



# Energy efficiency of an intermediate-temperature solid oxide iron–air redox battery



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## ABSTRACT

An ASPEN Plus based model is presented for an intermediate-temperature solid oxide iron–air redox battery (IT-SOIARB) system. The model shows that the energy efficiency of the system can be as high as 83%. Furthermore, the model is used to determine the factors that affect the energy efficiency of the battery. With air as the working fluid, a heat exchanger and thermal storage unit are included in the battery system to utilize effectively the heat generated from the discharge cycle in the charge cycle. The results show that air utilization (or air mass flow rate) plays a key role in regulating heat flow between the battery components.

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## 1. Introduction

Large-scale and cost-effective energy storage technology is vitally important to the implementation of a smart grid and renewable energy production. Among many types of energy storage options, Electrochemical energy storage (EES) technology is particularly attractive because of its fast response time, high energy capacity, modularity, and low cost. The major form of EES is rechargeable batteries, representative chemistries of which include the well-known lead-acid [1–3], Ni–Cd [4,5], Ni–MH [6–8], Li–ion [9–11], redox flow [12–14] and Na–S [15–17]. For large-scale grid storage applications, only redox flow and Na–S batteries have so far demonstrated the potential to be performance-competent and cost-effective. However, to be commercially viable, these technologies will need breakthroughs in materials discovery and engineering design.

In an effort to develop the next-generation advanced battery technology, we recently demonstrated a new type of battery based on reversible solid oxide fuel cells (RSOFCs) [18–20]. The core of the technology is the metal–air chemistry, storing and releasing oxygen in/by a metal/metal–oxide chemical bed integrated within a RSOFC operated under fuel-cell and electrolysis modes, respectively. Due to the use of solid oxide and redox materials, the new battery has also been named “Solid Oxide Metal–air Redox Battery” or SOMARB. Compared to other types of batteries, the new

battery possesses many distinguishing advantages over conventional redox flow and Na–S batteries: higher energy density, faster charge/discharge rates, safety, environmental friendliness and scalability, and therefore promises to be a next-generation battery system for large-scale renewable and grid energy storage. Since its first laboratory demonstration in 2011, significant progress has been made in the areas of performance enhancement [21–29], new redox chemistries [29–34] and computational analysis [35–41]. However, the ultimate commercialization of the SOMARB technology requires a full understanding of factors affecting system energy efficiency, which has not been addressed in the open literature.

In the present work, we present a system model to analyze the efficiency as well as performance determining factors for a Solid oxide iron–air redox battery or SOIARB operated at intermediate temperature, collectively IT-SOIARB. To increase the accuracy of the model, the electrochemical sub-model was validated by an experimental *V–I* curve. To achieve a heat balance between cycles, air was utilized as a working fluid to store, move and transfer heat among the three key components of the system: heat exchanger, thermal storage unit (TSU) and IT-SOIARB unit. The energy efficiency was particularly analyzed as a function of air utilization, current density and air outlet temperature.

## 2. The IT-SOIARB system

One of the most important thermal characteristics of the IT-SOIARB is the opposite heat signature for the discharge and charge

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## Nomenclature

$A$	Cross area of IT-SOIARB ( $\text{m}^2$ )
$C_p$	Heat capacity ( $\text{J kg}^{-1} \text{K}^{-1}$ )
$D$	Diffusion coefficient ( $\text{m}^2 \text{s}^{-1}$ )
$E$	Energy input or output ( $\text{kWh}$ )
$F$	Faraday's constant, 96485 ( $\text{C mol}^{-1}$ )
$F_{\text{air}}$	Molar flow rate of air ( $\text{mol s}^{-1}$ )
$F_{\text{O}_2}$	Molar flow rate of $\text{O}_2$ ( $\text{mol s}^{-1}$ )
$F_{\text{Fe}}$	Molar flow rate of Fe ( $\text{mol s}^{-1}$ )
$F_{\text{Fe}_3\text{O}_4}$	Molar flow rate of $\text{Fe}_3\text{O}_4$ ( $\text{mol s}^{-1}$ )
$G$	Gibbs free energy ( $\text{J mol}^{-1}$ )
$\Delta_{\text{Heat}}$	External heat flow provided to SOIARB at charge cycle ( $\text{kWh}$ )
$h_{\text{cycle}}$	Cycle time in hour (h)
$J$	Current density ( $\text{A m}^{-2}$ )
$J_{\text{ict}}$	Local charge transfer current density ( $\text{A m}^{-2}$ )
$M_{\text{air}}$	Molar weight ( $\text{kg mol}^{-1}$ )
$n$	Number of exchanged electrons (mol)
OCV	Open circuit voltage (V)
$p$	Pressure (Pa)
$P$	Power (kW)
PA	Power output/input
$Q$	Heat (W)
QCA	Heat stream to/from the battery
$R$	Gas constant, 8.314 ( $\text{J (mol}^{-1} \text{K}^{-1})$ )
$R_{\text{air}}$	Air utilization ratio
S1	Heat leakage of the battery
S4	Heat stored in TSU for discharge cycle
S17	Heat restored from TSU for charge cycle
$T$	Temperature (K)
$V$	Voltage (V)
$V_m$	Molar volume of air ( $\text{m}^3 \text{mol}^{-1}$ )

## Greek symbols

$\sigma$	Conductivity ( $\text{S m}^{-1}$ )
$\varepsilon$	Porosity of electrodes,
$\tau$	Tortuosity of electrodes
$\eta$	Overpotential (V)
$\eta_{\text{elec}}/\eta_{\text{energy}}$	Electric/energy efficiency
$\delta$	Thickness ( $\mu\text{m}$ )

## Subscripts

act	Activation overpotential loss
an	Anode
cat	Cathode
con	Concentration overpotential loss
$c$	Charge cycle
$d$	Discharge cycle
$e$	Electrode
eff	Effective
ele	Electrolyte
$i, m, n$	Species
$L$	Limiting
o	Oxygen electrode
ohm	Ohmic loss
h	Hydrogen electrode

## Superscripts

0	Ideal
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## Meaning of symbols

IT-SOIARB	Intermediate-temperature solid oxide iron–air redox battery
RSOFC	Reversible solid oxide fuel cell

RCU	Redox cycle unit
SOIARB	Solid oxide iron–air redox battery
SOEC	Solid oxide electrolysis cell
TSU	Thermal storage unit

cycles. An efficient utilization of the heat liberated from the discharge cycle ( $\text{H}_2$  and iron oxidation reactions) by the endothermic charge cycle ( $\text{H}_2\text{O}$  and iron oxide reduction reactions) can lead to a better energy efficiency. In the present study, a separate air heat exchanger and thermal storage unit (TSU) are included as integrated parts of the system to reuse and capture the heat liberated from the discharge cycle for the charge cycle. Air is used as the working fluid to store, transport and transfer heat. Fig. 1 shows a schematic of the IT-SOIARB system analyzed in this study. The operating temperatures of interest for the study are  $550^\circ\text{C}$  for the discharge cycle and  $500^\circ\text{C}$  for the charge cycle; at these temperatures the prevalent redox couple in the energy storage redox cycle unit (RCU) is  $\text{Fe}/\text{Fe}_3\text{O}_4$ . The operating temperature was assumed to be constant for simplicity.

The system under analysis consists primarily of an IT-SOIARB stack, TSU, heat exchanger and air pump. During the discharge cycle, ambient fresh air is first preheated by the hot air exiting from the IT-SOIARB stack. This preheated air then enters the air channel of the IT-SOIARB. This design recovers the waste heat in the exhaust air while delivering  $\text{O}_2$  to the cathode for the electrochemical reaction. At the exit of the air channel, the heat-loaded air enters the TSU to store a majority of the process heat for the charge cycle. Clearly, the total molar flow rate of air, temperature of exhaust air and the capacity of the TSU will have a significant impact on the thermal balance and therefore the energy efficiency of the system. For the charge cycle, the above process flows are reversed as shown in Fig. 1(b). In this case, the preheated air passes through the TSU to extract stored heat before entering the IT-SOIARB stack.

## 3. Model description

A 5 kW/60 kWh IT-SOIARB system intended for residential solar panel/battery applications was modeled by using the commercial software known as ASPEN Plus [42]. The simulation flow diagram for the system shown in Fig. 1 is illustrated in Fig. 2, which contains all the components and functionalities specified in the IT-SOIARB system.

In Fig. 2, the mass and heat streams are represented by black solid lines and red dashed lines, respectively, while the power input/output streams are represented by magenta solid lines. The heat streams S1 accounts for the heat leakage of the battery during cycles, S4 for the heat stored in TSU during the discharge cycle, S17 for the heat supplied by TSU for the charge cycle, and finally QCA for the heat demand by the charge cycle, or heat released by the discharge cycle. The power terms PA represent the power output from the discharge cycle and input for the charge cycle, respectively.

The commercial system software known as Aspen Plus was selected for the analysis. This software is capable of calculating thermodynamic properties at a defined states of chemical processes. Details of the model construction can be found in the Appendix A. The general considerations/assumptions used in the model are:

1. Air is composed of  $\text{O}_2$ ,  $\text{N}_2$  and  $\text{H}_2\text{O}$ , with a composition (mole fraction) of 0.21:0.78:0.01.
2. The reaction occurring in SOIARB is simplified to the overall reaction, as there is no built-in module for the battery in ASPEN Plus.

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