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Reversible Solid Oxide Fuel Cell Connected to Solar PV/T System: Cell Electrochemical Modelling and Analysis

A K Mishra[1], D Roy[1] and S Ghosh[1]

[1]Department of Mechanical Engineering, Indian Institute of Engineering Science and Technology, Shibpur, Howrah 711103, West Bengal, India

Corresponding Author: aradhykumar@gmail.com

Abstract. In this paper, a novel power generation cum storage system employing reversible solid oxide fuel cell (RSOFC) has been proposed and modelled. The RSOFC is integrated with solar PV/T system. Here only the electrochemical modelling of the fuel cell unit has been presented and analysed thermodynamically. The RSOFC unit operates in steam electrolyser mode (during day time) as well as in fuel cell mode (during night time). The electrochemical model has been developed by using Engineering Equation Solver. Performance of RSOFC unit has been investigated under varying operating parameters viz. applied current density and operating cell temperature. For electrolyser mode of operation maximum efficiency is found to be 93% at a current density (J) 8000 A/m^2 and at cell temperature (T_{cell}) 1273K. Maximum efficiency during fuel cell mode of operation is found to be 77% at cell temperature 1073K and at current density 500 A/m^2.

1. Introduction

According to IEA report [1], fossil fuels contribute a major share of electricity production till now. Fossil based power plants are the major emitter of greenhouse gases. Therefore, designing advanced power generation system employing renewable energy sources is essential to neutralize greenhouse gas emissions. In that context, fuel cell technology has a potential to provide a clean and sustainable form of energy without emitting any polluting agents. Reversible solid oxide fuel cell (RSOFC) is a promising new technology which can operate in solid oxide fuel cell (SOFC) mode as well as in solid oxide steam electrolyser (SOSE) mode. RSOFC generally operates at a very high temperature (873-1273 K). Thus, it requires a high temperature heat source to preheat the incoming feed (H_2 and air in SOFC mode of operation, H_2O in SOSE mode of operation).

Akikur *et al*. [2] proposed a solar powered RSOFC based cogeneration system. The overall efficiency of the system is found to be 20% and 23% in the solar-SOSE mode and the solar-SOFC mode respectively. Wendel *et al.* [3] studied the performance of an intermediate temperature RSOFC and found that efficiency, more than 70% can be achieved at intermediate stack temperature (680^{0}C). Kazempoor *et al*. [4] proposed a RSOFC based energy storage system in which they investigated the effect of operating parameters viz. temperature, gas composition and fuel utilization on cell voltage, at varying current densities. Visitdumrongkul *et al.* [5] investigated the performance of SOSE integrated system for H_2 production. The effect of operating parameters viz. oxygen to carbon ratio, operating temperature and pressure have been reported. Ni *et al.* [6] conducted the parametric study of SOFC. They found that the activation and ohmic overpotentials decrease significantly with increasing cell temperature, whereas the concentration overpotential increases with rising cell temperature. Ghosh *et al.* [7] investigated energetic analysis of a cogeneration plant using coal gasification and SOFC. Ni *et al.* [8] conducted a parametric study of SOSE and found that at increasing electrode porosity and pore size, the total voltage loss reduces. Stamatis *et al.* [9] studied a SOFC-GT system fed with ethanol and found that at higher current density, the SOFC-GT system is more efficient compared to SOFC unit. Roy *et al.* [10] performed energetic and exergetic analyses of a biomass based SOFC-GT-ORC system. Akkaya *et al.* [11] studied the performance of a combined system consisting of SOFC and ORC.

This paper proposes a novel power generation cum storage system employing a RSOFC and PV/T module. Electrochemical model of RSOFC system has been developed and analysed. Engineering Equation Solver (EES) was used to write codes for the model. Performance of RSOFC unit has been investigated under varying operating parameters viz. current density and cell temperature.

2. System description

The schematic of the proposed RSOFC integrated power generation cum storage system is depicted in Figure 1. RSOFC unit operates in SOSE mode (solid line in Figure 1) as well as in SOFC mode (dotted line in Figure 1). At this time, water is passed through solar thermal photovoltaic (PV/T) system where it takes heat from it. After that, it passes through parabolic trough solar collector (PTSC) where water is further heated and is converted into steam. Further superheating is done by Heat Exchanger 1 (HEx 1) where heat is extracted from outlet product of RSOFC. If further heating is required, then the steam is again passed through the Supplementary Heater 1 and then this superheated steam is supplied to cathode channel of RSOFC. Necessary electrical power required to run RSOFC, is consumed from PV/T unit. Water molecules will be dissociated into a mixture H_2+H_2O and O_2. Oxygen gas, leaving from anode channel exit, is stored in oxygen storage tank after exchanging necessary heat in the HEx 1. The mixture of H_2+H_2O, after exchanging necessary heat in HEx 1, is fed to the separator, where H_2 is separated from the mixture. H_2O will be stored in the H_2O storage tank.

During night time in SOFC mode of operation (dotted line in Figure 1), stored hydrogen from hydrogen storage tank and air from the atmosphere will be fed in the RSOFC after necessary heating in heat exchanger 2 (HEx 2) and Supplementary Heater 2. Due to chemical reactions taking place in RSOFC unit, DC power is produced which further converted to AC power through the rectifier.

3. Mathematical model development

3.1 SOSE Mode of Operation

For a SOEC fed by electricity and water, the overall electrode reaction is:-

$$\mathrm{H_2O} \rightarrow \mathrm{H_2} + \frac{1}{2}\mathrm{O_2} \tag{1}$$

The total electrical power demand (P_{SOSE}) is defined by:-

$$P_{\mathrm{SOSE}} = V_{\mathrm{SOSE}} J \mathrm{A_{cell}} \mathrm{N} \tag{2}$$

where V_{SOSE} is the input potential of SOSE, J is current density, $\mathrm{A_{cell}}$ is area of cell and N is number of cells. The required voltage V_{SOSE} can be written as:-

$$V_{\mathrm{SOSE}} = E + \eta_{\mathrm{ohmic}} + \eta_{\mathrm{act,a}} + \eta_{\mathrm{act,c}} + \eta_{\mathrm{conc,a}} + \eta_{\mathrm{conc,c}} \tag{3}$$

where E is Equilibrium potential or Nernst potential, η_{ohmic} is ohmic overpotential, $\eta_{act,a}$ is activation overpotential at anode, $\eta_{act,c}$ is the activation overpotential at cathode, $\eta_{conc,a}$ is concentration overpotential at anode and $\eta_{conc,c}$ is concentration overpotential at cathode. Nernst potential or Equilibrium potential can be calculated as:-

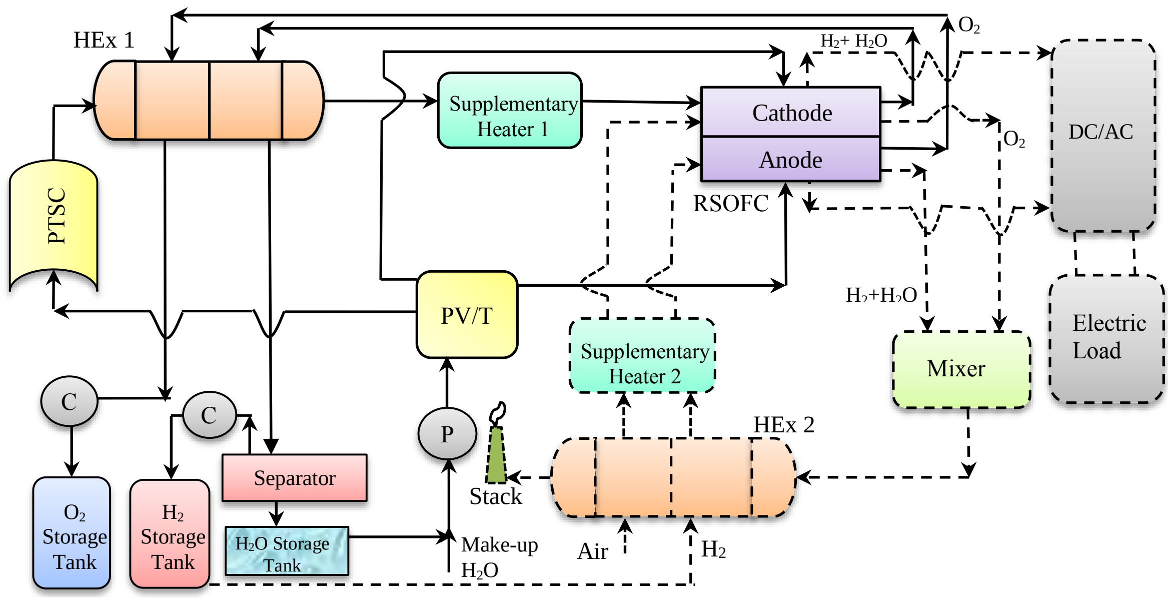

Figure 1. Schematic of the proposed RSOFC integrated power generation cum storage system

$$E = E^0 + \frac{RT}{2F}\ln\left[\frac{P^0_{H_2}\left(P^0_{O_2}\right)^{1/2}}{P^0_{H_2O}}\right] \quad (4)$$

where E^0 is the standard potential which is calculated by Stamatis *et al.* [9], R is universal gas constant, T is operating temperature, F is Faraday constant, and $P^0_{H_2}$, $P^0_{O_2}$ *and* $P^0_{H_2O}$ are the partial pressure of hydrogen, oxygen and water at electrode surface respectively. Ohmic overpotential can be calculated by [12], activation overpotential can be determined by Butler-Volmer equation [8], and concentration overpotential can be calculated by Akikur *et al.* [2]. Efficiency of SOFC is calculated by:-

$$\eta_{SOSE} = \frac{LHV_{H_2} \times \dot{N}_{H_2out}}{P_{SOSE} + Q_{Heat,SOSE} + Q_{Heat,H_2O}} \quad (5)$$

where LHV_{H_2} is the lower heating value of hydrogen, $\dot{N}_{H_2out}$ is molar flow rate of produced hydrogen, P_{SOSE} is power input, $Q_{Heat,SOSE}$ is heat supplied to SOSE and Q_{Heat,H_2O} is heat required to raise the temperature of H_2O. The irreversibilities in SOSE will result heat production because of entropy generation (σ) [8]:-

$$\sigma = 2F\left(\eta_{ohmic} + \eta_{act,a} + \eta_{act,c} + \eta_{conc,a} + \eta_{conc,c}\right) \quad (6)$$

If $\sigma \geq T\Delta S$ i.e. heat generation due to irreversibility is more than or equal to the heat required for water splitting reaction ($T\Delta S$) then no external heat is required but if $\sigma < T\Delta S$ then heat production is less than the heat requirement hence external heat is required which is calculated by [8]:-

$$Q_{Heat,SOSE} = \frac{J}{2F}\left(T\Delta S - \sigma\right) \quad (7)$$

3.2 SOFC Mode of Operation

For SOFC fed by H_2 and air, the overall electrode reaction is:-

$$H_2 + \frac{1}{2}O_2 \rightarrow H_2O \quad (8)$$

Power output (P_{SOFC}) in fuel cell mode can be expressed as:-

$$P_{SOFC} = V_{SOFC}J_{SOFC}A_{cell}N \quad (9)$$

where J_{SOFC} is the produced current density in SOFC mode of operation which can be calculated as:-

$$J_{SOFC} = 2\dot{N}_{H_2,utilized}F \quad (10)$$

where $\dot{N}_{H_2,utilized}$ is molar flow rate of hydrogen consumed by RSOFC. The output voltage (V_{SOFC}) of a fuel cell is the difference of Nernst Potential (E) and total overpotential where total overpotential is the sum of ohmic overpotential, activation overpotential at anode and cathode and concentration overpotential at anode and cathode.

$$V_{SOFC} = E - \eta_{ohmic} - \eta_{act,a} - \eta_{act,c} - \eta_{conc,a} - \eta_{conc,c} \quad (11)$$

where Nernst potential (E), the ohmic overpotential (η_{ohmic}), the activation overpotentials (η_{act}) can be calculated by the same equation those are used for electrolyser mode. The concentration overpotential can be calculated by [11]. Efficiency of SOFC (η_{SOFC}) is calculated by [2]:-

$$\eta_{SOFC} = \frac{P_{SOFC}}{\dot{N}_{H_2,inlet}LHV_{H_2}} \quad (12)$$

where $\dot{N}_{H_2,inlet}$ is the molar flow rate of hydrogen at inlet.

4. Model Validation

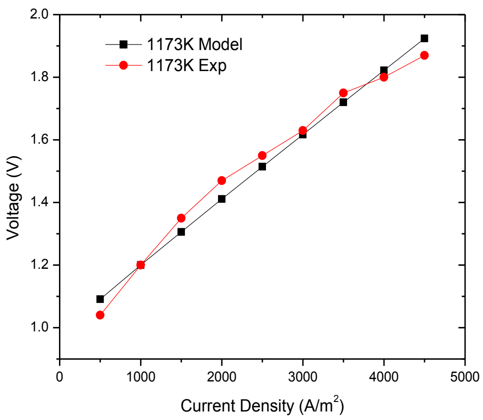

Figure 2. SOSE mode validation

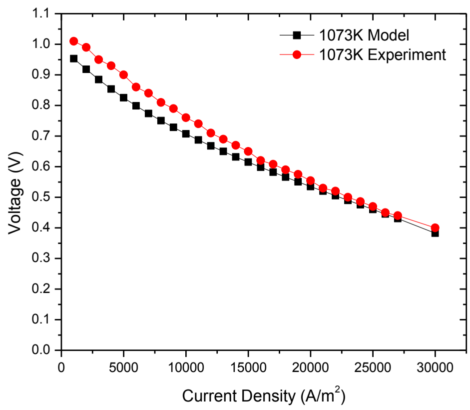

Figure 3. SOFC mode validation

RSOFC model has been validated both in SOFC mode and SOSE mode of operation. The SOSE mode of operation is compared with the experimental work of Momma *et al.* [14], as shown in Figure 2. The SOFC model of operation is compared with the experimental work of Zhao *et al.* [15], as shown in Figure 3. The maximum error in between simulation and experimental work in SOSE mode is 4.5% and in SOFC mode is 7.7%.

5. Result and Discussion

In this paper, we have only analysed the RSOFC unit by varying different operating parameters such as current density and cell temperature. Input parameters needed for analysis is shown in Table 1. Figure 4 shows the effect of SOSE current density on hydrogen production rate at a temperature of 1073K.

Table 1. Values of input parameters.

Parameter	Value
Pressure (bar)	1
Electrolyte thickness, L (μm)	50
Anode thickness, d_a (μm)	500
Cathode thickness, d_c (μm)	50
Number of cells, N	1000
Area of each cell, A_{cell} (m^2)	0.01

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Since hydrogen production rate is directly proportional to SOSE cell current density, increased current density increases the hydrogen production rate, as shown in Figure 4. Efficiency is also found to increases continuously up to J = 4000 A/m^2 and then remains almost unaffected by further increase in current density. Figure 5 depicts the influence of T_{cell} and J on the efficiency of RSOFC. It is observed that influence of T_{cell} is not highly significant on efficiency at lower current densities. It is due to the fact that, at lower current densities, the requirement of heat energy is higher compared electrical energy. Efficiency of RSOFC unit is highly influenced by increasing operating current density and cell temperature. At elevated current density, electrical energy requirement is higher compared to thermal energy. Further at higher current density and elevated T_{cell} amount of H_2 production increases. Hence high temperature and higher value of current density are desirable.

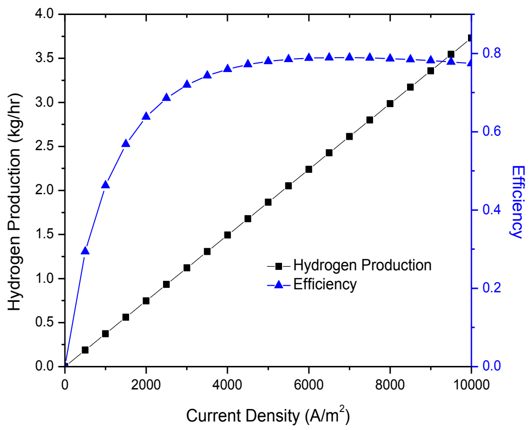

Figure 4. J vs H_2 production and J vs Efficiency at temperature of 1073 K.

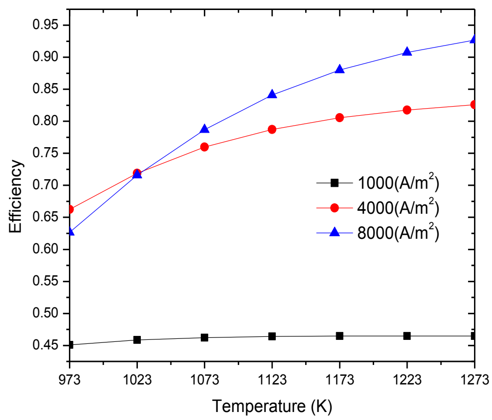

Figure 5. Temperature vs Efficiency at different current density.

Figure 6 illustrates the effect of current density on power and efficiency of RSOFC working in fuel cell mode when cell temperature is held constant (1073K). It is observed that on increasing current density, power from RSOFC increases while its efficiency decreases. As current density increases, molar flowrate of H_2 consumption increases. Thus, power obtained from RSOFC increases at elevated current densities. Again, increase of current density results in lower operating voltage due to which efficiency decreases. Figure 7 shows the effect of temperature on power and efficiency of RSOFC working in fuel cell mode. From Figure 7 it is clear that as temperature increases both power and efficiency increases. It is due to the fact that at rising operating temperature, overpotentials decreases. Hence, cell voltage increases which further results in increase of power and efficiency.

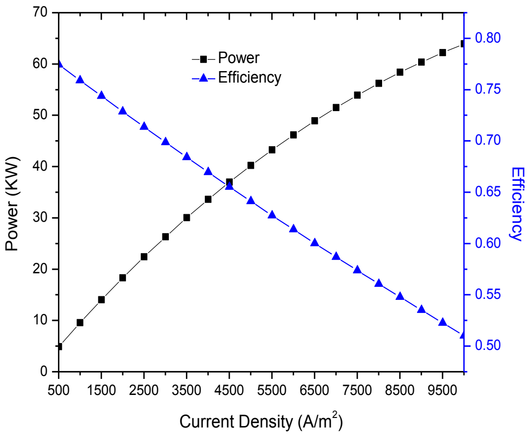

Figure 6. Power and Efficiency vs J

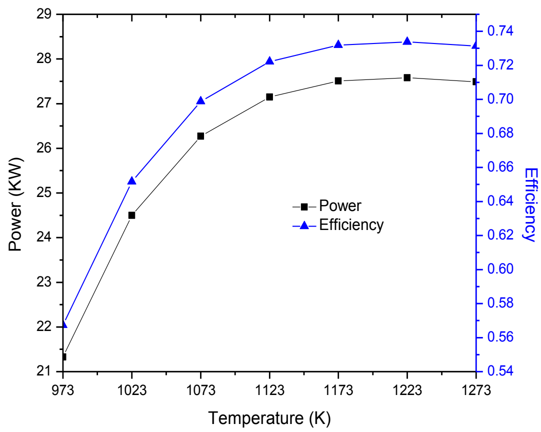

Figure 7. Power and Efficiency vs T

6. Conclusion

In this study, a novel power generation cum storage system employing reversible solid oxide fuel cell (RSOFC) has been proposed and modelled. Electrochemical modelling of the fuel cell unit has been presented and analysed thermodynamically. Analysis predicted that performance of RSOFC unit is highly affected by operating parameters viz. current density and cell temperature. In SOSE mode of operation, under varying operating cell temperature from 973K to 1273K efficiency of the RSOFC unit is found to be in increasing nature at elevated current densities. Though, the performance of the RSOFC unit is not influenced at lower operating current densities. Maximum efficiency of RSOFC unit in SOSE mode found to be 93%, at T_{cell}= 1273K and J=8000 A/m^2. In the SOFC mode of operation, efficiency of the RSOFC unit found to be decreasing at rising current densities. Maximum efficiency of the RSOFC unit in SOFC mode of operation found to be 77% at T_{cell} =1073K and J=500A/m^2.

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