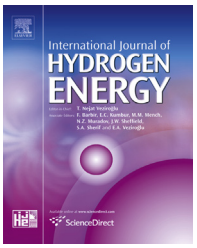
INTERNATIONAL JOURNAL OF HYDROGEN ENERGY XXX (2016) 1–12

Available online at www.sciencedirect.com

ScienceDirect

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



Planar SOFC system modelling and simulation including a 3D stack module

Amirpiran Amiri [a], *Periasamy Vijay* [a], *Moses O. Tadé* [a,*], *Khaliq Ahmed* [a,b], *Gordon D. Ingram* [a], *Vishnu Pareek* [a], *Ranjeet Utikar* [a]

[a] *Centre for Process Systems Computations, Department of Chemical Engineering, Curtin University, GPO Box U1987, Perth, WA 6845, Australia*

[b] *Ceramic Fuel Cells Ltd., Noble Park, Victoria 3174, Australia*

ARTICLE INFO

Article history:
Received 6 August 2015
Received in revised form
3 December 2015
Accepted 3 December 2015
Available online xxx

Keywords:
SOFC
System
Stack
Balance of plant
Aspen Plus

ABSTRACT

A solid oxide fuel cell (SOFC) system consists of a fuel cell stack with its auxiliary components. Modelling an entire SOFC system can be simplified by employing standard process flowsheeting software. However, no in-built SOFC module exists within any of the commercial flowsheet simulators. In Amiri et al. (Comput. Chem. Eng., 2015, 78:10–23), a rigorous SOFC module was developed to fill this gap. That work outlined a multi-scale approach to SOFC modelling and presented analyses at compartment, channel and cell scales. The current work extends the approach to stack and system scales. Two case studies were conducted on a simulated multilayer, planar SOFC stack with its balance of plant (BoP) components. Firstly, the effect of flow maldistribution in the stack manifold on the SOFC's internal variables was examined. Secondly, the interaction between the stack and the BoP was investigated through the effect of recycling depleted fuel. The results showed that anode gas recycling could be used for managing the gradients within the stack, while also improving fuel utilisation and water management.

Introduction

Fuel cells are electrochemical reactors that convert chemical energy directly into electrical energy, which is in contrast to conventional power plants where chemical energy is first converted to mechanical energy before it is converted into electrical energy. The key advantages of this technology are not only high efficiency and low emission of pollutant gases, but also its diversity of fuel sources, particularly renewables, such as biogas and ethanol. Nevertheless, the commercialization of fuel cell technology has been hindered by several technical challenges. Modelling and simulation approaches will play a central role in overcoming some of these barriers. Modelling tools reduce the costs and risks of experimental investigations through screening the more feasible and reliable cases. Further, material performance analysis, fluid flow design, system energy analysis, fuel pre- and post-processing analysis and optimization, durability assessment and system interactions are some of the tasks that can benefit from a reliable and flexible model.

* *Corresponding author*. Tel.: +61 8 9266 7581; fax: +61 8 9266 2681.
E-mail address: m.o.tade@curtin.edu.au (M.O. Tadé).

http://dx.doi.org/10.1016/j.ijhydene.2015.12.076

In the last two decades, the development and refinement of detailed mathematical models of fuel cells – a multidisciplinary endeavour – has increasingly received attention from researchers. In the more fundamental studies, the main goal is to understand and capture the cell's internal operational behaviour, transport phenomena and reaction aspects. These are of vital importance in exploring the fundamental mechanisms and providing deep insights into the small scale behaviour of a fuel cell that can be used in higher scale models. Typical of these studies are [1–4]. At the larger stack and system scales, engineering aspects of optimization, design and analysis of the system have been studied [5–15]. In these works, cell-to-cell and/or stack-to-BoP interactions are the modelling focus, resulting in an integrated analysis of all the unit operations involved. Furthermore, energy and cost analyses of the system, which are necessary for commercialization, are mainly based on stack and system level models. The more BoP components, chemical species, reactions and transport phenomena involved, the more complicated the system of equations that must be dealt with. Obviously this increases the complexity of the model, which is not always desirable. Further, the process flowsheet may vary depending on the application area of the fuel cell system. If a dedicated software package for fuel cells is created, any alteration in the process units or the flowsheet means that the model equations and software may need to be changed. This complexity can be avoided by implementing a flexible fuel cell model within a general process simulator. Such an approach minimizes the work needed to simulate the standard unit operations that form the BoP, and also facilitates making small changes, like to the species present, and large changes, such as reconfiguring the entire flowsheet. Changes to the fuel cell and stack can be done independently, thereby facilitating the simulation, analysis and optimization of the process.

Fuel cell system modelling in a process simulator, such as Aspen Plus, has been undertaken in several previous studies. Zhang et al. [16] created a SOFC system simulation by using inbuilt reactor modules. FORTRAN programming and data post-processing subsequently enabled the authors to simulate a tubular SOFC plant that was validated against a 100 kW Siemens-Westinghouse SOFC stack. Ameri and Mohammadi [17] used a similar methodology to simulate a SOFC integrated with a gas turbine. Moreover, Kivisaari et al. [18] and Doherty et al. [19] used Aspen Plus to model a molten carbonate fuel cell that was fuelled by gasification process products. In another work, Kivisaari et al. [20] compared the application of three process flowsheeting packages, Design-II, Aspen Plus and Spence, for fuel cell system simulation. They found that, in spite of good agreement of the overall results, significant differences between the packages became apparent on more detailed examination.

The majority of previous studies have used the simulator's inbuilt reactor modules to approximate the fuel cell. However data post-processing was also inevitably used to transform the simulator results into those representing a simplified lumped electrochemical reactor. In spite of the simplicity of this approach, there are some serious deficiencies. Table 1 compares some of the features of previous works to the current study. Some of the limitations compared to the current approach are outlined in the following. First, the parameters and variables of the fuel cell are limited to user-defined equations added to the flowsheet. Second, the bidirectional interaction of the fuel cell and the rest of the process is not effectively and systematically implemented. Third, the fuel cell's internal reaction and flow phenomena are often not included appropriately, or in some cases not included at all. Fourth, the spatial distributions of a cell's internal variables, which are influenced by BoP parameters, are not captured, but they are vital for the temperature and fuel management of the stack. Fifth, the fuel and oxidant flow patterns in the cell are not considered. Finally, stacking related issues, manifold flow distribution effects for instance, are neglected. In the cases in which a user-defined reactor is developed and used, the majority of the abovementioned flaws are still present. Most of the deficiencies mentioned here have been addressed in this paper (Table 1), the most important of which is the influence of BoP parameters on the cells' internal, spatially distributed variables. This is a key aspect of the current work.

It should be noted that the configuration of the fuel cell reactor is also an important consideration in modelling. Even though a fuel cell reactor could be approximated by ideal reactor models, such as the Plug Flow Reactor (PFR) or Continuous Stirred Tank Reactor (CSTR) under specific conditions, in practice a fuel cell reactor's performance may fall in between these two ideal models depending on the hydrodynamics. A flexible model is, therefore, required to account for ideal and non-ideal flow behaviour. The CSTR-in-series methodology is sufficiently general and flexible to address this requirement. Therefore, another contribution of the modelling approach proposed in this work is to enable the user to simulate a planar SOFC reactor as a PFR, CSTR or a more complex reactor according to the flow regime of interest, along with the BoP. Analysis of residence time distribution data can provide information about the number of consecutive CSTRs needed.

Modelling and simulation methodology and input parameters

Since fuel cell design and operation possess a multi-scale nature, its behaviour should be described through a multi-physics, multi-scale modelling strategy. However, unnecessary complexity in the final model must be avoided. The aim of the current study is to conceive and implement a multi-scale framework for modelling a SOFC system within a well-established process flowsheeting environment such as Aspen Plus or Aspen Hysys. Fig. 1 shows the modelling framework that was proposed and partly implemented in Amiri et al. [21]. The interested reader may refer to that paper where the authors describe and analyse compartment, channel and cell scale SOFC models using the proposed framework. In contrast, the focus of this paper is on multi-cell stack and system level modelling and simulation.

Stack and system modelling and simulation

A SOFC channel is assembled from a series of compartment blocks created in Aspen Custom Modeller [21]. The conservation and constitutive equations for a single compartment

Please cite this article in press as: Amiri A, et al., Planar SOFC system modelling and simulation including a 3D stack module, International Journal of Hydrogen Energy (2016), http://dx.doi.org/10.1016/j.ijhydene.2015.12.076