U. P. B. Sci. Bull., Series C, Vol. 69, No.4, 2007 ISSN 1454-234x

OPTIMIZATION OF A SOFC SYSTEM: INFLUENCE OF DESIGN AND OPERATION PARAMETERS ON SYSTEM EFFICINCY

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In this paper, a model for a solid oxide fuel cell (SOFC) system for decentralised electricity production has been developed and studied. The proposed system, fuelled with natural gas, consists of planar anode supported fuel cells and a balance of plant (BoP) which includes gases supply, fuel processing, heat management, start-up equipment, power conditioning and control system. A reference case has been evaluated by the use of a simple system flowsheet and state of the art operation parameters. The optimization of the electrical efficiency in the system has been carried out varying some of the operation parameters. Fuel utilization, gas temperature spring in fuel cell stack, anode off-gas recirculation, air inlet temperature and external pre-reforming reaction extent are tuned to reach the highest system efficiency.

1. Introduction

Electricity is an essential element required to ensure the normal operation of the present society system. The combined effect of industrialization, rising standards of living and demographic pressure over the last 50 years has generated an always increasing energy consumption in all regions of the world. In the light of available data, this increasing trend in energy demand will continue in the future. Therefore, research topics on new and more efficient power generation technologies operating on fossil and non-fossil fuels are globally encouraged.

Solid oxide fuel cells (SOFC) are promising electricity power devices because of their high theoretical electrical efficiencies and their high operation temperature which allows a wide range of cogeneration possibilities (CHP systems) and the development of gas turbine integrated systems. In order to perform a proper operation. This paper deals with the conceptual study of a SOFC unit of 1kW of nominal power focused on the thermodynamic model of the system (mass and energy balances).

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The main advantages of the built model are: i) flexibility of the model to simulate different types of stack varying easily stack parameters such as number of cells, active area of single cells, different thickness and electrochemical parameters and ii) high flexibility of fuel feedstock composition.

2. Modelling

The basic concept of this SOFC system is represented as a block diagram in figure 1.The analysed system is a SOFC based heat and power generator of 1 kWe of nominal power operated on natural gas. It is designed to independently work from the grid except for the start-up stage when it requires electricity from a back-up battery or from the grid to operate fans and electrical heaters.

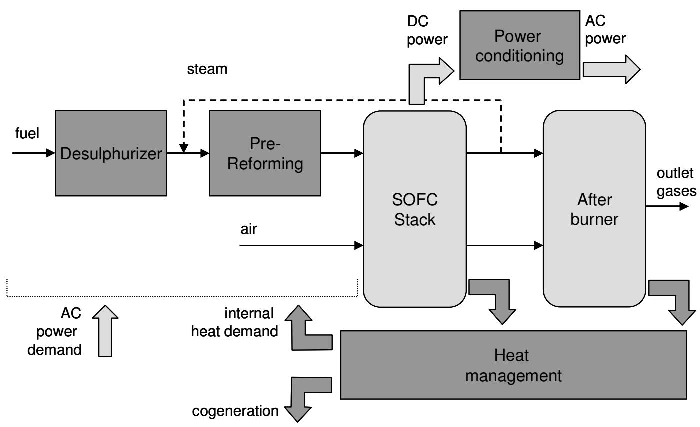

Fig1 Block diagram of a combined heat and power SOFC system

Air is supplied by a blower and preheated prior to enter the SOFC stack. Non-recycled gases are sent to the after-burner where the remaining fuel is burnt with part of the excess air. Internal demand of electricity and heat is self supported by the system. Electrical and thermal efficiencies of the system defined in this paper take it into consideration.

2.1 Development of SOFC stack model

A SOFC model previously developed at the University of Perugia was used to simulate the performance of the cell. The model is suitable to be integrated in the commercial software Aspen Plus^{TM} . As described , the fuel cell has been simulated as a black-box, a zero-dimensional stationary model, similar to a lot of previous works on this subject. The assumption of a zero-dimensional model implies that the cell has a uniform temperature and that the gases leave anode and cathode at this temperature. The code determines the cell voltage and temperature, substantially using the following input:

Gas composition, flow rate, temperature and pressure of the cathode and the anode inlet stream; Fuel utilization (U_F); Cell Area.

The reactions occurring in the cell are :

$$CH_4 + H_2O \xleftrightarrow{\xi} CO + 3H_2 \qquad (2.1)$$

$$CO + H_2O \xleftrightarrow{\psi} CO_2 + H_2 \qquad (2.2)$$

$$H_2 + \tfrac{1}{2}O_2 \xleftrightarrow{\zeta} H_2O \qquad (2.3)$$

The fuel utilization is the fuel fraction which is oxidized through reaction (2.3) and considering that four moles of hydrogen are theoretically produced by reactions (2.1)+(2.2) and one mole of H_2 can be generated by (2.2) from CO provided by the inlet, ζ is given by:

$$\zeta = U_F (4CH_4^1 + CO^1 + H_2^1) \qquad (2.4)$$

Therefore ζ is the number of H_2 moles oxidized inside the cell and superscript i indicates *"inlet fuel flow"*. The cell voltage has been determined as:

$$V= OCV - \eta_{act} - \eta_{ohm} - \eta_{con} \qquad (2.5)$$

Where OCV is the open circuit voltage and η indicates the voltage loss due respectively to activation polarization, ohmic resistance and concentration polarization.

OCV is given by the Nernst equation:

$$E = E_0 + \frac{RT}{2F} \ln \frac{p_{H_2} p_{O_2}{}^{0.5}}{p_{H_2O} p_{atm}{}^{0.5}} \qquad (2.6)$$

where

$$E_0 = 1.2723 - 2.7645 \cdot 10^{-4}\, T \qquad (2.7)$$

The SOFC model also includes the calculation of thermo-chemical balance:

$$H_{IN} + \Delta H_{REACT}(T) = H_{OUT}(T) + Q_{LOSS} + V(T) * I \qquad (2.6)$$

V(T)*I is the electric power produced by the cell, which is deeply influenced by its temperature.

The model has been validated with the experimental data relative to an anode supported SOFC tested at University of Perugia. The parameters listed in table 1 have been retrieved from technical literature and slightly adjusted for the calibration of the model.

Table 1

Parameters used for model calibration

Anodic gas	97 % H_2 – 3% H_2O		
Uf	0.4		
Uox	0.4		
Stack Pressure	1,11 bar		
Stack Temperature (°C)	800		
Active Area (cm^2)	50		
Ohmic loss coefficients	A (Ωcm)	B (K)	δ(cm)
Cathode [9]	2.38 10^{-5}	1200	0.0040
Electrolyte [9]	0.0299401/ T	10300	0.0005
Anode [9]	1.05 10^{-5}	1150	0.0545
Activation polarization coefficients	E act (J/mol)		γ(A/cm^2)
Anode	70000		70000
Cathode	90000		70000
i_L (A/cm^2)	1.6		
θ	0.88		

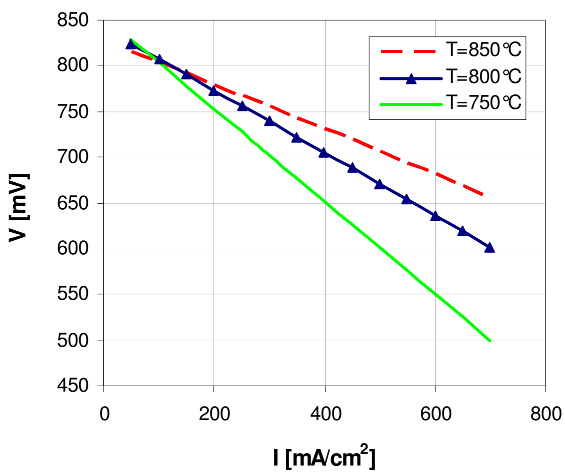

Fig. 3 Influence of temperature on SOFC voltage (Anodic gas: 97%H_2 – 3%H_2O; Uf=0.4; Uox=0.4).

The comparison between the experimental and the simulated voltage is illustrated in figure 2. Subsequently an analysis has been carried out to investigate the influence of temperature and fuel utilization factor on cell performance, as shown in figures 3 and 4. Furthermore the voltage-current curve has been plotted for the particular gas composition resulting from nominal conditions operation of the system (section 2.3).

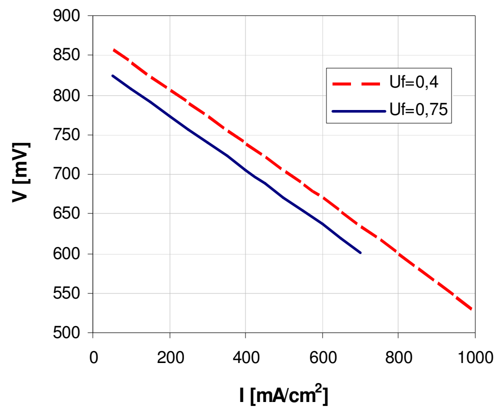

Fig.4 Influence of Uf on SOFC voltage (Anodic gas: 97%H_2 – 3%H_2O; T=800°C; Uox=0.4).

2.2. Aspen Plus^{TM} system model

Apart from the in-house code used to simulate SOFC stack performance which has been described in the previous section, the components of the balance of plant have been implemented using Aspen Plus^{TM} modules. These blocks which complete the system include: compressors, desulphurizer, pre-reforming block, heat exchangers and after-burner. Pressure losses of 5% are considered in every single stage of the system.

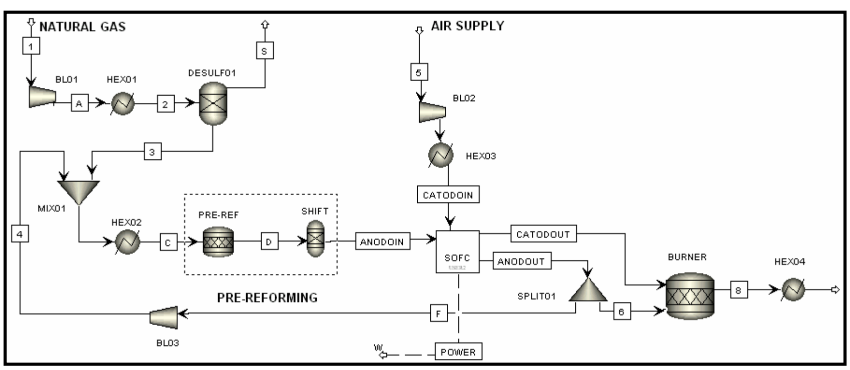

Fig.5 Aspen Plus^{TM} SOFC CHP system flowsheet.

Table2

Nominal operation parameters

SOFC stack	
Number of cells	40
Active cell area	100 cm^2
Pressure	1,11 bar
Fuel temperature at stack inlet	700º C
Air temperature at stack inlet	700º C
Fuel cell temperature	800º C
Fuel utilization (single step)	75%
Thermal losses	7%
Balance of Plant	
Anode recycle	70%
S/C prior entering pre-ref	1,14
Degree of pre-reforming	20%
DC/AC inverter efficiency	96%

2.3. Nominal Operation

A number of relevant parameters which control the system performance must be set to define the nominal point of operation. These parameters dealing with the SOFC stack and with global system are gathered in table 2. The characteristic curve of the fuel cell stack under nominal conditions is shown in figure 6 where is compared to the system operating on pure hydrogen.

Electrical and thermal efficiencies in the system are defined as follows:

$$\eta_{el} = \frac{P_{DC}\eta_{inverter} - P_{aux}}{\dot{m}_{fuel} LHV_{fuel}} \qquad (2.7)$$

$$\eta_{th} = \frac{\dot{Q}_{HEX\,04} - Q_{HEX\,03} - Q_{HEX\,02} - Q_{HEX\,01}}{\dot{m}_{fuel} LHV_{fuel}} \qquad (2.8)$$

where:

P_{DC}: DC power generated by the stack

P_{AUX}: power consumed by blowers

$\dot{m}_{fuel}$: inlet fuel mass flow

LHV_{fuel}: low heating value of fuel

3. Results of system performance simulation

In the following, the main parameters describing the SOFC system performance which have been calculated through Aspen Plus™ simulations are presented under the conditions chosen as nominal operation conditions.

These values represent the reference scenario to compare results from other situations but always maintaining a constant fuel flow.

Table 3

Nominal operation results

SOFC stack	
Fuel utilization (single step)	75%
Power output	1120 W
Electrical efficiency	48,4%
Oxidant utilization (U_{ox})	20%
S/C stack inlet	1,14
Global system	
Electrical AC efficiency	43,5%
Thermal efficiency	22,9%
Total fuel utilization	91%
S/C pre-reformer	1,22

3.1. Results under nominal conditions

The output power given by the stack is 1120 W. Under an anode recirculation of 70%, global fuel utilization increases to 91%. Oxidant flow utilization is obtained to be 20%. The case under nominal conditions described in section 2.3 achieves an electrical efficiency of the stack of 48,4% and a global electrical AC efficiency of 43,5%. A summary of these results is presented in table 3.

3.2. Effect of fuel utilization (Uf)

The fuel utilization is one of the most important operating parameters for fuel cells and has significant effects on the cell voltage and efficiency. It also affects thermal efficiency through the unburned fuel concentration in the exhaust of the fuel channel. Fuel utilization (single step) in the SOFC stack has been varied from 45% to 95%.

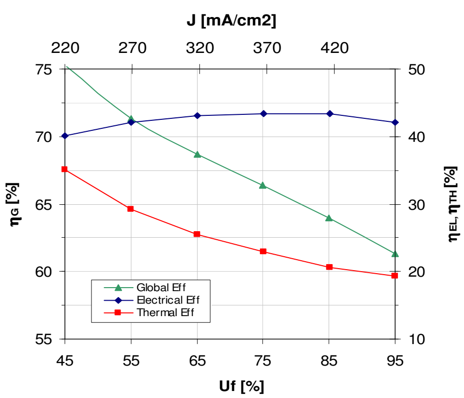

Fig7. System efficiencies in the system varying fuel utilization (single step) of the stack.

As fuel inlet flow and composition are constant, current density decreases with fuel utilization while stack voltage increases. The result of these two opposed trends is a variation of the generated power as figure 7 shows.

4. Conclusions

A model which simulates a global SOFC stack system was developed by integration of the in-house *fortran* code which models SOFC stack performance as unit operation model in Aspen Plus^{TM}. Detailed thermodynamic and sensitivity analysis of the SOFC operation can be performed. The model can easily be extended to study the entire system consisting of the SOFC stack and the balance of plant. The model was calibrated with experimental results of an anode supported SOFC tested in the Fuel Cell laboratory of the University of Perugia. From this paper, the complexity of choosing the optimal group of operation parameters of the system which lead to the highest efficiency is highlighted. Electrical and thermal efficiency follow opposite trends under some of the supposed cases because they are controlled by different processes.

It should be pointed out, that a further research which studies different flow configurations will lead to understand actual thermal efficiency in the system. Recirculation of exhaust gases from cathode must be studied and designed to optimize heat utilization within the system.

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