SOFC. They affect concentrations in the vicinity of triple phase boundary (tpb), and thus the electrical properties. Simulation shows that it is the dynamic behaviour of partial pressures in the vicinity of tpbs contributes more to the slow rise of voltage in the step response test and current interrupt experiment, not the charge transfer capacitance. Given different diffusion thicknesses, it is found that the voltage output and dynamic behaviour of gas consumption rates are affected greatly by the thicknesses of the diffusion layers. Simulations also indicate that temperature has large effect on the voltage output dynamics.

PAPER 22B.3 — 16:20

INFLUENCE OF MICROSTRUCTURAL PARAMETERS OF A SOFC COMPOSITE CATHODE ON THE COLLECTION OF RELIABLE EXPERIMENTAL DATA: A MODELLING ANALYSIS.

B. KENNEY and K. KARAN, Fuel Cell Research Centre, Queen's University, Canada

For SOFCs, composite cathodes comprising an electronically conducting electro-catalyst (e.g. LSM) and an ionically conducting electrolyte material (e.g. YSZ) are considered to improve the electrochemical performance by extending the active reaction zone to regions beyond the electrolyte-electrode interface, as in the case of conventional cathodes. Interpretation of composite cathode performance however is complicated by the mixed conducting behaviour which results in local overpotential distributions throughout the composite cathode. The magnitude of the overpotentials depends on many factors, such as the composition, particle size, porosity and thickness of the cathode. Reliable experimental data obtained from composite cathodes requires carefully crafted microstructural parameters in order to minimize the overpotential variations.

In this study, we utilize a one-dimensional composite cathode model to analyze the influence of composition, particle size, porosity and cathode thickness on obtaining accurate data such as the reaction order of the oxygen reduction reaction and the activation energy. Coupled differential equations describing transport and consumption of chemical species, oxygen ion and electrons are solved simultaneously. The ORR is described in terms of a Butler-Volmer type equation with an assumed rate determining step. The results are analyzed in terms of electrode polarization resistance (and exchange current density) as a function of pO_2 and temperature. An apparent pO_2 dependency exponent n and apparent activation energy is then extracted from the predicted Rp vs pO_2 and i_0 vs 1/T data. It was found that this exponent n and activation energy can be significantly influenced by the microstructural parameters.

PAPER 22B.4 — 16:40

DIESEL STEAM REFORMING FOR SOFC SYSTEMS.

B. PEPPLEY, P. HARASTI, J.C. AMPHLETT and C.P. THURGOOD, Royal Military College of Canada, Canada

The current most common method of hydrogen production for fuel cell systems, including SOFC systems, is autothermal reforming. Autothermal reformers have a number of advantages including fast start up and load following and ease of control. However, there are a number of problems inherent with the addition of air into a system connected to the anode feed such as dilution of the fuel with nitrogen and the potential for oxygen to reach the anode chamber directly. Pure steam reforming, which does not involve air addition, provides a richer fuel mixture to the SOFC anode and is inherently safer than autothermal reforming. Although in theory pure steam reforming can be shown to provide these advantages, a number of technical problems need to be overcome before such a system can be practical. In particular, issues such as catalyst degradation due to poisoning and thermal sintering, coking, as well as fuel-steam mixing need to be addressed. Experimental results from a prototype reformer will be presented to illustrate a number of these points.

This paper will compare differences in system efficiency, safety and complexity between an autothermal/SOFC systems versus a steam reformer/SOFC system. A system simulation will be utilized that is able to account for material and energy balances for a SOFC power generator operating on diesel fuel. The requirements for improved catalysts will be discussed and an analysis of the potential benefits of sulfur tolerance and lower temperature activity will be considered.

PAPER 22B.5 — 17:00

A REVIEW OF MATHEMATICAL MODELLING OF THE TRANSPORT PHENOMENA AND THE CHEMICAL/ELECTROCHEMICAL REACTIONS IN SOFCS.

J.G. PHAROAH, J.D.J. VANDDERSTEEN, B. KENNEY and K. KARAN, Queen's University, Canada

Over the last two decades a variety of models for solid oxide fuel cells (SOFCs) have emerged ranging from one dimensional (1-D) to 3-D models, from steady-state to transient models; single- and half-cell and entire stack models. A majority of these models have focused either on the transport processes or on the chemical/electrochemical processes.

The approach taken by our research group is to develop a comprehensive SOFC model framework based on the considerations of detailed electrochemical reaction mechanism and by accounting for complex transport processes occurring in the porous media at the micro-scale level. In this paper, we review the state-of-the-art in SOFC Modelling and identify the existing gaps that need to be filled in.