Available online at www.sciencedirect.com
ScienceDirect
Journal of Power Sources 180 (2008) 309–321
JOURNAL OF POWER SOURCES
www.elsevier.com/locate/jpowsour

Computationally efficient modeling of the dynamic behavior of a portable PEM fuel cell stack

S.P. Philipps, C. Ziegler *

Fraunhofer Institute for Solar Energy Systems ISE, Heidenhofstr. 2, D-79110 Freiburg, Germany

Received 13 April 2007; received in revised form 19 January 2008; accepted 25 January 2008
Available online 16 February 2008

Abstract

A numerically efficient mathematical model of a proton exchange membrane fuel cell (PEMFC) stack is presented. The aim of this model is to study the dynamic response of a PEMFC stack subjected to load changes under the restriction of short computing time. This restriction was imposed in order for the model to be applicable for nonlinear model predictive control (NMPC). The dynamic, non-isothermal model is based on mass and energy balance equations, which are reduced to ordinary differential equations in time. The reduced equations are solved for a single cell and the results are upscaled to describe the fuel cell stack. This approach makes our calculations computationally efficient. We study the feasibility of capturing water balance effects with such a reduced model. Mass balance equations for water vapor and liquid water including the phase change as well as a steady-state membrane model accounting for the electro-osmotic drag and diffusion of water through the membrane are included. Based on this approach the model is successfully used to predict critical operating conditions by monitoring the amount of liquid water in the stack and the stack impedance. The model and the overall calculation method are validated using two different load profiles on realistic time scales of up to 30 min. The simulation results are used to clarify the measured characteristics of the stack temperature and the stack voltage, which has rarely been done on such long time scales. In addition, a discussion of the influence of flooding and dry-out on the stack voltage is included. The modeling approach proves to be computationally efficient: an operating time of 0.5 h is simulated in less than 1 s, while still showing sufficient accuracy.

Keywords: PEM fuel cell; Modeling; Dynamic; Stack; NMPC

1. Introduction

In recent years the interest in using hydrogen fuel cells as power supply for portable electronics has grown substantially. Compared to batteries fuel cell systems can provide a higher energy density and instantaneous refilling while avoiding the problem of self-discharge. However, the use of fuel cells as power supply for electronic products is challenging because the power demand of these applications fluctuates. Due to the limited space in portable electronics the stack can in many cases not be buffered by a battery. Thus, the fuel cell does not usually operate at steady-state. A solid understanding of the dynamic response of a proton exchange membrane fuel cell (PEMFC) under load changes is crucial for reliable and optimized operation [1]. The dynamic behavior of a fuel cell is a highly complex phenomenon, as it involves different length and time scales. The power of a PEMFC also strongly depends on operating conditions such as flow rates, relative humidity and temperature of the gases as well as ambient temperature. Mathematical modeling is a powerful tool for understanding and handling this complexity. Nonlinear model predictive control (NMPC) and online optimization of dynamic processes have attracted increasing attention over the past decade, see e.g. Ref. [2]. In contrast to empirical control strategies based on experimental observations and extensive testing, a model-based control allows faster system development and optimal system operation over a wide range of operating conditions. As a prerequisite, NMPC requires detailed nonlinear process models.

A considerable amount of work has been done thus far to model PEMFCs [3,4]. Most of the models are steady-state, see for example Refs. [5–7]. Less work has been published on dynamic fuel cell modeling. Amphlett et al. [8] modeled the behavior of the stack temperature and the voltage during

* Corresponding author.
E-mail address: christoph.ziegler@ise.fraunhofer.de (C. Ziegler).
URL: http://www.ise.fraunhofer.de (C. Ziegler).

0378-7753/$ – see front matter © 2008 Elsevier B.V. All rights reserved.
doi:10.1016/j.jpowsour.2008.01.089

start-up, shut-down and load-step. In their model only the energy balance of the solid is modeled dynamically whereas all other equations are assumed to be at quasi-steady state for a given solid temperature. Lee et al. [9] used an object-oriented approach based on stationary equations. Dynamic profiles are created by calculating the quasi-stationary solution variables for each time-step. Ceraolo et al. [10] used an isothermal model to simulate the dynamic behavior of the cell voltage to a load change on a time-scale of seconds. Their model was extended to account for non-isothermal conditions by Shan et al. [11]. In recent years several authors have presented dynamic models using a similar approach as Amphlett et al. [8]. Golbert et al. [12] developed a transient along-the-channel model for control purposes, which includes mass balances of liquid water and water vapor. Yu et al. [13] presented another extension of the model of Amphlett, which accounts for the influence of latent heat on the energy balance. Pathapati et al. [14] included dynamic mass balance equations and energy balance equations for the gases. In addition, a term to account for the double layer capacity is presented. The influence of flooding on the dynamic behavior of the stack voltage under isothermal conditions was modeled by McKay et al. [15]. All of these models are reduced in terms of dimensionality and comprehensiveness. In recent years several research groups have published valuable in-depth analyses on the transient behavior of PEM fuel cells using commercial software tools either based on computational fluid dynamics, e.g. Refs. [16–21] or on finite-element, multiphysics simulation approaches, e.g. Refs. [22–25]. These studies help in understanding the fundamental physical processes and interactions within the fuel cell. However, due to the massive computational effort required they are not suitable for online control.

This work presents a dynamic model approach for portable fuel cell stacks. The aim of our work is to model the dynamic behavior of a portable PEM fuel cell stack on relevant time scales for technical applications under the restriction of keeping the computing time short. Therefore, a reasonable compromise between physical accuracy and numerical efficiency is found which makes the model suitable for NMPC. Despite of the number of very valuable contributions to the dynamic fuel cell modeling, a validated model approach, which meets these needs was not found in the literature. Many of the existing models require massive computational effort either in terms of memory usage or computing time or both, e.g. Refs. [16–21,23–25]. Most of the reduced models in the literature are either not designed for NMPC purposes, e.g. Refs. [9,10] or are not validated against experimental data of a PEMFC stack on realistic time scales, e.g. Refs. [11–13]. The reduced model presented here is validated against experimental data of a PEMFC stack for different load profiles on realistic time scales of up to 30 min. The model validation study does also include an analysis of the characteristics of the stack in critical states of operation. The model is non-isothermal and considers the mass transfer and the electrochemical reactions. Moreover, the model accounts for both water vapor and liquid water and for the phase transition. In contrast to previous modeling studies the average liquid water concentration is used to predict flooding of the fuel cell based on the liquid water balance. This can be useful for improved NMPC algorithms. To ease the transfer to different stacks we describe the methods of parameter identification in detail. In order to meet the challenge of realizing sufficiently exact modeling results with short calculation time some strong simplifications are made, which are justified by the good agreement between simulation and experimental results.

2. Model description

2.1. Modeling approach

The PEM fuel cell stack model presented here is dynamic and non-isothermal. The model is based on transient energy and mass balance equations, a membrane model and an electrical model based on the tafel equation. Convective heat and mass transfer within the stack are accounted for dynamically. A mass balance of water in the liquid and vapor phase is included. Condensation and evaporation in the channels as well as water generation at the cathode are accounted for. The membrane model is steady state and accounts for the electro-osmotic drag and back diffusion of water. The steady-state electrical model incorporates the influence of pressure and temperature changes as well as the voltage drop due to activation and ohmic losses.

Fuel cell stacks are commonly characterized by measuring the time evolution of the stack voltage and the stack temperature subject to specific operating conditions like power demand, ambient and gas temperature and gas humidity. In integrated fuel cell systems the stack voltage, the stack temperature and the gas flow rates are usually monitored. The stack model presented here allows the simulation of the most important parameters for the operation of a PEMFC stack. The model considers four monitoring points for the mass and heat balance of the gases: the inlet and outlet of the stack on the anode and cathode side. At these points, gas temperatures and molar fluxes of the different species are considered. The operating conditions at the stack inlets are used as input values of the model. Furthermore, the current density is an input variable. Based on the values of the operating conditions, the model predicts the molar fluxes and gas temperatures at the stack outlets, the average temperature of the solid material, the stack voltage and the average concentration of liquid water in the stack. Fig. 1 shows the solution variables and operating conditions and illustrates that these parameters are accessible even in a fully integrated fuel cell system. For the stack temperature, four monitoring points are indicated from which the average temperature is calculated.

The derivation of the model equations is done in a bottom-up approach that can be split up into three steps. First, we consider one particular cell of the stack. Balance equations are set up for a representative elementary volume of the cell (REV_1) and for a representative elementary channel (REC) in the cell (REV_2). The model is reduced to one geometrical dimension, the direction along the channel length. Second, the time-dependent balance equations for the REVs are integrated along the channel length. For a complete description of one cell all gas channels are assumed to behave like the REC. Third, the stack is modeled as several coupled cell modules. The approach and the model geometry is illustrated in Figs. 1–3. The model assumptions are