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Review

A Review on solid oxide fuel cell models

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ABSTRACT

Since the model plays an important role in diagnosing solid oxide fuel cell (SOFC) system, this paper proposes a review of existing SOFC models for model-based diagnosis of SOFC stack and system. Three categories of modelling based on the white-, the black- and the grey-box approaches are introduced. The white-box model includes two types, i.e. physical model and equivalent circuit model based on EIS technique. The black-box model is based on artificial intelligence and its realisation relies mainly on experimental data. The grey-box model is more flexible: it is a physical representation but with some parts being modelled empirically. Validation of models is discussed and a hierarchical modelling approach involving all of three modelling methods is briefly mentioned, which gives an overview of the design for implementing a generic diagnostic tool on SOFC system.

1. Introduction

Fuel cell systems are considered as an alternative to conventional fuel combustion power generation, thanks to their lower emissions and higher efficiency. Amongst various types of fuel cell, solid oxide fuel cell (SOFC) at high temperature operation allows systems design that well uses the fuel cell thermal output, which leads to higher system efficiency than other fuel cell systems such as comparable proton exchange membrane (PEM) fuel cell systems [1]. Due to the importance of efficiency and the need to operate fuel cells at altitude, the hybrid SOFC/gas turbine cycle is a potentially attractive option for applications of auxiliary power unit ofaircraft [1,2] and vehicle as well as for industrial power supply, in stationary and even non-stationary electricity generation applications [3,4]. Besides, SOFCs possess other advantages, i.e.

1. Due to its high temperature operating condition, internal reforming (IR) can be realised;
2. Its insensitivity to gas contaminants enables utilisation of unconventional fuels such as biomass or coal gas;

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Additionally, developers expect commercial SOFCs to have lifetimes of 10–20 years, two to four times longer than other fuel cells [5]. However, the capabilities of IR and gas insensitivity lead to more complex electrochemical reactions inside SOFCs. Moreover, carbon formation thermodynamically can take place on the anode material in hydrocarbon-fuelled case. These disadvantages can make SOFC system suffer from a low reliability. In order to avoid catastrophic system failures, an online diagnostic tool for assessing and tracking the state of health of SOFC stack or/and system is very necessary. Nowadays, the diagnosis technique mainly relies on model-based method [6], by analysing the residuals/deviations of the measured system response from the simulated one by model [7]. Following this diagnostic concept, a reliable and general model which is capable of predicting the normal performance of SOFC is required.

In the past decades, a great number of researchers had investigated in SOFC modelling and the internal process simulation based on physical principles. By using physical and analytical equations, they translated successfully the electrochemical reactions, the electronic and ionic properties of materials as well as gas flow process to detailed physical models. These models range from zero-dimensional (0-D) to three-dimensional (3-D) with different features and point to different research objectives. From the viewpoint of model function, 2-D and 3-D modelling is typically concerned with the cell and stack design issues while 0-D and 1-D modelling is aimed at control purposes (on system-level) such as prediction of both the transient and steady-state performance of fuel cell/stack and establishing the optimal operating conditions [5]. For the research target of setting up an online diagnostic tool, low dimensional models (0- and 1-D) are more appropriate due to the less computational time in comparison with the high dimensional ones (2- and 3-D). Moreover, high dimensional models require information about material properties or electrochemical parameters that are not always available or might be difficult to determine. Even so, high dimensional models are still helpful to learn the operation behaviour of fuel cells of different geometry design and very useful for creating training data for black-box modelling which will be introduced in the fifth section.

Another method is AC impendence modelling. It is based on electrochemical impedance spectroscopy (EIS) measurements. The electrochemical information on an operating fuel cell system can be obtained from the measured EIS data and interpreted by fitting this data to an impedance model. Recently, specific applications of EIS in SOFCs have appeared frequently in the literature. The obtained results demonstrate that this technique is an effective modelling approach. It is worth noting that EIS is a tool used to acquire electrochemical parameters. It is also known as AC impedance technique. When a perturbation signal (voltage or current) is imposed on a SOFC, a corresponding output signal (current or voltage) can be obtained. This signal is the reaction of the SOFC to the perturbation. Comparing these two signals can give a characteristic impedance $Z(\omega)$. In EIS measurement, a series of $Z(\omega)$ in various frequencies are collected. They are supposed to exhibit the SOFC characteristics and should give information on physical behaviours inside the operating fuel cell.

In fact, both physical and equivalent circuit fuel cell models are mainly based on the knowledge of physicochemical characteristics (electrically, chemically and kinematically), thus also called as “white” models. They presents a high generalisability level that enables modelling SOFC stacks of different geometric features, but require a high computational effort. In contrast, there is another approach only based on experimental database (no requirement for any physical property), known as the black-box modelling. Black-box models are developed particularly for control-oriented applications, i.e. system monitoring, online control and diagnosis. This approach is appropriate for complex fuel cell system. Nevertheless, the high dependency upon experimental data makes it less generalisable and the fourth approach is thus developed. It falls in between white and black-box approaches, named grey-box modelling. Models based on this method are partially physical and partially empirical.

In the following 4 sections (from the 2nd to the 5th section), four modelling approaches for SOFC will be introduced by presenting the models available in literature. It is worth noting that all models reviewed in this paper are with the aim of proposing a state-of-the-art of existing models which may be useful for model-based SOFC system diagnosis. In addition, whichever modelling approach to be used, it should be kept in mind that since phenomena occurring in nature are too complex to be completely described by mathematical equations, the required details to be described by the model must be goal-driven, i.e. the complexity of the model, and the related results, must be strictly connected to the main goal of the analysis itself [8]. In the 6th section, the functions of the reviewed models have been summed up and their application on SOFC stack and system diagnosis is proposed. The validation of models is discussed, too.

2. Physical models

A great number of papers can be found on SOFC physical modelling. Some were aimed at cell design modification or material development. In this case, the models involve simulations for the temperature distribution, the heat generation, and the flow diffusion. Others focus on predicting cell performance which is expressed either in term of output current density at fixed potential or in term of potential at given applied current. Research objective determines the complexity and the dimension of model [9,10]. In this paper, the focus is put on general models which depict cell performance for system analysis. The physical models covered in this section are classified into 4 categories on the basis of model dimensionality and will be introduced in the order of dimension decreasing from 3-D to 0-D.

Multi-dimensional (MD) models are set up in the consideration of spatial variation in the physical and chemical variables such as gas concentration, temperature, pressure and current density, for example [8]. In this review, the covered MD models have an identical assumption that the stack is made of repeating single cells stacked together thus a single cell is simulated and its outcome is multiplied by the number of cells to obtain stack results. Such a cell model usually consists of three sub-models, i.e. thermal model, fluid