Performance Investigation of Fuel Cell Models and Systems

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Abstract – **High temperature fuel cells such as the solid oxide fuel cell (SOFC) are considered extremely suitable for electrical power plant application. In order to better understand the thermodynamics of fuel cell and cycle's co-flow planar SOFC model are built in Aspen Custom Modeller for the externally reformed (ER) SOFC and internally reformed (IR) SOFC. These models are integrated in Aspen Plus^{TM} as externally and internally reformed SOFC systems. In this article the influence of the steam carbon ratio (S/C) on the performance of a Solid Oxide Fuel Cell System is investigated. The simulation results show that, the cell voltage and net efficiency of both SOFC are higher in case of S/C=2 compared to S/C=3.56 . So lowering steam-carbon ratio is advantageous for the SOFC cycle. Moreover, the cycle with internal reforming gives better efficiency than the cycle with external reforming.**

Keywords: SOFC **,gas turbine, Analysis.**

I. Introduction

Fuel cells are electrochemical energy conversion devices which typically run on hydrogen or methane and produce electricity, heat and benign emissions (water and, in the case of methane and methanol, CO_2). The fuel cells used for stationary energy production are typically high temperature fuel cells (HTFCs) such as solid oxide fuel cell (SOFC).
The SOFC is one of the fuel cells of which the concept is proven and several of them are in operation [1-6].

In previously paper [7], the SOFC performances are investigated using models which are built in Aspen soft wear, and it introduces a new simulation software, which is called Al-Nour V.1.0-2012 software application. The interface of Al-Nour V.1.0-2012 software was mainly implemented based on the educational theory of User's Split Attention, that is; the entire software works with only one screen for all the operations without any scrolling (user-friendly interface), this application reflects the fact that Al-Nour software does not require the user to has any previous training. In the power cycles [4 and 5] hydrogen can be produced by reforming natural gas in a reformer which is fed with steam produced with waste heat available in the cycle. This is called external reforming (ER). Due to the high temperature in the SOFC and the water production during the electrochemical reaction, SOFCs can allow for internal reforming (IR). This means that natural gas is directly fed into the fuel cell, where it will convert to hydrogen. The heat necessary for this reforming reaction is delivered by the electrochemical reaction in the cell.

In this paper a thermodynamic model for an SOFC is developed in Aspen Customer Modeller and then integrated in Aspen Plus^{TM} to be able to study the performance of IR and ER reformed SOFC cycles. Moreover, the influence of the steam carbon ratio on the performance of SOFC mode and cycles can be evaluated.

II. SOFC Systems Description

Solid oxide fuel cells are considered to be high temperature cells, having an operation temperature lying between 800 °C and 1000 °C [1]. The cells currently in operation are fuelled with natural gas. In order to provide the cell with the necessary hydrogen gas, the methane is converted to hydrogen in a reformer prior to introduction of the fuel to the cell. Steam is used to reform CH_4 to H_2 according to eq. (5). Heat for the reaction is coming from the combustor. The high temperatures inside the cell stack also make it possible to reform the methane directly inside the cell if steam is provided at the inlet. The heat necessary for this reforming reaction is delivered by the electrochemical reaction in the cell.

The SOFC systems considered in this work are externally reformed ER-SOFC and internally reformed IR-SOFC systems. The different cell types have different internal chemical reaction schemes which are discussed further in the paper. The different cells also need different configurations of surrounding heat exchangers, pre-heater and compressors. In this paper two typical configurations are compared, looking from the same point of view.

The fuel cell is integrated into a system, containing the necessary compressors and heat exchangers for providing fuel and steam, reforming, and heat recovery. A combustor is added delivering heat for reforming. A turbine recovers energy in the exhaust. Fuel is provided at atmospheric conditions. The fuel is pure methane (CH_4). The fuel mass flow rate being burned in the combustor is varied. Steam for reforming is produced at 4 bar and temperature depending on the operational condition of the fuel cell. The fuel cell systems are simulated in two ways. Firstly the performance with varying steam to carbon ratio of both SOFC systems is analysed for a current density of 150 mA/cm^2 and corresponding fuel utilisation of 0.7. Secondly the load is varied by lowering the current density to 107mA/cm^2. This means that the fuel utilisation or the fuel flow rate decreases. The characteristics of the fuel cell system are given in Table I. Pressure is kept constant at 4 bar. The cathode inlet temperature is controlled to be 800 °C.

A. IR-SOFC System

In the IR-SOFC system, water and methane are admitted into the heat exchangers H/E2 and H/E3 to generate steam and to preheat the methane (Fig. 1.). The pre-heated methane is mixed with steam. The mixture passes to the pre-heater, where it is heated to a given temperature, and then enters into the anode side in the stack, see Fig .1. The remaining anode and cathode gases are recycled to the combustor. Part of the heat released in the combustor (stream 2) is used in the pre-heater; the remaining heat is used to heat up the burned gas. This burned gas from the combustor passes to five heat exchangers H/E1, H/E2, H/E3, H/E4, and H/E5 respectively. In three of these heat exchangers the hot effluent of burned gas releases the heat necessary to preheat the cathode inlet gases, generate steam, and preheat the methane.

The combustor exit gas which contains a large portion of H_2O, enters into the flash tank at 4 bar, 30 °C. In the flash tank the combustor exit gas is separated into water and remaining gas. Part of this water is supplied to the heat exchanger H/E6. The remaining combustor exit gas is supplied to the heat exchangers H/E4, H/E8, turbine and heat exchanger (H/E6) respectively. The combustor exit gas expands at the turbine to generate additional power. Part of the compressed air from the compressor (COMP2) is supplied to the heat exchanger (H/E7).The air coming from the H/E7 is further heated to 800°C at (H/E1) before it flows into the cathode side of the stack.

The boundary conditions for all the heat exchangers are summarised in Table II.

B. ER-SOFC System

The ER-SOFC system is similar to the IR-SOFC system (Fig.1), except that instead of the pre-heater in the IR-SOFC system there is a methane steam reformer. In this case the pre-heated methane and steam are fed to the reformer, where hydrogen, carbon dioxide and carbon monoxide are produced. This hydrogen-rich gas is used as fuel at the anode of stack.

III. FUEL CELL STACK MODEL

The model of the stack used in this paper is based on an existing isothermal SOFC Co-flow model [3]. It is extended in a way that both externally and internally reformed cells can be simulated. The model divides the cell over the length of the gases flow path and solos the energy performance for each part.

IV. ANALYSIS

In both models the chemical reactions are assumed to be in equilibrium. This means that the reactions occur instantaneously and reach the equilibrium condition spontaneously at each position. For both models the electrochemical reaction and water gas shift reaction are implemented:

$$\tfrac{1}{2}O_2 + 2e^- \rightarrow O^{2-} \quad \text{cathode} \tag{1}$$

$$H_2 + O^{2-} \rightarrow H_2O + 2e^- \quad \text{anode} \tag{2}$$

$$H_2 + \tfrac{1}{2}O_2 \rightarrow H_2O \quad \text{overall reaction} \tag{3}$$

$$CO + H_2O \Leftrightarrow CO_2 + H_2 \quad \text{gas shift} \tag{4}$$

For the IR-SOFC an additional reaction equation is taken into account for the fuel reforming

$$CH_4 + H_2O \Leftrightarrow CO + 3H_2 \tag{5}$$

The steam-carbon ratio is defined as the ratio between the mole flow rate of steam and the CH4 mole flow rate to the anode.

$$S/C = \frac{\dot{n}_{H_2O}}{\dot{n}_{CH_4}} \tag{6}$$

The fuel utilisation factor is defined by

$$u_f = \frac{\dot{n}_{H_2 consumed}}{\dot{n}_{H_2 in} + \dot{n}_{CO in} + 4\dot{n}_{CH_4 in}} \tag{7}$$

The Nernst voltage is defined by

$$V_{eq}(u) = E_0 + \frac{RT_{cell}}{2F}\ln\left(\frac{p_{H_2} p_{O_2}^{1/2}}{p_{H_2O}}\right) \tag{8}$$

The gross system efficiency (η_{gross}) is defined as the ratio of power produced by the fuel cell to the lower heating value (LHV) of the total amount of fuel ($Q_{tot} = m_{tot} * LHV$) supplied to the system.

$$\eta_{gross} = \frac{P_{el}}{Q_{tot}} \tag{9}$$

Where m_{tot} is the sum of the mass flow rate of CH_4 supplied to the fuel cell and to the combustor.

The net system efficiency (η_{net}) is defined as the ratio of the power produced by the fuel cell and the turbine, minus compressors power, to the (LHV) of the total amount of fuel (Q_{tot}) supplied to the system.

$$\eta_{net} = \frac{P_{el} - P_{comp} + P_{turb}}{Q_{tot}} \tag{10}$$

TABLE 1. INPUT PARAMETERS OF THE SOFC SYSTEMS.

Fuel cell	
A_{cell}	250 m^2
S/C ratio	0.5, 2 and 3.56
P	4 bar
u_f	50 and 70%
m_{CH4}	28.7 and 40 kg/hr
m_{cathode}	5000 kg/hr
T_{cathode}	800 °C
other devices	
λ (air factor)combustor	1.1
η for compressor	0.8
η for turbine	0.85
T_{react} combustor	900 °C

TABLE 2. THE BOUNDARY CONDITIONS FOR ALL THE HEAT EXCHANGERS OF THE SOFC SYSTEMS.

Heat exchanger	Specification	Value
H/E1	Cold stream outlet temperature	800 °C
H/E2 and H/E3	Hot inlet cold outlet temperature difference	50 °C
H/E4 and H/E6	Hot inlet cold outlet temperature difference	10 °C
H/E5	Hot stream outlet temperature	30 °C
H/E7	Hot outlet cold inlet temperature difference	10 °C
H/E8	Hot stream outlet temperature	750 °C

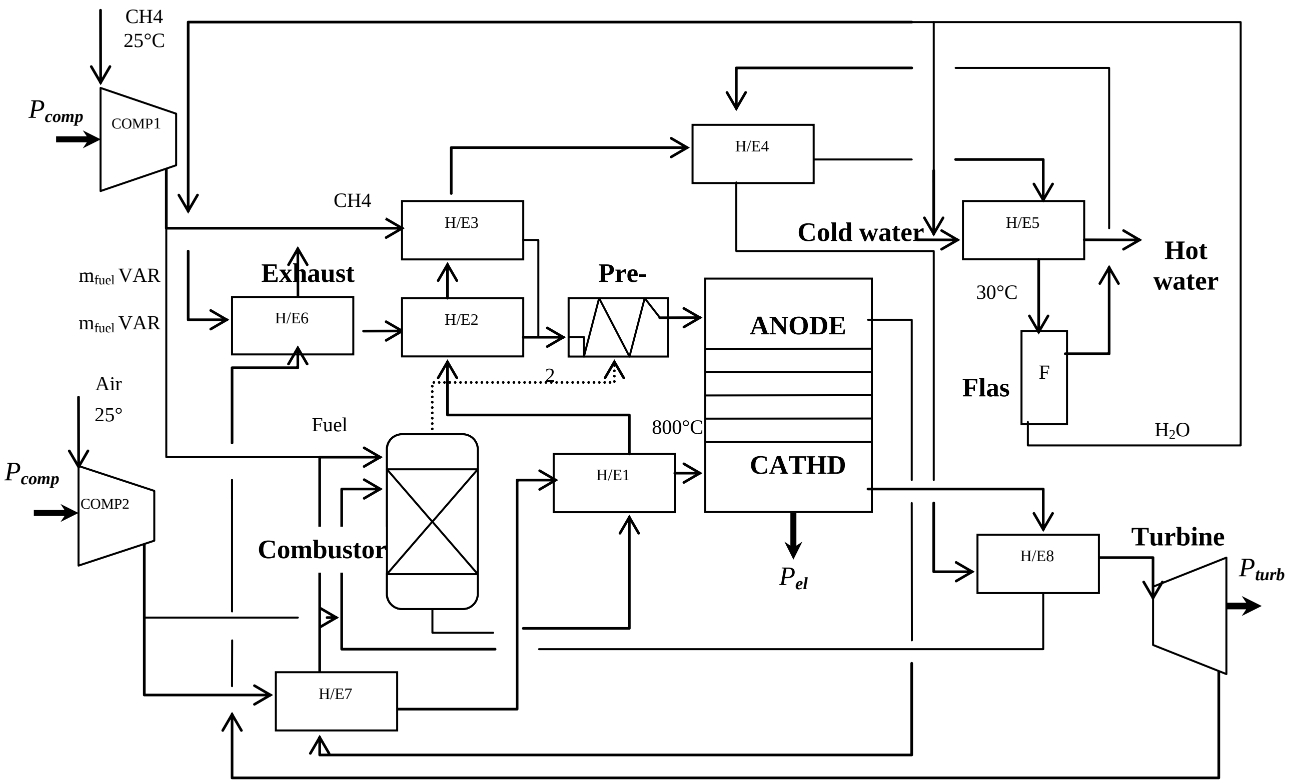

Figure 1: Schematic diagram of internal reformed SOFC system (COMP: compressor; H/E: heat exchanger).

V. RESULTS AND DISSCUSION

For all the fuel configurations studied the operating temperature of SOFC systems is varied. Aspen Plus^{TM} *Design-spec* function [4] is used to vary the fuel burnt in the combustor to control the temperature of anode gas inlet. In the IR-SOFC system simulations the gas temperature at the anode inlet will be varied in a range between 940°C and 1360°C. In ER-SOFC system simulations the gas temperature at the anode inlet will be varied in a range between 910°C and 1310°C. In these two ranges of the gas temperature at the anode inlet the operating temperature in both SOFC systems will range between 850°C and 950°C.

In a first paragraph the performance with varying steam to carbon ratio of both SOFC systems is analysed for a current density of 150 mA/cm^2 and corresponding fuel utilisation of 0.7. Secondly the load is varied by lowering the current density to 107mA/cm^2. This means that either the corresponding fuel utilisation is lowered to 0.5 or the fuel flow rate is lowered from 40 kg/hr to 28.7 kg/hr.

A. Performance of the SOFC in case of current density (150 mA/cm^2)

Figure 2 shows the effect of decreasing the steam-carbon ratio on the cell voltage of the SOFC. The ER-SOFC has a higher cell potential than the IR- SOFC in case of steam-carbon ratio 2 and 3.56. This is caused by the difference in H_2 concentration in the two cell types if for both cells the steam flow rate is kept constant. In the IR- SOFC there is always CH_4 present in the cell, resulting in a lower partial pressure of H_2 in the cell. From equation (8) follows that a reduction in partial pressure of H_2 results in a reduction of the V_{eq}.

As operating temperature goes up in both cases the cell voltage goes up. This is mainly caused by the reduction of the cell ohmic and polarization resistance with rising temperature. By decreasing the steam-carbon ratio, the cell voltage goes up. For both SOFC cells reducing the steam-carbon ratio results in a lower H_2O flow rate going into the cell. Looking again at eq. (8), this causes a raise in cell voltage.

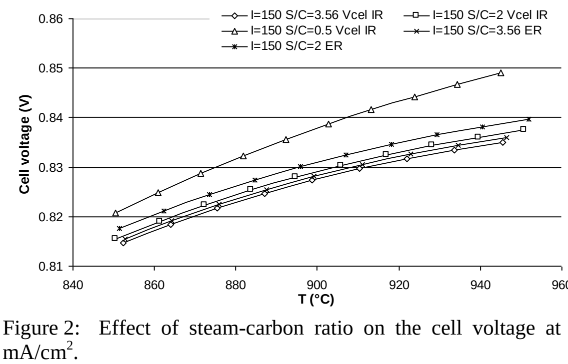

Figure 2: Effect of steam-carbon ratio on the cell voltage at I=150 mA/cm^2.

Figure 3 shows the CH_4 concentration in the outlet of the anode. By decreasing the steam-carbon ratio the CH_4 concentration curves moves upwards.

This means an increase in the mass flow rate of steam results in moving the reforming and gas-shift reaction equilibrium to the H_2 side.

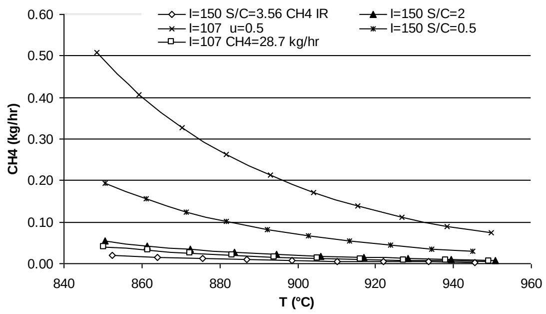

Figure 3. The mass flow rate of remaining CH_4 in the anode exit.

Figure 4 shows the effect of decreasing S/C ratio on the efficiencies of both cycles. The gross and net efficiencies of both SOFC cycles are bigger in case of S/C ratio=2.

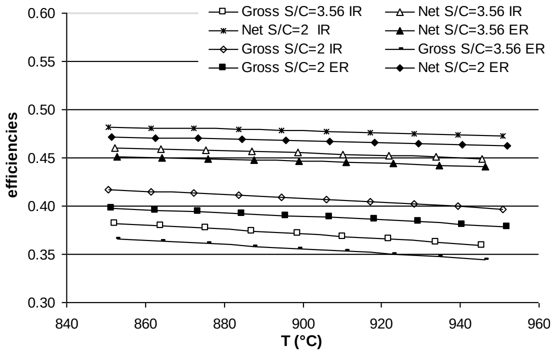

Figure 4. Effect of steam-carbon ratio on the efficiencies at I=150 mA/cm^2.

The fuel consumption in the combustor (Fig.5) is bigger in case of S/C ratio=3.56, causing the reduction in the efficiencies. The combustor needs more fuel in case more steam has to be heated.

The efficiency of the IR cycle is in all cases bigger than of the ER cycle. Though the electrical output of the cell is bigger in the ER cycle, the fuel consumption is also bigger, causing the reduction in efficiency.
Internal reforming uses heat directly produced in the fuel cell. With the ER-cycle the heat has to be recovered out of the exhaust gasses. This is less efficient.

B. Performance of the SOFC in case of current density (107 mA/cm^2)

In case of lowering the fuel flow rate, the fuel supplied to the combustor (Fig. 6) is increased compared to in case of I=150 mA/cm^2 because the remaining fuel which is not used in the fuel cell (Fig. 3) goes down with the reduction of CH_4 mass flow rate to the anode and u=0.7. As less fuel is used in the fuel cell in case of lowering the fuel utilisation to 0.5 (Fig. 3), more can be burned in the combustor resulting in a reduction of extra fuel supplied to the combustor.

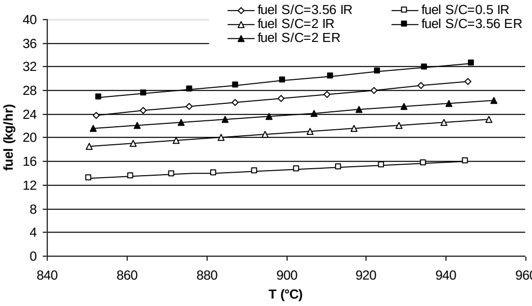

Figure 5. Effect of steam-carbon ratio on the fuel flow rate at I=150 mA/cm^2.

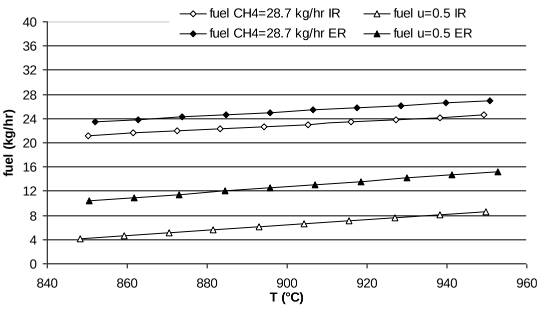

Figure 6. Mass flow rate of fuel as a function of operating temperature at I=107 mA/cm^2.

The cycle efficiencies are reduced compared to I =150 mA/cm^2. As the power production goes down and the fuel flow rate only changes slightly, efficiency goes down. The net and gross efficiencies of both SOFC cycles are higher in case of lowering the fuel utilisation to 0.5 (Fig.7). The fuel consumption in the combustor (Fig. 6) is bigger in case of lowering the fuel flow rate, causing the reduction in the efficiency.

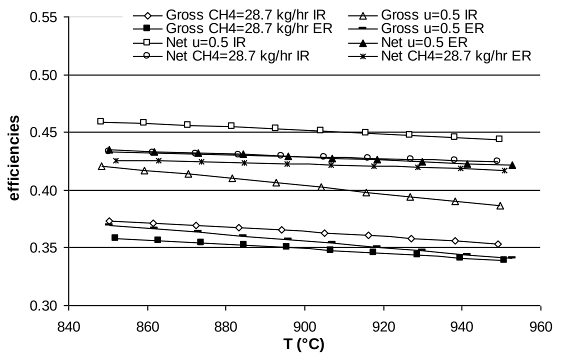

Figure 7. Efficiencies of the cycles at I=107 mA/cm^2, u=0.5 and CH_4 flow rate=28.7

VI. CONCLUSION

In this article a validated model for an SOFC is used in Aspen soft wear to be able to study and investigated the performance of IR and ER reformed SOFC cycles. Moreover, the influence of the steam carbon ratio on the performance of SOFC mode and cycles can be evaluated.

The simulations results indicated that the cell voltage and the efficiency of both (ER and IR) SOFC are higher in case of S/C=2 compared to S/C=3.56. Hence lowering steam-carbon ratio is advantageous for the SOFC cycle. The cycle with internal reforming gives better gross and net efficiencies than the cycle with external reforming.

For part load the cycle efficiencies of SOFCs are higher in case of lowering the fuel utilisation to 0.5 compared to lowering the fuel flow rate to the anode.

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BIOGRAPHIES

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