Physical Model Development, Model Reduction, and Observer Design of a Molten Carbonate Fuel Cell

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Keywords: Molten carbonate fuel cell; mathematical modeling; dynamic simulation; model reduction; observer; process control

Due to its high electrical efficiency, the molten carbonate fuel cell (MCFC) is an attractive candidate for decentralized power generation. The MCFC's operation temperature of 600-650 °C allows for a combined generation of electricity and heat. An industrial MCFC stack is characterized by a high degree of system integration that includes the internal generation of hydrogen by steam reforming, the mass coupling between anode and cathode gas channel, and the heat integration of endothermic reforming reactions and exothermic electrochemical reactions. The system integration reduces build costs and improves the overall efficiency on the one hand, but on the other hand it makes process operation more challenging. Currently, the operation of MCFC stacks is mainly based on empirical knowledge. However, that empirical mode of operation requires large safety factors, as the intuitive process understanding of such a highly integrated system is difficult and because the amount of measuring information available is typically limited. Consequently, the potential of the cells is not fully exploited today. This contribution reports on some results of a collaborative research project by several academic and industrial partners that aims at overcoming those limitations by providing reliable physical process models, by deepening the process understanding, and by developing model based concepts of process operation. It is concerned with the experimental and theoretical analysis of the 300 kW MCFC stack 'Hot Module' by MTU CFC Solutions, Germany (Bischoff, 2002). In the first part of this contribution, a detailed spatially two-dimensional model of the MCFC is presented. In the second part, from that reference model a reduced model is derived that is suitable for process control purposes. In the last part, a state and parameter estimator is developed based on the reduced model.

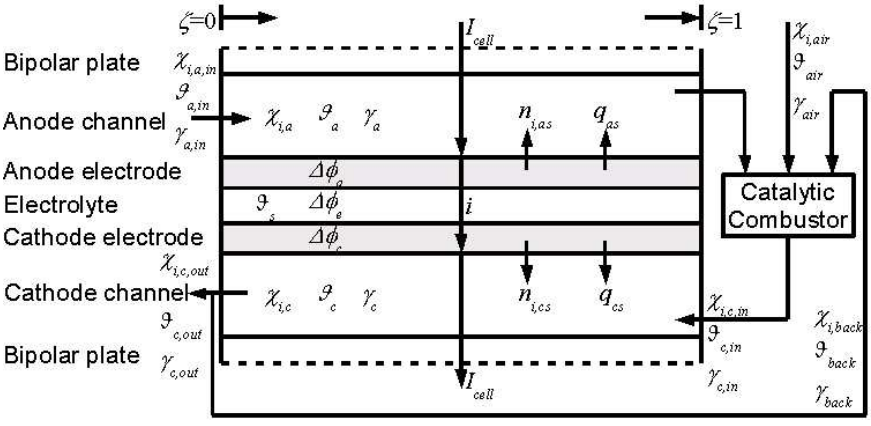

Fig. 1: Scheme of a single cell MCFC counter flow model with catalytic burner. State variables like molar fractions, molar flows, temperatures, and electric potentials as well as the input quantities at anode and burner inlet and total cell current are indicated together with mass, enthalpy and charge fluxes.

The dynamic modeling of a cross flow single cell MCFC is based on the description of chemical and physical phenomena. It includes convection, heat and mass exchange between different phases, heat conduction and a detailed model for electric potentials. The reference model describes the transient behavior of concentrations, molar flows, temperatures as well as cell voltage and current density distribution (figure 1) (Heidebrecht and Sundmacher, 2002).

For many process control purposes, the high degree of detailedness of the reference model described above is not necessary. Instead, a reduced model formulation is desirable that requires less computational time and consists of a low-order system of equations. Such a reduced model has been developed for the MCFC. In the first step, the reference model is slightly simplified by additional physical assumptions like quasi-stationary mass and charge balances and a pseudo-homogeneous energy balance. A further model reduction is achieved by mathematical methods. For the reduction of parabolic partial differential equations, orthogonal projection methods like the Galerkin method have become a frequently used technique (Baker and Christofides, 2000; Hoo and Zheng, 2001). In this work, the spatial basis functions for the Galerkin procedure are obtained numerically by applying the Karhunen-Loeve decomposition technique (Park and Cho, 1996) to simulation results of the reference model. It is found that a small number of basis functions suffices to describe the spatial temperature, charge, and concentration profiles of the cell with good accuracy (Mangold and Sheng, 2003). Compared to the original distributed reference model, the computation time required for the reduced model is reduced by a factor of up to one hundred. Special care is taken to test the extrapolation qualities of the reduced model. Test simulations show that the reduced model is able to predict the influence of even large parameter changes on the system satisfactorily for the relevant kinetic and operation parameters. Therefore, the reduced model seems well suitable for process control applications.

Based on the reduced model, a state and parameter estimator for the MCFC is developed. The purpose of the state and parameter estimator is to provide on-line information on the process that is not directly accessible by measurements. This is accomplished by comparing measured and simulated values and using the results of the comparison to correct the simulated states. In this work, the concept of a Luenberger state observer is used as a starting point for the development of the estimator. This concept has to be extended slightly due to the time varying nature of the MCFC. During its life cycle, a fuel cell suffers from aging and degradation effects resulting in time dependent values of the kinetic parameters in the fuel cell model. In order to take this effect into account in the observer, the observer model is extended by dummy equations for the kinetic parameters. The observer gain matrix is obtained from an algebraic Riccati design. The state and parameter estimator is tested in simulations where simulation results of the distributed reference model are used as measuring information for the observer.

Fig. 2: Test of the state and parameter estimator; measuring information consists of the temperature at 3 locations and the total cell voltage; the state estimator is able to correct wrong initial conditions as well as a wrong initial value for a kinetic pre-exponential factor k_0^A.

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