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Modelling of solid oxide electrolyser cell using extreme learning machine

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ABSTRACT

Solid Oxide Electrolyzer Cell (SOEC) can covert H_2O and/or CO_2 into usable fuel by consuming the excess electricity of renewable resource or off-peak grid power. The SOEC is a promising device for the sustainable development of energy and hydrogen economy. In this work, the steady-state performance of SOEC is tested under different gas compositions and modelled by extreme learning machine (ELM) algorithm. According to the experimental results, the concentrations of H_2O and CO_2 influence the performance of SOEC. For the model, the inputs are the operating voltage and volume percentage of H_2, CO_2, and H_2O, while the output is the performance (current) of SOEC. The obtained model has correlation coefficients of higher than 0.999 and root mean square error less than 0.018, which means that the predicted data by the model well matches the experimental results. Then, the obtained ELM model is used to analyse the performances of SOEC under different concentrations of feedstock. Thus, this data driven ELM model is suitable for many instances of fast modelling for individual group and may be helpful to save the cost, time and effort to build a model for the purpose of performance analysis and system level design.

1. Introduction

For years, environmental concerns causing by the fossil fuel have attracted a lot of attention. The sulfur oxides (SOx), nitrogen oxides (NOx), and carbon dioxide are the biggest contributors to the global emissions. Hydrogen is considered as a leading candidate of energy carrier, which has the potential to reduce the issues of environment [1]. Currently, more and more researchers turn to study the water electrolysis process [2–4]. On the other hand, the CO_2 can be reduced to CO and catalytically converted to hydrocarbon fuels via Fischer Tropsch or methanation reactions [5–7]. These electrolysis processes can be integrated with the existing electric generation system to store surplus power to produce emissions-free hydrogen and synthetic hydrocarbon [8,9].

The solid oxide electrolyzer cell (SOEC) recognized as the reverse operation of solid oxide fuel cell has attracted tremendous attention for these electrolysis processes [10–14], which means that it can handle H_2O electrolysis, CO_2 electrolysis and co-electrolyzing H_2O and CO_2 simultaneously [5,11,15,16]. It has the advantages of a lower electrical energy requirement and without the requirement of expensive catalysts.

Currently, most researches related to SOEC are on materials and understanding the physical–chemical processes by modelling. In the material studies of SOEC, yttria-stabilized zirconia (YSZ) is a popular electrolyte material due to its good ionic conductivity at high temperatures. The hot topics of YSZ are related to the performance, durability and gas tight electrolyte [3,17–22]. While the Ni–YSZ and LSM (lanthanum strontium manganite) – YSZ are the widely used materials for the anode and cathode of SOEC, respectively [18,23–25]. For the modelling studies, Grodin et al. [26] reported a one-dimensional steady state model to predict the cathodic behaviour of Ni–cermet by considering the mass and

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charge conservations and two reaction kinetics. They also analysed the kinetic influences of electrochemical steps on the performance of polarization curves. Narasimhaiah et al. [27] presented a modified Butler–Volmer model for the simulation of CO_2 reduction by considering multi-step single-electron transfer reactions. Laurencin et al. [28] developed a 2D multi-physic model to analyse the performance of SOEC stack. The thermal equilibrium of the stack and parametric studies were carried out. Ni. [2,15,17,29] developed electrochemical model, 1D model and 2D thermal model of SOEC to study H_2O electrolysis, CO_2 electrolysis and H_2O/CO_2 co-electrolysis by considering its heat/mass transfer and chemical/electrochemical reactions. Stempien et al. [30–35] proposed a new model included the effects of operating the electrolyser under the extreme oxygen chemical potential difference. The model was applied to analyse several energy conversion systems, i.e. mitigation of CO_2 emissions, alleviation of renewable energy intermittency, grid balancing and synthetic hydrocarbon fuel production via Fischer-Tropsch fuels. However, these aforementioned models need a lot of physical parameters. Though Some models were built using the parameters of common materials from existing references, with the improvement of materials technology, the parameters of new materials may be different from the existing common parameters and lead to some errors. In addition, it is not easy to obtain the materials' properties under real operating condition. The easily obtained data sets of SOEC during operating are the fuel flow-rate, fuel composition, temperature, voltage and current. These data sets can represent the real performance of a SOEC operating on different conditions, which can be used to develop a data-driven model for the purpose of performance analysis and system design. These data sets can be divided into inputs (e.g. fuel flow-rate, fuel composition, temperature and current) and outputs (e.g. current). Currently, the data-driven models related to SOEC for the fuel compositions, such as H_2O electrolysis, CO_2 electrolysis and H_2O/C_2O co-electrolysis, are rare. Thus, a tool or framework to build a model is proposed and trained with the limited parameters (aforementioned fuel composition only). Definitely, this type of model can be extended to more parameters cared by other different researches.

In this study, data-driven model based on extreme learning machine algorithm is developed to model the performance of SOEC under H_2O electrolysis, CO_2 electrolysis and H_2O/C_2O co-electrolysis processes. The results show that the obtained model is good to represent the SOEC and can be extended to performance analysis and system design.

2. Experiment and modelling methodology

2.1. Experiment

In this study, a button cell of SOEC operating on H_2O electrolysis, CO_2 electrolysis and H_2O/CO_2 co-electrolysis processes were tested and analysed. In the cell, YSZ ($Zr_{0.92}Y_{0.08}O_{2-\delta}$), LSCF-GDC ($La_{0.6}Sr_{0.4}Co_{0.2}Fe_{0.8}O_{3+\delta}/Ce_{0.9}Gd_{0.1}O_{2+\delta}$), Ni-YSZ (Ni-$Zr_{0.92}Y_{0.08}O_{2-\delta}$) were used as electrolyte, positive electrode (cathode) and negative electrode (anode), respectively. The anode also served as the supporting layer of the cell. The thicknesses of the three layers were 10, 50 and 500 micrometres, respectively. The diameter of the active electrode was 0.8 cm. The schematic of the test rig is shown in Fig. 1. The button cell was sealed onto the bottom end of the top ceramic tube (1) by ceramic glue (2). In the tube (1), there was another ceramic tube (3) covered with Pt mesh at the bottom end. The Pt mesh was used as current collector. In the inner tube (3), steam and/or carbon dioxide gas mixed with H_2 were supplied to the cathode side of the SOEC. The presence of H_2 was to prevent the electrode oxidization, especially at low electrolysis current density [36]. The anode side of the cell was exposed to the ambient air with natural gas diffusion via ceramic tube (4). Similarly, there was another fine ceramic tube (5) covered with Pt mesh for current collection. The cell was housed in a temperature controlled furnace to maintain the operating temperature. The main reactions in the cell are also shown in Fig. 1. At the cathode, the supplied gases of H_2O, CO_2, and H_2 are reduced to H_2 and CO via reaction (a)-(b) at the triple-phase-boundary (TPB) of the electrode, while the oxygen ions (O^{2-}) are produced and transported across the ceramic electrolyte to the TPB of the anode electrode. Then oxygen ions lose electrons and form oxygen molecules via reaction (d). At the same time, a reversible chemical reactions named as RWGS may also occur in the cathode chamber via reaction (c). The overall reactions are presented as reaction (e)-(f) [1,15,37].

The SOEC cell was first heated up to operation temperature 800 °C under N_2 condition at a controlled heating rate. Before electrolysis testing, the Ni-based cathode was fully reduced in humidified H_2. Then the cell was tested with ambient air at the positive electrode and H_2 mixed with $H_2O/CO_2/CO_2$-H_2O at the negative electrode. The gas feeding conditions are listed in Table 1. The performance of the button cell was measured at fixed flow-rate of 50 sccm and which was controlled by mass flow controller (MFC, Alicat). After each gas shift, waited for 30 min to ensure stable gas conditions were reached. The polarization curves were measured

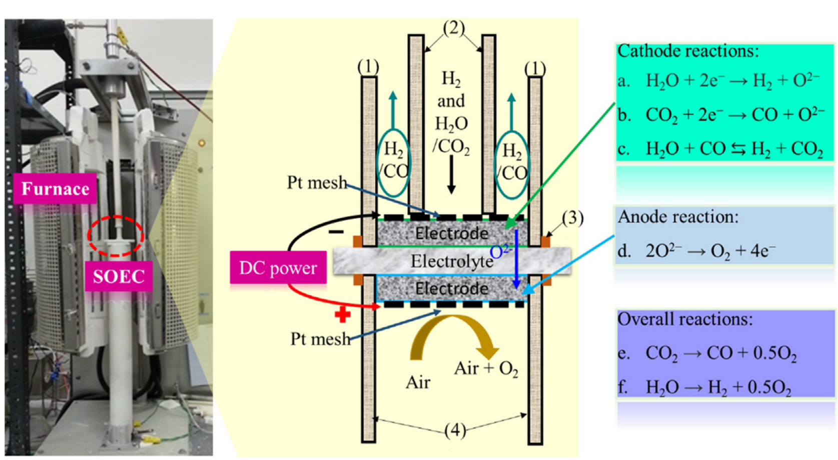

Fig. 1. Test rig and schematic of working mechanism of SOEC.