CYCLE ANALYSIS OF SOFC COMBINED CYCLE

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ABSTRACT

Solid oxide fuel cells (SOFC) are considered extremely suitable for electrical power plant application. The SOFC performance is calculated using numerical models which are built in Aspen customer modeler for the internally reformed (IR) SOFCs. These models are integrated in Aspen Plus™ . In our present study, a combined cycle consisting of two-staged high-temperature SOFC (HT-SOFC) and low-temperature SOFC (LT-SOFC) was investigated. In the combined cycle the anode flow of the HT-SOFC and LT-SOFC is in parallel connected while the cathode flow is serially connected. The combined cycle and single-staged cycle with SOFC are simulated in order to evaluate and compare their performances. The simulations show that the net efficiency of two-staged combined cycle and single-staged SOFC cycle are 62% and 52% respectively under standard operation conditions. In other words, the cycle with two-staged SOFCs gives better net efficiency than the cycle with single-staged SOFC.

INTRODUCTION

Fuel cells convert chemical energy into electrical energy and have the advantage of continuous supply of reactant gases. The fuel cells used for stationary energy production are typically high temperature cells.

Recently, a low temperature SOFC, which runs in the temperature range of around 600°C or above and give high power generation efficiency, has been developed. In [1] a model is developed which accurately simulates the polarisation behaviour of a Ceres cell including electrical leakage. This cell model is incorporated into a model of a 2.5 kW stack, and the stack model into a natural gas fuelled combined heat and power system model. The system model demonstrates that high operating efficiencies are achievable for such a system based upon IT-SOFC cells. In [2], a power generation system consisting of two stages SOFCs with serial connection of low and high temperature SOFCs was investigated. The numerical results show that the power generation of the two staged-

SOFCs is 50.3% and the total efficiency of power generation with gas turbine is 56.1% under standard operating conditions.

In this paper thermodynamic models for SOFC are developed in an Aspen customer modeller and then integrated in Aspen Plus™. Two types of SOFC cycles are analysed: combined cycle and single-staged cycle with high temperature (HT) SOFC only.

NOMENCLATURE

F	[kC/kmol]	Faraday's constant , 96487
i	[A/cm²]	Current density
$\dot{Q}$	[kW]	Heat
p	[Pa]	Partial pressure
K	[-]	Equilibrium constant
g	[kJ/kmol]]	Molar Gibbs free energy
h	[kJ/kmol]	Enthalpy
n	[mol s⁻¹]	Mole flow rate
s	[kJ/kmolK]	Entropy
P_{SOFC}	[kW]	SOFC stack electrical power
$\dot{Q}_{cv}$	[kW]	Heat in a control volume
R_t	[Ω m²]	Total resistance
$\dot{W}_{cv}$	[kW]	Work in a control volume
σ_{cv}	[kW/K]	Entropy production in a control volume
P_{Comp}	[kW]	Compressor Power
P_{turb}	[kW]	Turbine power
A_{cell}	[m²]	Active cell area
T_{cell}	[°C]	Cell temperature
u_f	[-]	Total fuel utilization
V_{cell}	[V]	Cell voltage
S/C	[-]	Steam-carbon ratio

Subscripts and Superscripts

0	[-]	At standard temperature and pressure
i	[-]	Initial
p	[-]	Product
R	[-]	Reaction or reactants

Greek symbols

η	[-]	Efficiency

V_{act}	[V]	Activation overpotential
V_{ohm}	[V]	Ohmic overpotential
V_{conc}	[V]	Concentration overpotential

CYCLES DESCRIPTION

The SOFCs cells currently in operation are fuelled with natural gas. The high temperature inside the cells stack allows for reforming 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. 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. In both cycles part of the anode gases is recycled, as the anode gasses contain steam needed in the reforming reaction. This is a way of introducing a steam generator in the cycles. The characteristics of the systems are given in Table 1. Pressure is kept constant at 4 bar. The cathode inlet temperature of the high temperature SOFC stack is controlled to be 800 °C.

Combined Cycle Configuration

Fig.1 shows a cycle diagram of the combined cycle consisting of a low and high temperature SOFC. In this cycle the anode flow of the HT-SOFC and LT-SOFC is in parallel connected while the cathode flow is serially connected. Methane is admitted into the heat exchanger H/E4 to preheat the methane. The preheated methane is split into two equal parts. Part of the preheated methane is supplied to the anode side of LT-SOFC stack. The remaining part of the preheated methane is mixed with part of recycling anode gases. This mixture passes to the pre-heater, where it is heated to a given temperature, and then enters into the anode side in the HT-SOFC stack. In both SOFC stacks the remaining part of anode gases is 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 heat exchangers H/E2 and H/E3 respectively. In the heat exchanger H/E2 the hot effluent of burned gas releases the heat necessary to preheat the cathode inlet gases.

The compressed air from the compressor (COMP2) is supplied to the heat exchanger (H/E1). The air coming from the H/E1 is further heated to 800°C at (H/E2) before it flows into the cathode side of the HT-SOFC stack. The cathode gases composition at the HT-SOFC outlet was taken as the LT-SOFC inlet condition. The combustor exit gas is heated at H/E3, and then is sent to gas turbine and heat exchanger (H/E4) respectively. The cathode gases of the LT-SOFC stack is recycled to the combustor. The boundary conditions for all the heat exchangers are summarized in table. 2.

Single-staged SOFC Cycle Configuration

The single-staged SOFC cycle (Fig. 2) is similar to the combined cycle (Fig. 1), except that there is no LT-SOFC stack. Therefore the combustor exit gas is heated at H/E3, and is then sent to a gas turbine and heat exchanger (H/E4).

Table 1: Input parameters of the cycles

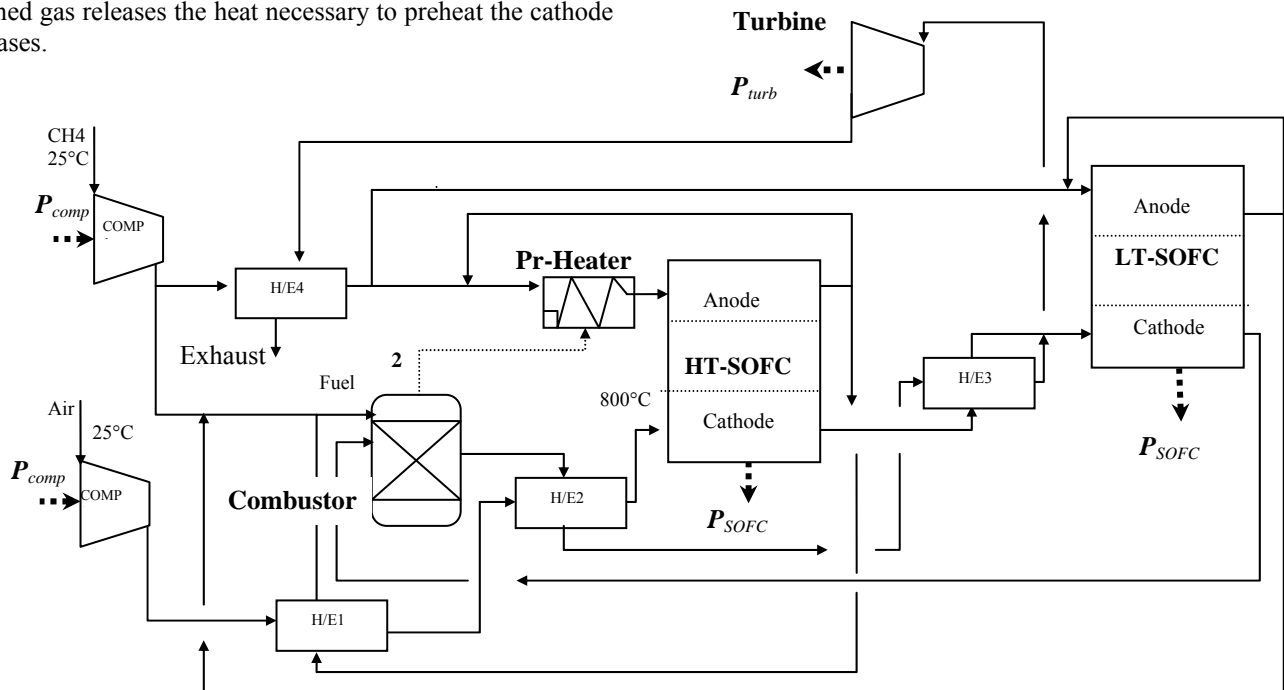| Fuel cell	
A_{cell}	250m²
p	4 bar
other devices	
η for compressor	0.8
η for turbine	0.85
T_{react} combustor	900 °C

Figure 1 Schematic diagram of SOFCs combined cycle (COMP: compressor; H/E: heat exchanger)

SOFC STACK MODEL

The fuel cell is treated as a single control volume on which the steady state flow energy equation is applied with the assumption of negligible change of kinetic energy and potential energy. In a SOFC, to determine actual cell performance, the overpotential must be deducted from the Nernst potential which represents the ideal performance. Overpotential data for the LT-SOFC used in this article are based on an existing SOFC model [4].

The first law of thermodynamics for fuel cell can be written as follows:

$$\dot{Q}_{cv} - \dot{W}_{cv} + \sum_i \left(\dot{n}_i \bar{h}_i \right)_R - \sum_i \left(\dot{n}_i \bar{h}_i \right)_P = 0 \tag{1}$$

The entropy balance for the control volume can be written as follows:

$$\frac{\dot{Q}_{cv}}{T} + \sum_i \left(\dot{n}_i \bar{s}_i \right)_R - \sum_i \left(\dot{n}_i \bar{s}_i \right)_P + \dot{\sigma}_{cv} = 0 \tag{2}$$

Combining (1) and (2) and assuming that the electrochemical reaction is based on unit molar flow rate of the fuel (for example H_2) yields.

$$\dot{W}_{cv} = zFV_{cell} = -\left[\sum_i \left(\dot{n}_i \bar{g}_i \right)_p - \sum_i \left(\dot{n}_i \bar{g}_i \right)_R \right] - T\sigma_{cv} \tag{3}$$

The electrical power density produced by the fuel cell is calculated as follows:

$$\dot{W} = V_{cell} I \tag{4}$$

The cell voltage of the SOFC can be calculated by

$$V_{cell} = \frac{\bar{R}T}{2F} \ln K - \frac{\bar{R}T}{4F} \ln \left[\frac{\left(p_{H_2O}^i \right)^2}{\left(p_{H_2}^i \right)^2 p_{O_2}^i} \right] - \frac{\sigma_{cv} T}{2F} \tag{5}$$
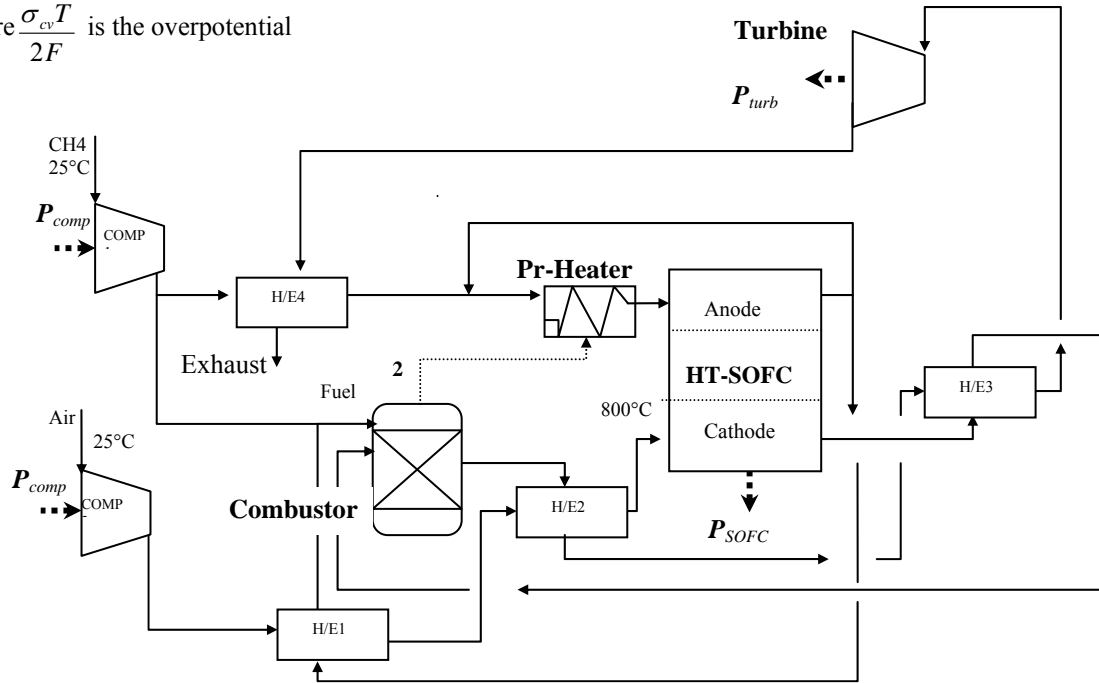
Where $\dfrac{\sigma_{cv} T}{2F}$ is the overpotential

Evaluation of voltage drops in HT-SOFC

The overpotential is a very important parameter in the analysis of fuel cell performance and is expressed by activation (V_{act}), ohmic (V_{ohm}) and concentration (V_{conc}) overpotentials. Activation overpotential, which estimates losses due to slow electrochemical kinetics, is calculated as follows:

$$V_{act} = aie^{b/T} \tag{6}$$

where: $a = 2.83 \times 10^{-4}$ Ωcm^2 ; $b = 8360$ K are the coefficients which obtained by Solheim from experimental data from Umimura, and the temperature T [6]

Ohmic overpotential, which estimates losses associated with ionic and electronic resistance throughout the fuel cell, can be calculated by [4].

$$V_{ohm} = iR_t \tag{7}$$

The resistance of all material used in the SOFC components can be calculated as follows:

$$R_t = \frac{a \exp(b/T)\delta}{A} \tag{8}$$

Where: a and b are the constants which are specific to the materials. δ is the equivalent thickness of diffusion layer and A is the active area.

Concentration overpotential, which estimates losses due to mass transport limitations, becomes significant when large amounts of current are drawn from the cell, can be calculated by [4]

$$V_{conc} = -\frac{\bar{R}T}{n_e F} \ln \left(1 - \frac{i}{i_L} \right) \tag{9}$$

Figure 2 Schematic diagram of SOFC cycle (COMP: compressor; H/E: heat exchanger)

Table 2: The boundary conditions for all heat exchangers of the SOFC systems

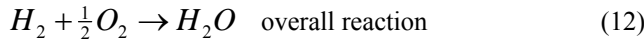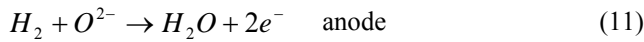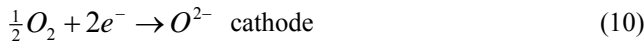| Heat exchanger	Specification	Value
H/E1	Hot outlet cold inlet temperature difference	50°C
H/E2	Cold stream outlet temperature	800°C
H/E3	Hot/cold outlet temperature approach	20°C
H/E4	Hot inlet cold outlet temperature difference	10°C

Assumptions and calculation conditions of SOFC models

The assumptions and conditions of SOFC models used in the simulation program are as follows:

- The fuel cell is isothermal
- Steady state conditions with negligible frictional losses
- Negligible changes of potential and kinetic energies in any process
- Changes in the composition of the anode and cathode gases are only significant in the flow direction.
- All reactions in the gas phase are in equilibrium.
- Oxidant and fuel are considered to be ideal gases.
- Nernst potential is independent of hydrostatic pressure gradient.

ANALYSIS

In the 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. The electrochemical reaction is implemented:

$$\tfrac{1}{2}O_2 + 2e^- \rightarrow O^{2-} \quad \text{cathode} \tag{10}$$

$$H_2 + O^{2-} \rightarrow H_2O + 2e^- \quad \text{anode} \tag{11}$$

$$H_2 + \tfrac{1}{2}O_2 \rightarrow H_2O \quad \text{overall reaction} \tag{12}$$

Both HT-SOFC and LT-SOFC operate at a temperature high enough to reform the steam inside the anode. The chemical reactions for steam reforming and shift reaction of methane are shown below:

$$CH_4 + H_2O \Leftrightarrow CO + 3H_2 \tag{13}$$

$$CO + H_2O \Leftrightarrow CO_2 + H_2 \tag{14}$$
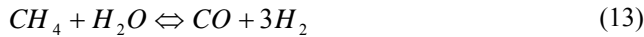
The steam carbon ratio is defined as the ratio between the mole flow rate of steam and the CH4 mole flow rate to the anode.

$$S/C = \frac{\dot{n}_{H_2O}}{\dot{n}_{CH_4}} \tag{15}$$

The fuel utilisation factor is defined by:

$$u_f = \frac{\dot{n}_{H_2 consumed}}{\dot{n}_{H_2 in} + \dot{n}_{CO in} + 4\dot{n}_{CH_4 in}} \tag{16}$$

The net cycle efficiency (η_{net}) is defined as the ratio of the power produced by the fuel cells and the turbine, minus the total compressor power, to the (LHV) of the total amount of fuel ($\dot{Q}_{tot}$)

$$\eta_{net} = \frac{P_{HT-SOFC} + P_{LT-SOFC} + P_{turb} - P_{comp}}{\dot{Q}_{tot}} \tag{17}$$

RESULTS AND DISCUSSION

Performance of the combined and single staged SOFC cycles

Referring to the flow sheets shown in Fig. 1 and Fig. 2, the performance of the SOFC cycle and combined cycle are evaluated and compared. The operating conditions of the SOFC stack in both cycles used in this comparison are the same. The fuel in the combustor is varied to control the temperature of anode gas inlet. The operating temperature of HT-SOFC stack will range between 850 and 950 °C in both cycles. The operating temperature of LT-SOFC stack in the combined cycle runs in the temperature range of around 625°C or above. The simulations of the cycles are performed at current density 150mA/cm², steam carbon ratio S/C=2, fuel recirculation ratio 53% and fuel utilisation factor u_f =0.85.

Figure 3 shows the net efficiency of the combined cycle and SOFC cycle. The net efficiency curves are relatively flat. The net efficiency of the combined cycle is bigger than of the SOFC cycle. The total fuel consumption in the SOFC stacks and the combustor of the combined cycle is bigger than of single staged SOFC cycle (Fig. 4). Though the total fuel consumption is bigger in the combined cycle, the electrical output (Fig. 6) of the fuel cells and gas turbine (GT) is also bigger, causing the increase in net efficiency.
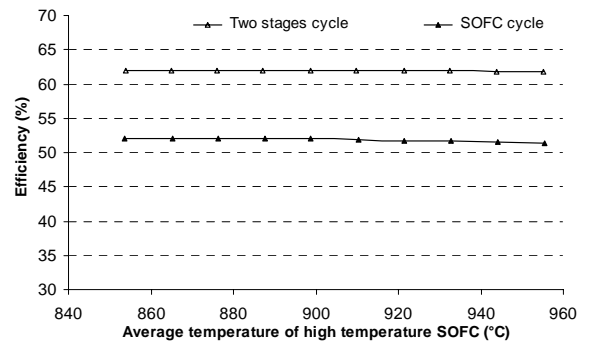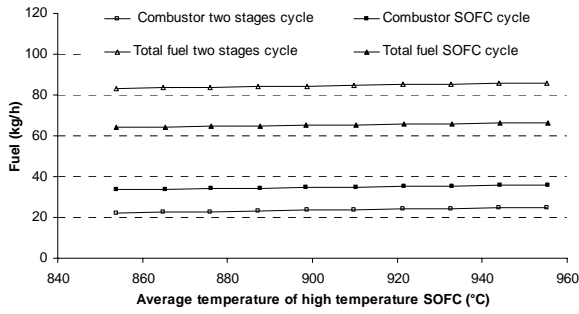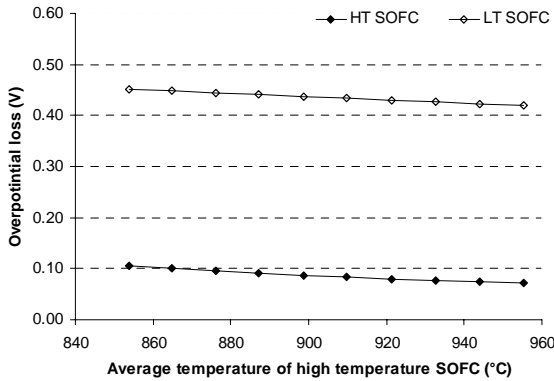

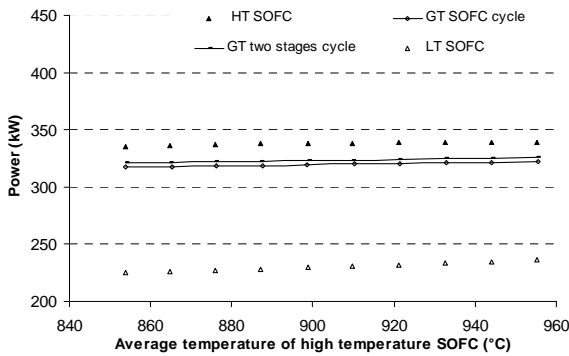**Figure 3** Net efficiency of the cycles.

Figure 4 The fuel flow rate to the cycles

The overpotential (Fig. 5) is lower in the HT-SOFC than in the LT-SOFC, the cell voltage of the HT-SOFC is higher than that of LT-SOFC. Therefore, the electrical output of the HT-SOFC stack (Fig. 6) is higher than that of LT-SOFC stack.


**Figure 5** Overpotential of SOFCs stacks.

Figure 6 Fuel cells and turbines power of the cycles

Efficiency changes with current density

Fig. 7 shows the changes in total electrical output of the SOFCs and gas turbine with current density. Increasing the current density increases the SOFC overpotential , resulting a decrease of the cell voltage. Since the increase in the current density is larger than the decrease in the cell voltage, the electrical outputs of the SOFCs incline (equation 4). The increase in the total fuel consumption in the cycles with mean current (Fig. 8) causes increase in the temperature and amount of inlet gas to the gas turbine, this means the electrical output of turbine goes up.
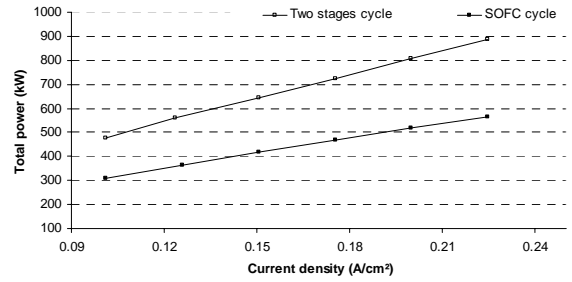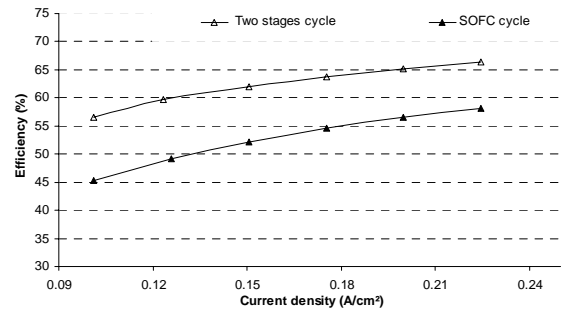

**Figure 7** Fuel cells and turbines power of the cycles
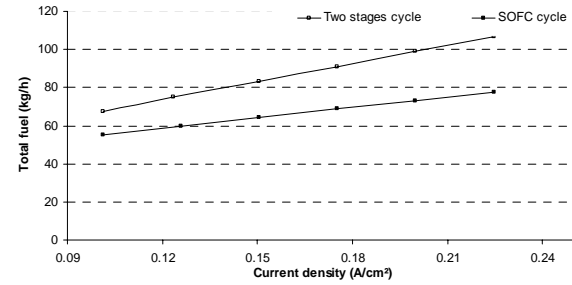
Figure 8 Total fuel of the cycles with current density.

Fig. 9 shows the changes in net efficiency of the cycles with current density. As the power production of fuel cells and turbine goes up (Fig. 7) and total fuel flow rate only changes slightly (Fig. 8), net efficiency of the both cycles goes up.

Figure 9 Change of net efficiency with current density
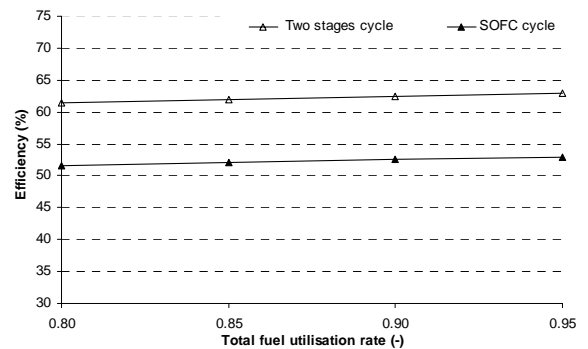
Figure 10 Change of net efficiency with total fuel utilisation rate

Efficiency changes with total fuel utilisation rate

Fig. 10 shows the changes in net efficiency with the total fuel utilisation rate. The energy converted at the SOFC stack increases with rising fuel utilisation rate. As a result of the raise in fuel utilisation rate the electrical output of the SOFC stack

goes up. Therefore, the net efficiency of the cycles increases with increasing fuel utilisation rate.

Efficiency changes with fuel recirculation rate

Fig. 11 shows the changes in net efficiency with fuel recirculation rate. The range for the fuel recirculation rate is limited by the steam flow needed for the reforming reaction. The lower limit of the fuel recirculation rate is 53%, corresponding to a steam carbon ratio of S/C=2.

By increasing the fuel recirculation rate the CH_4 concentration in the outlet of the SOFC anode goes down (Fig. 12). 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. Therefore, increasing the fuel recirculation rate brings about an increased fuel concentration, resulting in a slight incline in net efficiency of the cycles.
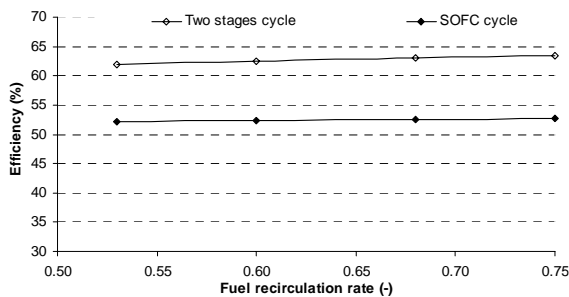

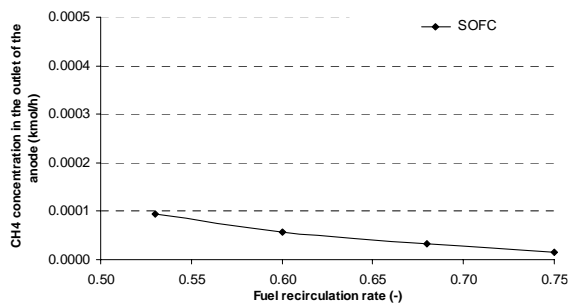**Figure 11** Change of net efficiency with fuel recirculation rate.

Figure 12 The mass flow rate of remaining CH_4 in the SOFC anode exit.

CONCLUSION

In this article, a new combined cycle consisting of two-staged high temperature HT-SOFC and low temperature LT-SOFC was proposed. In this cycle the anode flow of the HT-SOFC and LT-SOFC is in parallel connected while the cathode flow is serially connected. The performance of the single-staged and two-staged SOFCs cycles are evaluated and compared.

The simulations results indicate that the net efficiency of two-staged combined cycle is 62% under standard operation conditions of mean operating temperature for HT-SOFC of 850°C, current density 0.150 A/cm², total fuel utilisation rate of 85%, steam carbon ratio S/C=2 and fuel recirculation rate of 53%. On the other hand, the net efficiency of single-staged SOFC cycle is 52.1%.

In addition, by changing the mean current density, total fuel utilisation rate and fuel recirculation rate for HT-SOFC and LT-SOFC, their effects on net efficiency of combined and single-staged cycles are studied. The results indicate that the combined cycle has higher net efficiency. In other words, the cycle with two-staged SOFCs gives much better net efficiency than the cycle with single-staged SOFC.

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