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Maximizing Hydrogen Production of A Solid Oxide Electrolyser Cell

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Abstract. Hydrogen production using solid oxide electrolyser cells (SOECs) has attracted increasing research interests as it may provide a cost-effective and green route to hydrogen production especially when coupled to a source of renewable or nuclear energy. Developing operation strategies of the SOEC stack corresponding to changes or disturbances that may occur during its operation supports the development and demonstration of this technology. A one-dimensional (1D) dynamic model of a planar SOEC stack developed at Imperial College has been employed to study optimal control strategies. This paper reports some preliminary results on one control strategy to maximize hydrogen production prior to step changes/disturbances. The results offer feasible optimal control pathway for chosen situations and provide a good starting point for identifying the optimal control strategy in practical operation.

Keywords: Hydrogen production, solid oxide electrolyser cell, dynamic model, optimal control

1. Introduction

To ease the crisis of rising energy cost due to the depletion of fossil fuels and to slow the changing of the climate due to the use of fossil fuels, alternative sustainable fuels must be sought. Hydrogen is regarded as a leading candidate for alternative future fuels as it has the potential to address the environmental and energy security issues associated with fossil-derived hydrocarbon fuels. High temperature (500-1000 °C) electrolysis of steam using a solid oxide electrolysis cell (SOEC) is a promising technique to produce hydrogen by offering reduced electrical energy consumption per unit of hydrogen compared to low temperature water electrolysis due to the combination of favourable thermodynamics and kinetics at high temperatures. This approach is particularly advantageous if a high temperature electrolyser may be simply and efficiently coupled to a source of renewable (solar[1], geothermal[2,3], wind[1] or nuclear[4] electrical energies, to produce carbon-free hydrogen.

A planar SOEC consists of a three-layer solid structure (composed of porous cathode, electrolyte and porous anode) and an interconnect plate. Steam is introduced at the cathode side of the solid structure where it is reduced into hydrogen, releasing oxide ions in the process. The oxide ions then migrate through the electrolyte to the anode where they combine to form oxygen molecules, releasing electrons. A number of repeating cells are normally packed into a stack to achieve a sufficient hydrogen production rate. An SOEC stack can function in either exothermic, endothermic or thermoneutral operating modes, resulting from a balance between the thermal energy consumed by the electrolysis reaction and the heat generated due to the irreversible losses in the stack. A change in operating conditions (such as stack temperature, average current density, operating voltage, steam utilisation and the inlet gas composition) can alter the operating mode of the stack. Thermal stress is a major factor to affect the structural reliability and durability of an SOEC stack due to the high operating temperature and the use of ceramic materials (e.g. yttria-stabilized zirconia (YSZ), gadolinium doped ceria (CGO)). Ceramics like those used in SOECs are typically brittle materials exhibiting

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little plasticity and low fracture toughness, and subjected to stresses. During the normal operation of an SOEC, the suppression of temperature gradients or transients can cause excessive stresses within the SOEC components and lead to cell breakdown. Such problem becomes more severe when the operation of the SOEC is integrated with intermittent energy sources whose power production rates change with seasons, months, days, hours etc.

For SOEC technology which is under development, theoretical models are important design tools to predict the response of the system under possible operations and to assist in the optimization of the system performance as well as in the development of operational control strategies. We have developed a one-dimensional distributed dynamic model of a cathode-supported planar SOEC stack, with which some preliminary investigations on the operation of SOECs have been reported[5-9]. The model developed is employed here to identify the optimal control strategies as the SOEC system is opposed to implementing specific controllers, and a parametric window of operating conditions that offers efficient large-scale stack operation.

2. The SOEC Model

To ensure a sufficient rate of H_2 production, an SOEC system must consist of several repeating cells assembled in stacks. Models of such stacks are usually constructed by considering the smallest unit cell, which is assumed to describe the response of the whole stack subject to the use of adequate boundary conditions. Here, the modelled unit cell is considered to be in the centre of a sufficiently large stack, so that end effects are negligible. Although interconnects normally provide the gas flow channels above and below the solid structure, the effect of individual passages is here neglected. The pressure drop along the gas channels is also assumed negligible at the operating pressure of 0.1 MPa. For modelling purposes, the unit cell is considered to consist of four components, the cathode and anode gas streams, the solid structure (which includes the two electrodes – cathode and anode, and electrolyte) and the interconnect. A schematic view of such a unit cell is shown in Figure 1. The cathode stream inlet gas is composed of H_2 and H_2O. The addition of hydrogen in the cathode stream avoids the oxidation of materials that might be induced by using pure steam. On the anode side, air flow is introduced to enable temperature control of the stack.

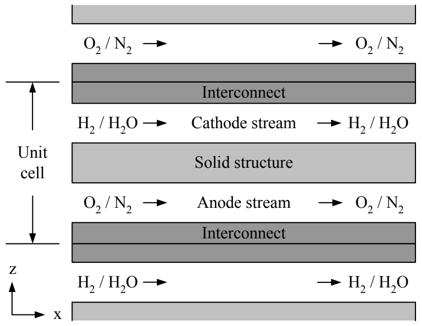

Fig. 1: Schematic view of a unit cell of a planar SOEC stack with the air flow through the anode gas channel. The length of the cell along the *x* direction is 10 cm. The other dimensions of the cell are referred to our previous papers.

The model developed consists of an electrochemical model, mass balances for the gas streams, and energy balances for the cathode and anode streams, solid structure and interconnect. An electrochemical model is used to relate variables such as gas species concentrations, cell component temperatures and average current density to the electrical potential of the cell, which can then be used to calculate the electrical energy consumption. The cell potential corresponds to the sum of the reversible potential and all the irreversible losses that occur as the electrical current is passed through the cell. Such irreversible losses include Ohmic losses, concentration overpotentials and activation overpotentials, which are all partly responsible for the heat produced within the cell.[5,6] Mass balances are solved to predict the evolution of the composition of the cathode stream (i.e. the mixture of H_2 / H_2O) [5], and the anode stream (i.e. the mixture of O_2 and N_2) 20, at each location along the cell[6]. In the energy balances, it is considered that the thermal fluxes between the gas streams and the solid parts of the cell are fully described by convection. The thermal fluxes along the solid parts of the cell are modelled using Fourier's law of heat conduction while radiative heat exchange is taken into account between the solid structure and interconnect. The entire enthalpy change of the reaction is assumed to occur in the solid structure. Air flow is introduced through the anode gas channel to provide the temperature control for an SOEC stack through the manipulation of the air ratio. The inlet air compositions are assumed to be 21 mol % O_2 / 79 mol % N_2. The lower bound and upper bound for the air ratio are selected to be 0.4 and 14 respectively, considering system constraints[7].

The optimal control strategy aims to maximize hydrogen production, with both– piecewise constant and piecewise linear parameter controllers applied. In the optimal control situations considered, a change in operating regime, namely an increase in the average current density from 1000 to 7000 A/m^2, must be effected over a time horizon of 3000 seconds. A path constraint is imposed on the overall temperature gradient (calculated as the difference between the outlet temperature and the inlet temperature of the cathode stream) across the cell, which must not be larger than 100 K, to avoid thermal excursion of the materials.[7]

The system of partial differential and algebraic equations is solved via the finite difference method using gPROMS Model Builder 3.3.1. Parameters such as cell geometry, material properties, thermal properties and operating conditions need to be specified as model input. The detailed description of the model is provided in our previous papers.[5-9] The model input parameters and operating conditions are the same as those given in Table 3 of our previous paper,[5] except that in this paper the operating temperature is 1073 K and the average current density is seen as a disturbance and thus a control variable varying between 7000 and 1000 A/m^2.

3. Results and Discussions

Before starting an optimization process, the steady state performance of the SOEC at 1073 K is investigated. As shown in Fig. 2, the cathode stream temperature decreases along the cell from the inlet (normalised position x=0) to the outlet (x=1, corresponding to a length of 10 cm), featuring endothermic operation. When operating at 1000 A/m^2 with a minimum air ratio of 0.4, the temperature gradient between the inlet and the outlet is about 164 K , which exceeds the maximum temperature gradient of 100 K allowed for a 10 cm cell, and thus puts the cell in danger of breakdown. Air ratio is increased to 5.26 to control the temperature down, giving a temperature gradient of 94 K. At current density of 7000 A/m^2, the cell features a temperature gradient of 47.4 K along the cell with a minimum air ratio of 0.4, indicating that there is no need to increase the air ratio for temperature control.

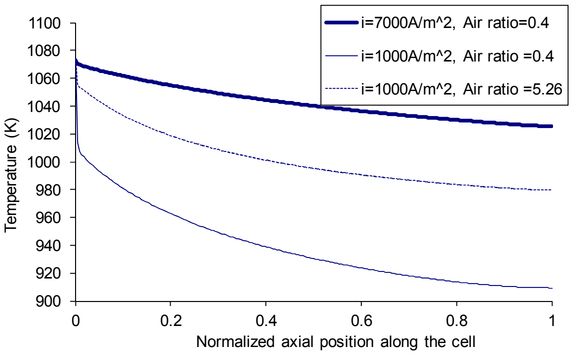

Fig. 2: Cathode stream temperature distribution along the cell at average current density of 7000 A/m^2 (thick lines) and 1000 A/m^2 (thin lines) when the inlet temperature is 1073 K.

Fig. 3 shows the optimal pathway for cumulative hydrogen production. The optimal pathways using both piecewise constant and piecewise linear controllers are almost identical – the amount of hydrogen produced is increasing almost linearly with time and the cumulative amount of hydrogen produced at the given time horizon 3000s is 55.54 moles. From the slope of the graph in Fig. 3, one can determine the rate of production of hydrogen at the cathode stream. It is clearly expected that hydrogen production rate increases with an increase in the average current density. The hydrogen production rate is at maximum when average current density is at 7000 A/m^2 and at minimum when average current density is at 1000 A/m^2. Hence, it is favourable to operate the SOEC stack at the high average current density for the longest possible period of time and the ideal case will be that the stack operates for 3000 seconds at 7000 A/m^2. As shown in Fig. 4, the two optimal controllers increase the operating current density from 1000 to 7000 A/m^2 within the first one

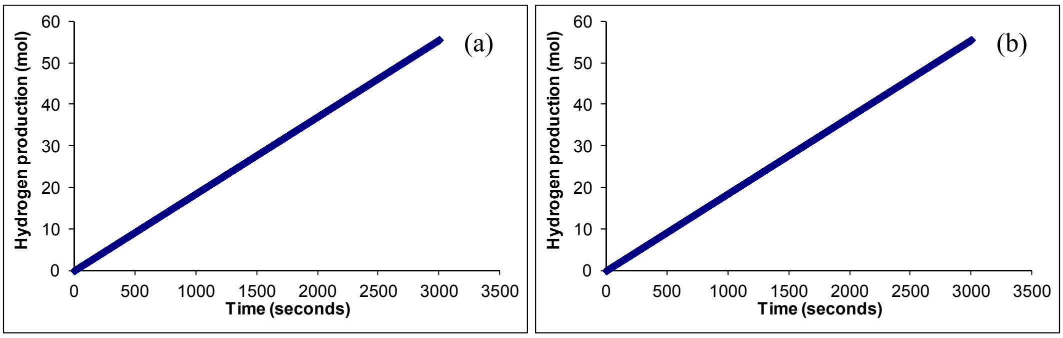

Fig. 3: The optimal control pathway for cumulative hydrogen production using (a) piece wise constant control and (b) piece wise linear control.

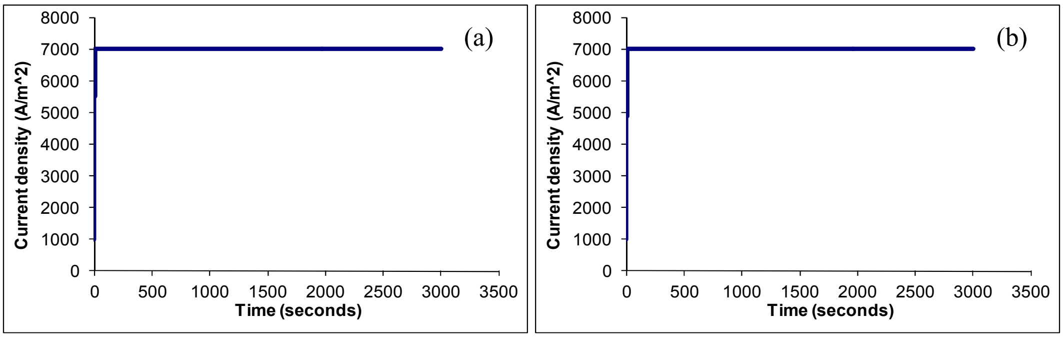

Fig. 4: The optimal control pathway of average current density using (a) piece wise constant control and (b) piece wise linear control.

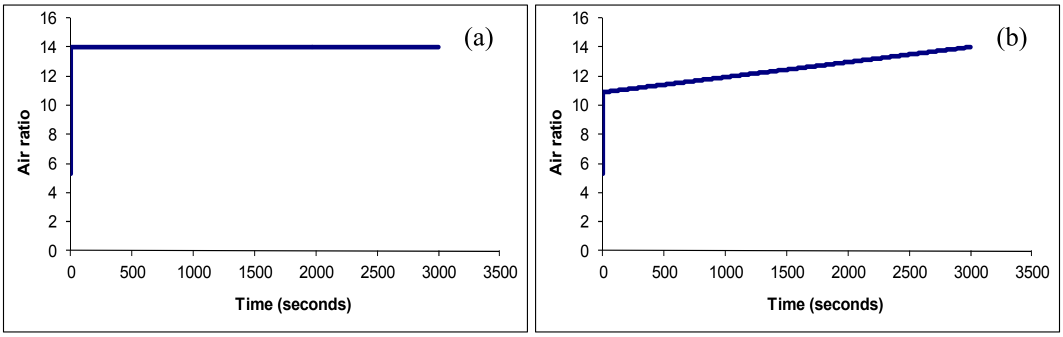

Fig. 5: The optimal control pathway of air ratio for maximising hydrogen production using (a) piece wise constant control and (b) piece wise linear control.

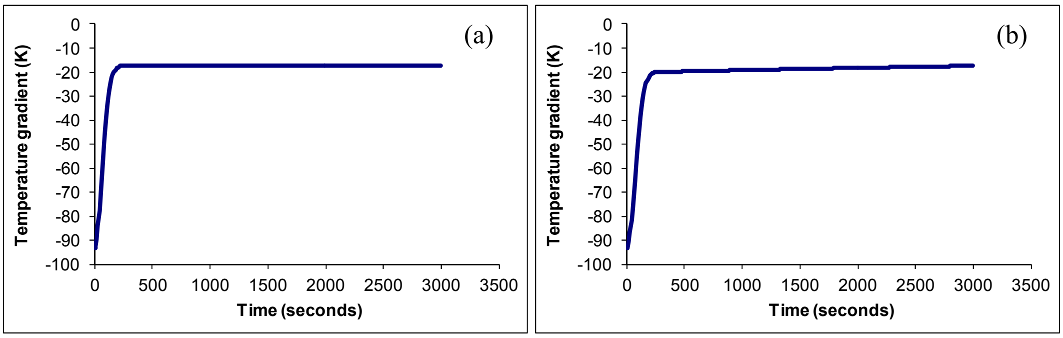

Fig. 6: The optimal control pathway of temperature gradient for maximising hydrogen production using (a) piece wise constant control and (b) piece wise linear control.

second and operate at 7000A/m^2 constantly till the end of 3000 seconds. As the current density increases, the air flow rate increases. The two parameter controllers give slightly different optimal control pathways for air ratio; an instant step increase in air ratio from 0.4 to 14 is made at the beginning of the control period by piecewise constant control (as shown in Fig.5 (a)) and a gradual increase from 0.4 to 14 is made by piecewise linear control over the entire 3000 seconds (as shown in Fig.5 (b)). As a result of increasing air ratio, the optimal pathway for temperature gradient cross the cell shows a decrease in the absolute value of the temperature gradient from 93 K to 17 K, as shown in Fig.6 (a) and (b). Similar trend is observed for both piecewise constant control and piecewise linear control. In both control conditions, one would expect that an air ratio to 5.26 would be enough to satisfy the temperature constraint when operating at current density of 1000 A/m^2, and the air ratio would decrease when the operating current density increase to 7000 A/m^2, from the steady state performance shown in Fig.2. However, air ratio decides to increase when current density increases and the upper bound value of 14 is seen. In practice, there is a penalty to the system efficiency when increasing the air flow rate. Further investigations will be done to examine how the optimal control will respond when such a penalty is applied to the model.

4. Conclusions

A one-dimensional distributed dynamic model of a cathode-supported planar SOEC stack has been employed to study one optimal control strategy of maximizing hydrogen production using two parameter controllers – piecewise constant and piecewise linear. Step changes in the operating current density from 1000 A/m^2 to 7000 A/m^2 are allowed. The optimal control trajectories show feasible control. The maximum amount of hydrogen produced for a single cell over 3000 seconds is 55.54 mols. The two parameter controllers show similar optimal pathways for cumulative hydrogen production, current density and temperature gradient, with slightly different pathways for air ratio.

5. Acknowledgements

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