SOFC PERFORMANCE UNDER VARIOUS GASIFIER COMPOSITIONS USING AN ELECTRO-THERMAL MODEL

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ABSTRACT

An electrochemical-thermal model has been developed to simulate the performance of a solid oxide fuel cell under different operating conditions. Temperature, current, gas distribution and fuel utilization were calculated with the model in the different regions of interest for a co-flow configuration. In addition, the model developed was used to investigate the optimal operating conditions under different gasifier compositions. The model was successfully used to identify the principal operating conditions that affected the performance of the fuel cell.

INTRODUCTION

The main advantage of solid oxide fuel cells (SOFC) is the high operating temperature (600–1000°C). This allows the use of fuels (e.g. methane, and carbon monoxide) that otherwise will contaminate the membrane. In addition, the hot depleted products from the fuel cell (hydrogen and water) can be used in cogeneration applications or bottoming cycles. These characteristics make SOFCs very attractive for stationary applications and in particular for integrated systems (1,2). The Energy & Environmental Research Center at the University of North Dakota (EERC) has designed a thermally integrated biomass gasification system with a SOFC (3). The hot effluent gases from the gasifier (producer gas) will be fed into the SOFC (without further processing); See Fig. 1 for a schematic of the system. The depleted fuel and products from the fuel cell will be combusted and re-injected to the gasifier’s pyrolysis zone. Because SOFCs show a high tolerance to tars and carbon deposition (4,5) no cleanup system will be required for the producer gas and a substantial reduction in costs is expected of such integration (Gasifier-SOFC). However, in order to optimize the efficiency of the SOFC unit it is important to analyze its response under the different gasifier compositions. This paper presents the results of the use of an electrochemical-thermal model for determining the performance of the cell under different gasifier compositions for a co-flow array with two different membranes (i.e., anode-supported and electrolyte-supported).

ELECTRO-THERMAL MODEL

The model is based on the unit-cell approach for a conventional co-flow design. Three modules that solve the material balances, the energy balances and the electrochemical relations along the fuel cell channels integrate the model (6). The model was developed for the different fuels present in the gasifier output (i.e. hydrogen, methane, carbon
The model was validated using a benchmark developed by the International Energy Agency (IEA) for the modeling and evaluation of advanced SOFC systems (7).

The material module considers hydrogen as the only electrochemical active fuel [1]. The model assumes that methane will be internally reformed into carbon monoxide and hydrogen [2] and that the water-gas shift reaction [3] is always in equilibrium (8):

\[ H_2 + \frac{1}{2}O_2 \rightarrow H_2O \]  \[ CH_4 + H_2O \rightarrow CO + 2H_2 \]  \[ CO + H_2O \rightarrow CO_2 + H_2 \]

The thermal module follows the treatment proposed by Motloch (9). Only convection and conduction was included, but radiation is planned to be included in a future model according to the results reported by Murthy and Fedorov (10).

The electrochemical module determines the I-V characteristics of the cell based on the Butler-Volmer equation (activation polarization), the dusty gas model (concentration polarization), and Ohm’s law (ohmic polarization). The details of this module are presented elsewhere (11).

The electrochemical model is used in Fig. 2 to show the IV-characteristics for a conventional SOFC operated at 80% of fuel utilization (μf).

Figure 1. Schematic of a downdraft gasifier thermally integrated with a solid oxide fuel cell.
Figure 2. IV-characteristic for a conventional SOFC operated at 80% of fuel utilization.

The model was implemented with Mathematica. A set of sixteen non-linear equations was solved simultaneously for each unit cell along the gas channels. The input variables to the model are: inlet temperature, inlet gas composition, pressure and either voltage or current density. The model outputs are: temperature profiles in the regions of interest (i.e., electrodes, electrolyte, and gas channels), gas and current density (voltage) distribution through the gas channels. From these results, the power density, fuel utilization and efficiency of the single cell were determined.

In the following section, the integrated model (electrochemical+thermal+material modules) was used to predict the performance of the fuel cell under different gasifier conditions.

RESULTS

A downdraft gasifier was thermally integrated with the SOFC. One of the main advantages of downdraft gasifier is the low percentage of tars in the producer gas (12,13). A low concentration of tar reduces the risk of carbon deposition in the SOFC (4,5). The producer gas composition depends upon the amount of moisture in the biomass feed. Accordingly, software was used to simulate a set of gasifier compositions at different biomass moisture contents (3,14) for woody biomass CH1.4O0.59N0.017 with ash content of 0.10–1.0 wt% and sulfur content of 0.00–0.02 wt%. Six moisture concentrations, from 0–50 wt% were used. These compositions (Table I), labeled with letters (A–F), are representative of a wide range of output conditions, i.e., high initial concentration of carbon monoxide combined with low initial concentration of water, high initial concentration of hydrogen under high and low initial concentrations of carbon monoxide, and low initial concentration of hydrogen under high and low initial concentrations of carbon monoxide. The response of the fuel cell using methane was presented elsewhere (6).
Table I. Gasifier's expected gas compositions based on the moisture content of the biomasses.

| Moisture wt% | A: 0 | B: 10 | C: 20 | D: 30 | E: 40 | F: 50 |
|--------------|------|-------|-------|-------|-------|-------|
| CO           | 40.0 | 40.0  | 44.0  | 42.0  | 34.0  | 26.0  |
| H₂           | 26.5 | 33.0  | 50.0  | 52.0  | 49.0  | 45.0  |
| CH₄          | 0.0  | 0.0   | 0.3   | 0.0   | 0.0   | 0.0   |
| CO₂          | 0.0  | 1.0   | 0.5   | 2.0   | 5.0   | 7.0   |
| H₂O          | 1.5  | 1.5   | 1.5   | 4.0   | 12.0  | 21.0  |
| N₂           | 32.0 | 24.5  | 0.0   | 0.0   | 0.0   | 0.0   |

The integrated model was used to calculate the performance of the cell at the gasifier conditions reported in Table I. In all calculations the operating conditions were 900°C initial temperature, 1 atm of pressure and operating voltage of 0.65 volts. In Fig. 3 the current density distribution for the six compositions (A–F) is presented for an anode-supported (A-S) and electrolyte-supported (E-S) membrane. The mean current density (Fig. 3, Mean) corresponds to the average value of the local current density along the gas channels. The maximum current density and minimum current density correspond to the local maximum and minimum value of the current density distribution.

Figure 3. Current density for six compositions (according to Table I) and two membranes i.e., anode supported (A-S) and electrolyte supported (E-S).

In Fig. 4 the mean temperature and the maximum temperature is presented for both membranes. The temperature distribution in the graphs corresponds to the cell temperature, which was calculated from the average of the temperature in the electrodes and electrolyte regions of the cell.

The fuel utilization (μf) of the system is reported in Fig. 5 for both membranes and the six gasifier compositions. It was calculated taking into account the depletion of hydrogen and carbon monoxide.
DISCUSSION

Figure 5 shows that the best performance (using the $\mu_f$ as indicator) was obtained for composition E (Table I) for both membranes. However, composition F showed the highest value of mean current density (Fig. 3). For a conventional fuel cell, the current density in the cell is calculated by taking the average of the current density distribution over the entire cell. A high current density translates into a smaller cell for generation of equivalent power and also minimizes the chance of carbon formation. Both, composition E and F, showed the highest values of maximum temperature ($\approx 1011°C$, Fig. 4) which is considered a disadvantage because higher temperatures in the cell result in a greater
thermal stress for the fuel cell components. Compositions C and D, on the other hand, showed high values of fuel utilization (comparable to compositions E and F) but a lower value of maximum temperature. Therefore, in terms of stability of the cell, compositions C and D would be better because of the lower temperature at the end of the channels without sacrificing fuel utilization; typically a fuel utilization of 80% is considered the optimum between performance, stability and costs. In addition the depleted fuel is not wasted because it is combusted and the heat re-injected to gasifier. Unfortunately, composition C had a minimum value of current density that could favor the formation of carbon in the cell (Fig. 3). In summary, compositions D, E and F for both membranes showed better performance (in terms of high fuel utilization, high mean current density and low maximum temperature).

The reason why these three compositions (i.e., D, E, and F) showed the best overall performance is because of the high concentration of hydrogen in the initial composition (≈ 50%), which is directly related to the amount of current produced (electrochemical reaction). In addition, these compositions showed a high steam-to-carbon ratio (S/C), which helps to promote a better water-gas shift reaction at the entrance of the cell. Accordingly, although the initial hydrogen concentration of compositions D, E was higher than F, a better S/C ratio in the initial concentration of composition F possibly contributed to increase the amount of hydrogen at the entrance of the cell, hence composition F showed a higher mean current density. Compositions A and B showed the lowest performance among the six compositions analyzed. This is a consequence of the low initial concentration of hydrogen. Furthermore, high concentration of carbon monoxide with low concentration of steam in the initial compositions imposes the risk of carbon formation. The analysis of carbon deposition at these conditions plus a small amount of tars content was studied by Singh et al. (5). Singh used the method of minimization of the Gibbs free energy in order to find equilibrium curves of 32 species in gaseous phase and one in a condensed phase. For composition A (assuming 1% of tars) the threshold current density was located at about 850 A m⁻² (Fig. 6); below this threshold value carbon will be formed in the cell. Because the minimum current density for composition A was 399 A m⁻², carbon deposition could develop under these conditions. Table II shows the threshold current density for compositions A, B, and C and the minimum current density from the model results. As shown in Table II all three compositions could potentially favor the formation of carbon in the cell because their minimum current densities (Fig. 3) are below the threshold current density. Fortunately, as the electrochemical reaction proceeds the steam formed in the cell (overall oxidation reaction) can reverse the formation of carbon.

Table II. Carbon formation at 900°C and 1% tars. TCD: Threshold current density, MCD: minimum current density (according to Fig. 3 A-S); NA indicates the threshold current density was minimum than the range analyzed.

| Indicator | A (A m⁻²) | B | C | D | E | F |
|-----------|-----------|---|---|---|---|---|
| TCD       | 860       | 740 | 780 | 380 | NA | NA |
| MCD       | 399       | 697 | 624 | 1535 | 1729 | 2076 |

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FINAL REMARKS

An electro-thermal model has been used to identify the optimal gasifier compositions for a biomass gasification-SOFC integrated system. The results showed that the performance of the cell is influenced by the initial concentration of hydrogen and the relation between the concentrations of carbon monoxide and water (steam to carbon ratio). A high initial concentration of carbon monoxide combined with a low initial concentration of water (low S/C ratio) promotes the risk of carbon formation at the entrance of the gas channels. Compositions with a higher steam to carbon ratio showed a minimum current density above the threshold current density and therefore carbon formation is not expected. In general, the best overall performance was obtained for compositions D, E and F based on high fuel utilization and high current density. However, composition D would be more stable because a lower maximum temperature is expected at the end of the channels.

This paper showed the usefulness of an electro-thermal model designed for a SOFC in determining the best operational conditions when integrated with a biomass gasification system.

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REFERENCES

1. B. Zhu, X. Y. Bai, G.X. Chen, W. M. Yi, and M. Bursell, International Journal of Energy Research, 26, 57–66, (2002).

2. T. Mäkinen, J. Leppälathi, E. Kurkela, and Y. Solantausa, in 8th European Conference on Biomass for Energy, Environment, Agriculture and Industry, pp. 1784–1790, Agence de l’Environnement et de la Maîtrise de l’Énergie, (1994).

3. P. N. Hutton, M. A. Musich, N. Patel, D. D. Schmidt, and R. C. Timpe, Feasibility Study of a Thermally Integrated SOFC-gasification System for Biomass Power Generation, Interim Report, No. DE-FC26-98FT40321, Energy & Environmental Research Center-University of North Dakota, (2003).

4. Devinder Singh, Tolerance of Solid Oxide Fuel Cells to Tars, Master’s thesis, University of North Dakota, (2004).

5. D. Singh, E. Hernandez-Pacheco, P. N. Hutton, N. Patel, and M. D. Mann, Journal of Power Sources, in Press, (2004).

6. Eduardo Hernandez-Pacheco, Electro-Thermal model for a Solid Oxide Fuel Cell, Ph. D. thesis, University of North Dakota, (2004).

7. E. Achenbach, SOFC Stack Modeling, Final report of activity A2, annex II, in Modelling and Evaluation of Advanced Solid Oxide Fuel Cells. International Energy Agency Programme on R, D & D on Advanced Fuel Cells, (1996).

8. Robert J. Braun. Optimal Design and Operation of Solid Oxide Fuel Cell Systems for Small-Scale Stationary Applications. Ph. D. thesis, University of Wisconsin-Madison, (2002).

9. Chester George Motloch. Thermochemical Modeling and Performance of a Methane Reforming Solid Oxide Fuel Cell, Ph. D. thesis, Idaho State University, (1998).

10. S. Murthy and A. G. Fedorov, Journal of Power Sources, 124, 453–458 (2003).

11. E. Hernandez-Pacheco, D. Sing, P. N. Hutton, N. Patel, and M. D. Mann, Journal of Power Sources, 138(1-2), 174–186 (2004).

12. T. A. Milne, N. Abatzoglou and R. J. Evans, Biomass Gasifier Tars: Their Nature, Formation and Conversion, Technical Report NREL/TP-570-25357, National Renewable Energy Laboratory, (1998).

13. Z. A. Zainal, Ali Rifau, G. A. Quadir, and K. N. Seetharamu, Biomass and Bioenergy, 23, 283–289 (2002).

14. S. Gordon and B. J. McBride, Computer Program for Calculation of Complex Chemical Equilibrium Composition, Rocket Performance, Incident and Reflected Shocks and Chapman-Jouguet Detonations, Technical report, NASA SP-273, (1971).