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Transient reversible solid oxide cell reactor operation – Experimentally validated modeling and analysis

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HIGHLIGHTS

- A hydrogen based system model was built using a dynamic validated reactor model.
- A simple system configuration led to a roundtrip storage efficiency of 42%.
- Mode switch from SOFC to SOEC mode possible in 1 min.
- Spatial and temporal temperature gradient in rSOC respected during mode switch.
- Temporal thermal gradient restricted to 15 K/min during mode switch.

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ABSTRACT

A reversible solid oxide cell (rSOC) reactor can operate efficiently in both electrolysis mode and in fuel cell mode. The bidirectional operability enables rSOC reactors to play a central role as an efficient energy conversion system for energy storage and sector coupling for a renewable energy driven society. A combined system for electrolysis and fuel cell operation can result in complex system configurations that should be able to switch between the two modes as quickly as possible. This can lead to temperature profiles within the reactor that can potentially lead to the failure of the reactor and eventually the system. Hence, the behavior of the reactor during the mode switch should be analyzed and optimal transition strategies should be taken into account during the process system design stage. In this paper a one dimensional transient reversible solid oxide cell model was built and experimentally validated using a commercially available reactor. A simple hydrogen based system model was built employing the validated reactor model to study reactor behavior during the mode switch. The simple design leads to a system efficiency of 49% in fuel cell operation and 87% in electrolysis operation where the electrolysis process is slightly endothermic. Three transient operation strategies were studied. It is shown that the voltage response to transient operation is very fast, provided the reactant flows are changed equally fast. A possible solution to ensure a safe mode switch by controlling the reactant inlet temperatures is presented. By keeping the rate of change of reactant inlet temperatures five to ten times slower than the mode switch, a safe transition can be ensured.

1. Introduction

Higher penetration of intermittent renewable energy sources in the energy mix poses certain critical challenges. The intermittent nature of the renewable sources requires an efficient energy conversion system for energy storage and grid stabilization [1]. Moreover, with reduction in fossil fuel use, alternate synthesis routes for important industrial chemicals have to be developed [2]. Storing electrical energy in form of chemical energy is advantageous due to higher storage capacity and facilitates sector coupling of the energy storage industry with the chemical industry. An rSOC reactor can address the above challenges by operating both as a Solid Oxide Electrolyser Cell (SOEC) and as a Solid Oxide Fuel Cell (SOFC). During the energy storage mode, the electrical energy is converted to chemical form by means of electrolysis. When electrical energy is required, the chemical energy is converted back to electrical energy via fuel cell operation. The high operating

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Nomenclature

Symbols	Description, Unit
Latin	
ASR	area specific resistance, Ω m^2
b	effective width of the single repeat unit, m
c	specific heat capacity, J/(kg K)
c_p	specific heat capacity at constant pressure, J/(kg K)
D	diffusion coefficient, m^2/s
E	energy, J
F	Faraday's constant, C/mol
H	height of the flow channel, m
h	specific enthalpy, J/kg S
I	current, A
j	current density, A/m^2
j_o	exchange current density, A/m^2
k^+	velocity of forward direction of reaction, mol/(s m^2 bar)
k^-	velocity of reverse direction of reaction, mol/(s m^2 bar)
l	length of the single repeat unit, m
m	mass, kg
$\dot{m}$	mass flow rate, kg/s
M	molecular mass, kg/mol
N	moles, mol
p	pressure, pa
$\dot{q}$	heat flow rate, W
r	reaction rate, mol/(s m^2)
R	ideal gas constant, J/(mol K)
T	temperature , K
U	voltage, V
x	mole fraction, 1
Greek letters	
α	convective heat transfer coefficient, W/(m^2 K)
β	charge transfer coefficient, 1
Δ	mathematical operator implying a change in quantity
δ	thickness of a functional layer, m
ε	emissivity of the material, 1
ϵ	porosity of the material, 1
γ	frequency factor of the electrode reactions, A/m^2
λ	conductive heat transfer coefficient, W/(m K)
κ	equilibrium constant of a reaction, 1
ν	stoichiometric coefficient of species in a reaction, mol
υ	dynamic viscosity of gas flow, kg m/s^2
ρ	density, kg/m^3
ψ	tortuosity coefficient, 1
σ	specific charge conductivity of a the functional layers, S/m
σ_o	specific conductivity at a reference condition, S/m

Superscripts	
'	represents quantity entering the control volume
''	represents quantity leaving the control volume
a	air electrode side or air flow side
bulk	represents the bulk fluid flow in flow chamber
f	fuel electrode side or fuel flow side
eff	effective
ic	interconnects
mea	membrane-electrode assembly
tpb	triple phase boundary
Subscripts	
a	air flow
act	activation process
ae	air electrode
diffusion	diffusion process
f	fuel side flow
fe	fuel electrode
cond	conduction
conv	convection
hor	hydrogen oxidation reaction
ic	interconnect
id	thermodynamic conditions or ideal conditions
k	Knudsen diffusion coefficient
o	oxygen atoms
ocv	open circuit voltage
ohm	ohmic process
op	operation point
rad	radiation
smr	reverse steam methane reforming reaction
wgs	reverse water gas shift reaction
Abbreviations	
ASR	area specific resistance
CV	control volume
EOO	equation based object oriented
EIS	electrochemical impedance spectroscopy
GDC	gadolinium doped ceria
LSCF	lanthanum-strontium-cobalt ferrate
MEA	membrane-electrode assembly
OCV	open circuit voltage
rSOC	reversible solid oxide cell
SOC	solid oxide cell
SMR	reverse steam methane reforming reaction
SOFC	solid oxide fuel cell
SOEC	solid oxide electrolysis cell
SRU	single repeating unit
WGS	reverse water gas shift reaction
3 YSZ	3 mol% Yttrium stabilized zirconia

temperatures of SOCs offer many advantages. At higher operation temperatures a greater portion of the energy required for the electrolysis reaction can be supplied as heat when operated in endothermic mode, therefore enabling higher roundtrip efficiency.

To realize such systems, process system analyses have to be performed and complex system architectures have to be investigated. Mottaghizadeh et al. [3] proposed a methane based rSOC system with a downstream methanation process achieving a roundtrip efficiency of 60% operating at 25 bar. Jensen et al. [4] and Monti et al. [5] developed an rSOC system based on a fuel electrode supported rSOC stack design with maximum efficiencies of 60% and 65% respectively. Frank et al. [6] reported an rSOC system based on hydrogen with fuel recirculation and integrated reactor heating whereby a roundtrip efficiency of 51% is reached. The system concepts reported in literature considered highly integrated process system designs to achieve high system efficiencies. Finally, the process system analyses were performed with simplified block models which do not account for the practical limitations of rSOC reactor operation. This can often lead to overestimation of system performances or to operating conditions that would result in reactor failure due to local effects that 0-D models will not reveal. Li et al. [7] quantitatively showed the effect of implementing a detailed reactor model in a SOFC system and its impact on