Plant-level performance of a reversible solid oxide cell-based stack with H$_2$-H$_2$O-O$_2$ and H$_2$-H$_2$O-Air system for a renewable energy-based microgrid[#]

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ABSTRACT

Reversible solid oxide cells (ReSOCs) stack consume electrical energy to produce chemical fuel in the electrolyser (SOEC) mode of operation and convert stored fuel into electrical energy during the fuel cell (SOFC) mode of operation. On the whole, the stack operation is endothermic in the SOEC mode and exothermic in the SOFC mode. A mutually compatible balance-of-the-plant (BoP) with thermal integration for the dual mode of operation is necessary for the ReSOC stack. A detailed process model of ReSOC of MWe scale capacity is developed with two layouts for the BoP: an oxygen-based system and an air-based system. Auxiliary power generation in both modes improves the efficiency of the system. Plant-level compatibility shows the plant can be operated at a 1:2.5 charging-to-discharging time ratio, thus making it highly suitable for islanded power operation of the daily residential energy requirement driven primarily by a solar PV-based renewable energy system. In terms of overall performance, the oxygen-based system shows a roundtrip efficiency of around 70% compared to around 55% for the air-based system. This difference may be attributed to air compression in both modes which requires significantly higher parasitic power consumption.

Keywords: Reversible solid oxide cell, renewable energy storage, balance-of-the-plant, fuel cell, electrolyser

NONMENCLATURE

Abbreviations	
EC	Electrolysis mode
FC	Fuel cell mode
RTE	Roundtrip efficiency
LHVE	Lower heating value efficiency
Symbols	
x	Mole fraction

η	Efficiency (%)
$\dot{n}$	Molar flow rate (mol/s)
z	Number of electrons
F	Faraday's constant (C/mol)
U$_F$	Utilization factor
$\dot{W}$	Work flow rate (kW)
$\dot{Q}$	Heat flow rate (kW)

1. INTRODUCTION

Decarbonizing fossil fuel-based energy systems by large-scale penetration of renewable energy sources into the grid is a major and necessary step in moving towards the net zero target. The intermittent nature of solar and wind energy results in a mismatch between supply and demand [1,2]. This makes efficient electrical energy storage of excess intermittent renewable energy (RE) sources an imperative for grid stabilization for future energy systems. Various electrical energy storage technologies are proposed, but each one has its own constraints in implementing and handling intermittent renewable energy-based microgrids, like scale-up, handling fluctuations, long-term durability, cost, energy density, and geological factors [3-7].

Reversible solid oxide cells (ReSOCs) work in dual mode (fuel cell and electrolyser) to produce/store electricity, capable of providing efficient and cost-effective electrical energy storage [8,9]. The schematic diagram of the proposed system is shown in Fig. 1. The MEA of the stack is made of advanced ceramic components, which enables the stack to operate at high temperatures and high-pressure conditions. Two layouts of the thermodynamic model of ReSOCs with the BoP have been developed in this study on the DWSIM simulation platform for the oxygen-based (henceforth referred to as H$_2$-H$_2$O-O$_2$ system) and air-based (or H$_2$-H$_2$O-Air) system. Exothermic fuel cell operation and endothermic electrolysis make system design challenging as optimal operating conditions in one mode

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clash with enhancing the performance in another mode. Since the unit is being considered as principal power provider, its operation cannot be compromised by coupling it with other systems. Therefore, a part of the hydrogen produced in the electrolyser mode is proposed to be utilized to provide high temperature heat source to make the overall system auto-thermal. Thermal management strategies for making effective waste heat utilization are employed for the system in both modes. Expansion turbines, water separators, and multi-stage compressors are employed to enhance system efficiency and energy storage density. The overall performance of ReSOC in SOEC and SOFC mode for both layouts at different current densities is investigated.
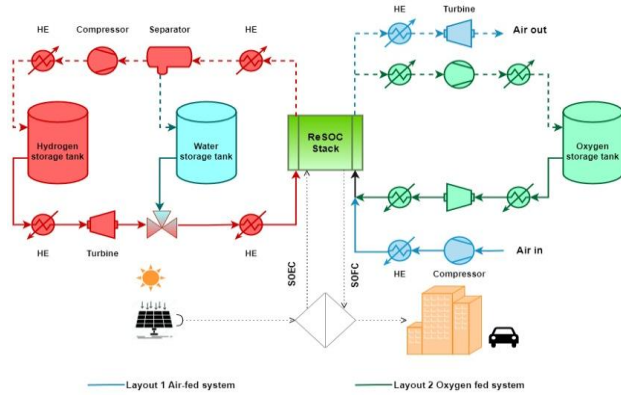

Fig. 1 Proposed system layouts

2. RESOC THEORY AND METRICS

2.1 ReSOC electrochemical model

Electrochemical oxidation and reduction reactions take place in the ReSOCs. When ReSOC operates in fuel cell mode, the forward electrochemical reaction occurs; the reverse electrochemical reaction occurs when ReSOC operates in electrolyser mode.

$$H_2 + \tfrac{1}{2}O_2 \underset{EC}{\overset{FC}{\rightleftarrows}} H_2O + Electricity + Heat$$
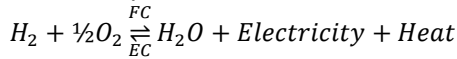
In the SOFC mode of operation, hydrogen undergoea electrochemical oxidation by reacting with oxygen ions at the triple-phase boundary, which produces electricity and water vapour. When the applied cell voltage between the electrodes exceeds the open-circuit voltage, electrolytic reduction starts, and the solid electrolyte's oxygen transport is reversed. The open-circuit voltage (OCV) of hydrogen oxidation is calculated as:

$$V_{Nernst} = E^0 + \frac{RT}{zF}\ln\left(\frac{x_{H2,b} x_{O2,b}^{0.5}}{x_{H2O}}\right) + \frac{RT}{zF}\ln\left(\frac{P}{P_{amb}}\right) \quad (1)$$

The cell voltage (V_{op}) is significantly higher than the Nernst potential in SOEC mode and significantly lower in SOFC mode, arising from the cell overpotentials.

$$V_{op} = V_{Nernst} - \eta_{act} - \eta_{ohm} - \eta_{conc} \quad (2)$$

The total losses in the cell during electrochemical reactions are taken as negative for electrolysis, making cell voltage greater OCV, and positive for fuel cell operation, resulting in lower cell voltage than OCV. The current generated in the stack is proportional to the molar flow rates of hydrogen in SOFC mode. It also correlates with the utilization factor, the number of electrons transferred in the electrochemical reaction, and Faraday's constant.

$$I_{FC} = zF\dot{n}_{H_2,in}U_{F_{FC}} \quad (3)$$

and

$$I_{EC} = zF\dot{n}_{H_2O,in}U_{F_{EC}} \quad (4)$$

The fuel utilization in the fuel cell is expressed as the ratio of the electrochemical hydrogen reduction rate to the rate at which hydrogen is sent to the fuel side channel of the ReSOC stack:

$$U_{F_{FC}} = \frac{\dot{n}_{H2,consumed}}{\dot{n}_{H2,inlet}} \quad (5)$$

2.2 ReSOC performance characteristics

2.2.1 Efficiency based on LHV for ReSOC operation

Energy efficiency in individual modes (SOFC and SOEC) of operation is estimated based on the lower heating value (LHV) of hydrogen for the stack and system level [10].

$$\eta_{FC} = \frac{\dot{W}_{FC}}{\dot{n}_{H_2,in}LHV_{H_2}} * 100 \quad (6)$$

and

$$\eta_{EC} = \frac{\dot{n}_{H_2O,in}U_{F_{EC}}LHV_{H_2}}{\dot{W}_{EC}+\dot{Q}_{EC}} * 100 \quad (7)$$

and

$$\eta_{FC,sys} = \frac{\dot{W}_{FC}+\dot{W}_{BoP,FC}}{\dot{n}_{H_2,in}LHV_{H_2}} * 100 \quad (8)$$

and

$$\eta_{EC,sys} = \frac{\dot{n}_{H_2O,in}U_{F_{EC}}LHV_{H_2}}{\dot{W}_{EC}+\dot{W}_{BoP,EC}+\dot{Q}_{EC}} * 100 \quad (9)$$

2.2.2 Roundtrip efficiency

The efficiency of an ReSOC is better expressed in terms of energy produced during the fuel cell operation and the energy consumed during electrolysis operation. Based on the specific charging-discharging ratio, the efficiency is expressed either in power or energy in steady-state simulation. The system round-trip efficiency is the ratio of the total power delivered by ReSOC during

discharging mode to the total power consumed for charging the system during electrolysis operation [10,11].

$$\eta_{RT,sys} = \frac{(\dot{W}_{FC} - \dot{W}_{BOP,FC})t_{FC}}{(\dot{W}_{EC} - \dot{W}_{BOP,EC})t_{EC}} \qquad (10)$$

Stack round-trip efficiency is an effective measure of the ReSOC stack performance and is determined by considering power produced and consumed by the stack in discharging and charging modes, respectively [10,11].

$$\eta_{RT,stk} = \frac{\dot{W}_{fc}t_{fc}}{\dot{W}_{ec}t_{ec}} \qquad (11)$$

3. SYSTEM

System-level modeling and simulation of the ReSOC stack with its balance-of-the-plant is carried out using an open-source process simulator, DWSIM. In order to obtain an accurate estimate of the stack efficiency under different operating conditions, an electrochemical model for the ReSOC has been developed using MATLAB and is validated with experimental results from the literature. Hydrogen and water are drawn out from their respective storage tanks. Hydrogen, stored at 200 bar and 30 °C, is preheated before each stage of expansion in a multi-stage expander to stack operating pressure. Water is also pressurized to stack pressure and then evaporated to form steam. Hydrogen and steam get mixed in proportion according to the mode of operation. The stack exhaust stream from the fuel side electrode preheats the inlet mixture stream to stack operating conditions and is fed to the fuel side electrode. During the electrolysis, electricity is consumed by the stack to produce fuel, and the exhaust stream from the fuel side electrode is a hydrogen-rich stream. While in fuel cell mode, hydrogen (fuel) is consumed to produce electricity and heat, and the fuel side electrode exhaust stream contains small fractions of hydrogen. The water vapour in the fuel side exhaust stream gets condensed, separated, and sent to the water storage tank. Subsequently, pure hydrogen is compressed in a multi-stage compressor with an intercooler to 200 bar and 30 °C storage conditions.

In the H_2-H_2O-Air system, air is drawn from the atmosphere and compressed to stack pressure in a multi-stage compressor with an intercooler. The air flow rate is maintained to provide oxygen to the stack in proportion to hydrogen and abate the hydrogen combustion temperature. The compressed air is preheated to stack temperature, and oxygen ion transport depends on the cell polarity. Exhaust air from the oxygen side electrode is oxygen-enriched stream during electrolysis and oxygen-depleted stream during the fuel cell mode of operation. In the H_2-H_2O-O_2 system, oxygen is drawn from the oxygen storage tank (150 bar and 30 °C), expanded in a multi-stage expander with a preheater to stack operating pressure, and then preheated to stack temperature. Similar to the previous case, the oxygen flow rate is maintained proportional to the hydrogen flow rate. In order to maintain stack operating conditions, hydrogen combustion provides additional heat. Carbon dioxide is utilized as the stack's heat carrier/coolant based on its operating condition. A Brayton cycle is introduced in both modes, providing auxiliary power to the system.

4. RESULTS

A mega-watt scale reversible solid oxide cell-based system operates at 750 °C, and 20 bar is developed, which electrochemically converts 90% of the feed during the cyclic operation. The stack contains 175 cells, each cell has an active area of 1 m^2. The system is operated at 0.75 and 1.25 A/cm^2 current densities in the electrolyser mode, and the steam flow rate for each current density is determined. To prevent the fuel electrode oxidation, 10 volume% hydrogen is mixed with the steam [12]. The cell voltage, power required for electrolysis, and amount of hydrogen available for the next cycle are obtained from the process simulation and high-pressure electrochemical model. From the process simulation, the amount of hydrogen required for the combustion to make the system auto-thermal in both modes of operation is estimated. The SOFC mode configuration is a hybrid fuel cell and gas turbine system. The gas turbine provides additional auxiliary power to the system in both modes of operation. The efficiency of the stack in SOFC and SOEC is determined based on the LHV in addition to the roundtrip efficiency.
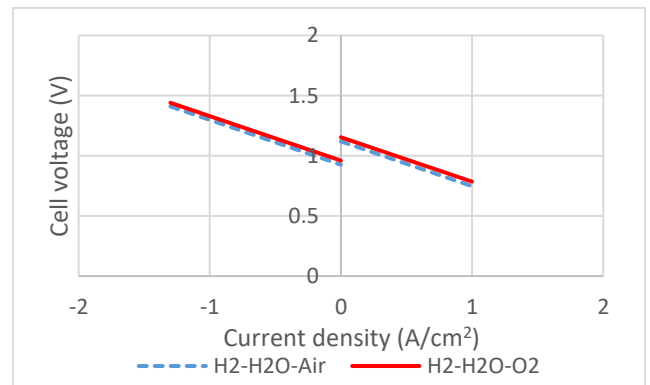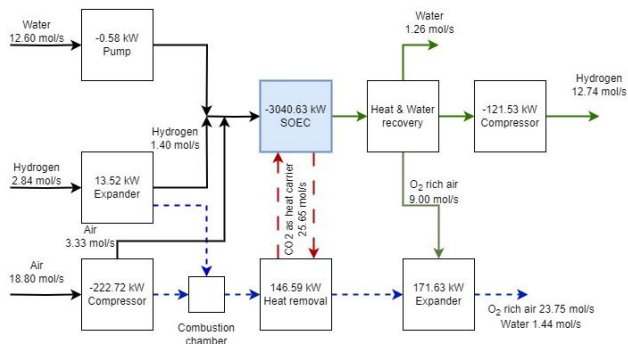

Fig. 2 j-V curve of ReSOC

Fig. 3 Schematic diagram during charging mode at 1.25 A/cm² for H_2-H_2O-Air system
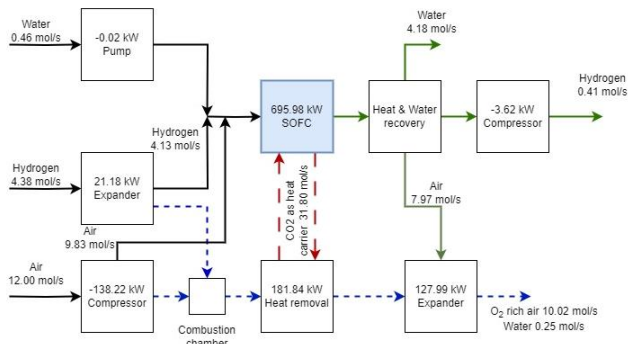

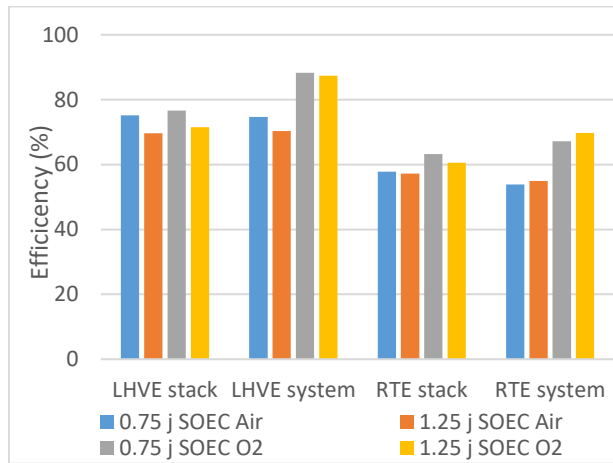Fig. 4 Schematic diagram during discharging mode for H_2-H_2O-Air system when SOEC operates at 1.25 A/cm²

Fig. 5 Performance of ReSOC system operating electrolyser mode at 0.75 and 1.25 A/cm² for H_2-H_2O-Air and for H_2-H_2O-O_2 systems

5. DISCUSSION

The results show that operating stack for 6 hours as electrolyser and as fuel cell for 15 hours makes the ReSOC system suitable for solar PV-based microgrid application. Figure 5 shows that the roundtrip efficiency and LHV efficiency do not vary significantly with the operating current density, making ReSOC suitable for

intermittent renewable energy storage-discharge applications as the system is capable of handling both high power and low power in SOEC mode. The H_2-H_2O-O_2 system shows significantly better results than the H_2-H_2O-Air system in terms of both stack and system-level performance.

6. CONCLUSIONS

ReSOC stack with BoP is developed for H_2-H_2O-O_2 and H_2-H_2O-Air based system operating at 750 °C and 20 bar. The characteristics of electricity storage and delivery of the proposed systems are analysed. Utilizing part of the hydrogen produced in electrolysis makes the system thermally self-sustainable, remaining hydrogen is stored for the power generation mode. Overall performance shows that the H_2-H_2O-O_2 system performs much better than the H_2-H_2O-Air system, with a roundtrip efficiency of around 70% compared to around 55% in the H_2-H_2O-Air system. This difference may be attributed to air compression in both modes which requires significantly higher parasitic power consumption. Operating ReSOC as electrolyser for 6 hours at high power and then as fuel cell for 15 hours at low power makes the system compactable for solar PV-based REES applications. A detailed techno-economic analysis for a case study is considered for future work.

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