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PEM fuel cell model and simulation in Matlab–Simulink based on physical parameters

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ABSTRACT

An advanced PEM fuel cell mathematical model is described and realised in four ancillaries in the Matlab–Simulink environment. Where possible, the model is based on parameters with direct physical meaning, with the aim of going beyond empirically describing the characteristics of the fuel cell. The model can therefore be used to predict enhanced performance owing to, for instance, improved electrode materials, and to relate changes in the measured performance to internal changes affecting influential physical parameters. Some simplifying assumptions make the model fairly light in computational demand and therefore amenable to extension to simulate an entire fuel-cell stack as part of an energy system. Despite these assumptions, the model emulates experimental data well, especially at high current density. The influences of pressure, temperature, humidification and reactant partial pressure on cell performance are explored. The dominating effect of membrane hydration is clearly revealed.

1. Introduction

The minimal generation of by-products (ideally only water for hydrogen fuel) and the high electricity generation efficiency of the hydrogen fuel cell make this technology attractive for a range of applications such as automobiles and small-scale stationary electricity generation. Based on the lower heating value of hydrogen, fuel cells have conversion efficiencies of 40–60%, higher than most other energy conversion systems [1].

The solid polymer membrane makes the PEM fuel cell simpler and less hazardous than the alkaline type, although the PEM type is more difficult to manage because of the need for proper hydration of the membrane [2].

PEM fuel cell performance is conveniently visualized *via* the different overpotentials/voltage drops, *i.e.* the difference between the electrode potential and the equilibrium potential. An important goal of fuel cell design is to minimise the lossy contributions to the overpotential for a given current and so maximise efficiency. Membrane hydration, achieved *via* humidification of the reactant gases, plays a dominating role in PEM fuel cell performance. Too little water leads to dehydration and high membrane resistance. Excessive water leads to flooding of the electrode pores and increased electrode resistance. Hence water management, and *via* the partial vapour pressure thermal management, are critical to the good performance of PEM fuel cells.

Better design, selection of appropriate materials and optimization of the overpotential are necessary in order to improve the PEM fuel cell performance. These issues can only be addressed efficiently if realistic mathematical process models are available to predict the effects of different materials, construction and so on. A realistic model provides a framework not only for analysing the overall performance of the PEM fuel cell, but also for studying its various components and their mutual influences. An effective model thus becomes a research tool to explore parameters which are difficult to measure *e.g.* water concentration at the membrane–electrode interface, water uptake into the channel, *etc.*

In the past two decades many fuel-cell models have been presented in the literature. The early history of PEM fuel-cell modelling work has been reviewed by Bıyıkoğlu [3]. The advantages and disadvantages of various conceptual approaches to PEM fuel-cell modelling have been discussed by Cheddie and Munroe [4].

More recently, Djilali and Lu [5] and Costamagna [6] proposed a multi-dimensional model and more complex approaches in 3D modelling have also been developed for the PEM fuel cell [7–13]. Sophisticated modelling approaches have been applied to understanding various aspects of fuel-cell behaviour. Carton and Olabi

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Glossary

A	Active area of MEA, cm^2
a	Water activity
C	Molar Concentration, mol m^{-3}
D	Diffusion coefficient, m^2 s^{-1}
E	Cell potential, V
E_c	Activation energy, kJ mol^{-1}
F	Faraday constant, 96485 C mol^{-1}
G	Gibbs free energy of activation, kJ mol^{-1}
I	Current, A
i	Current density, A cm^{-2}
i_0	Exchange current density, A cm^{-2}
k	Reaction rate coefficient
MEA	Membrane electrode assembly
$\dot{N}$	Molar flow rate, mol s^{-1}
n	Molar flux, mol m^{-2}-s
P	Pressure, atm
p	Partial pressure, atm
p_{sat}	Saturation pressure, atm
R	Universal gas constant, 8.3144 J $mol^{-1}K^{-1}$
S	Stoichiometry ratio
T	Temperature, K
X	Molar fraction
δ	Thickness, mm
ρ	Density of water, kg m^{-3}
σ_{mem}	PEM conductivity, S m^{-1}
n_d	Electro-osmotic drag coefficient
α	Charge transfer coefficient
λ	Degree of humidification
φ	Relative humidity
γ	Roughness factor
ε	Porosity
ξ	Tortuosity

[14] developed a 3D model based on computational fluid dynamics (CFD) for open pore cellular foam material as a flow plate and they found that the reactant gases were uniformly distributed from inlet to outlet. The volume-of-fluid (VOF) method has been used to numerically investigate the two-phase flow in an anode gas channel of a PEM fuel cell by Ferreira, Falcão [15]. They found that for hydrophilic or hydrophobic channel walls water moves as a film or droplets respectively. Carton, Lawlor [16] also developed a model based on CFD and VOF to investigate water droplet movement and slug formation in PEM fuel cell mini-channels. Kang [17] developed a quasi-three dimensional dynamic model to investigate the transient behaviour and dynamic characteristics of a PEM fuel cell. Xing, Cai [18] developed a 2D model to investigate the effects of relative humidity, stoichiometric flow ratio and channel length, as well as their interactive influence, on the performance of a PEM fuel cell. Salva, Iranzo [19] developed a one dimensional model to investigate the effect of relative humidity on the performance of a PEM fuel cell and validated it using neutron imaging. Abdollahzadeh, Pascoa [20] developed a multi-component mixture model to simulate two phase flow and transport in the cathode gas diffusion layer of a PEM fuel cell.

Liu, Li [21] used a numerical model to optimise flow channel dimensions for best fuel cell performance. The latter model provides a simple example of the inclusion of physical parameters so that the origin of the improved performance is identifiable as a physical entity. In contrast, in empirical modelling the improved performance of a real fuel cell owing to, for instance, a better electrocatalyst, does not directly associate the improvement with its physical origin, since it manifests in the model as parameters that may have no direct physical meaning. Ref. [11], based on empirical equations and requiring high-performance computing, exemplifies this approach.

Generally, a multi-dimensional model is useful, perhaps necessary, in order to understand the detailed behaviour of the individual elements of a fuel cell, electrolyser, *etc.* and to guide the process of designing for enhanced performance. However, to model an entire energy system in this way would be very cumbersome. Thus there is a role for realistic modelling that is not overly computation-intensive, so that a whole-of-system model becomes feasible with commonly available computing resources. A recent comparison of 1D and 3D fuel-cell models by Shekhar [22] concludes that 1D models are useful and cost-effective for practical applications, such as relating fuel-cell performance to the operating and underlying physical parameters.

This paper continues a series in which mutually compatible modular models of the components of an energy system, specifically one incorporating solar-derived hydrogen [23], are presented. One overall objective is to link the suite of component models together to form a whole-of-system model and simulation that can realistically predict the behaviour of a planned energy system, as a prerequisite to specifying the characteristics and capacities (sizes) of its components. Alternatively, such a model can simulate the behaviour of an existing energy system for research and other purposes. The component models are realised in Simulink® and are fully described so they can be recreated and used by others. The first such model [24] is of a PEM electrolyser cell. The next, for the PEM fuel cell, is presented here.

A second very important objective of the work is to use the component models as research tools to predict the effects of influential design parameters, materials and environmental conditions, thus lessening the need for experimentation, which is expensive and time-consuming.

Design parameters are necessarily physical in nature. The key to achieving the second objective is therefore to place the equations that embody the characteristics of the various elements of the electrolyser, fuel cell *etc.* on a proper physical basis by embedding the theory of the underlying physical mechanisms. Doing this has significant advantages. Firstly, it makes the model more generic in its application, in contrast to the present general reliance on empirical equations, with coefficients lacking physical significance, that only describe the characteristics of the particular component under consideration, perhaps with no applicability to the greater class of such components. Secondly, a sound physical basis for the model better allows the effects of changing materials, dimensions *etc.* to be predicted in the quest for enhanced performance, by performing sensitivity analyses, for instance, as was demonstrated in our paper on PEM electrolysers [24].

A third benefit is that a realistic model may be used to diagnose problems in the modelled component or system *via* changes in the fitted parameters arising from, for instance, degradation of an electrode, potentially allowing the degradation to be traced to its physical origin.

An example relevant to both electrolysers and fuel cells is the atomic-level mechanisms that control membrane processes