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A novel design of solid oxide electrolyser integrated with magnesium hydride bed for hydrogen generation and storage – A dynamic simulation study

Chen Bin [a], Haoran Xu [a], Houcheng Zhang [a,b], Peng Tan [a], Weizi Cai [a], Meng Ni [a,c,*]

[a] Building Energy Research Group, Department of Building and Real Estate, The Hong Kong Polytechnic University, Hung Hom, Kowloon, Hong Kong, China
[b] Department of Microelectronic Science and Engineering, Ningbo University, Ningbo 315211, China
[c] Environmental Energy Research Group, Research Institute for Sustainable Urban Development (RISUD), The Hong Kong Polytechnic University, Hong Kong, China

HIGHLIGHTS

- A novel tubular electrolyser is designed integrating SOEC and the metal hydride bed.
- The hydrogen generation and storage can be achieved in situ.
- The dynamic performance of the tubular electrolyser is simulated.
- Effects of pressure, voltage and cooling air temperature are discussed.

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ABSTRACT

This paper proposes a novel solid oxide steam electrolyser with in-situ hydrogen storage by integrating a magnesium hydride (MH) section with proton-conducting solid oxide electrolysis cell (SOEC) section. Dynamic simulation results show that it takes 1950 s to fully charge the MH section with a 56% H_2 storage efficiency without any flow recirculation, when the electrolyser is operated at 1.4 V and 4 atm, yielding a current density of 4956.40 A/m^2. The evolution of temperature, H_2 partial pressure and reaction of Mg powder through the charging process are analysed. It is found that the exothermic H_2 absorption process of MH section can enhance the performance of the electrolysis process of SOEC section. The effects of operating parameters including operating pressure, electrolysis voltage, and cooling air temperature on the performance of the novel design are investigated by sensitivity studies. Results show that it is beneficial to operate the electrolyser at elevated pressure for shorter absorption time and higher H_2 storage efficiency. Increasing the operating voltage can shorten the absorption time, but lower H_2 storage efficiency. An optimal cooling air temperature is found at 521 K when the electrolyser is operated at 1.4 V and 4 atm.

1. Introduction

Hydrogen is a clean energy carrier, yielding only H_2O as a by-product when releasing its chemical energy via combustion or electrochemically conversion. This merit is attracting extensive research on hydrogen production and utilization when environmental issues are becoming urgent worldwide.

Hydrogen is conventionally produced from fossil fuels by steam reforming process, which will inevitably generate greenhouse gas emissions and pollutants [1–3]. Thermochemical and photocatalytic splitting of water for hydrogen production both have drawbacks of low energy efficiency [4]. Alternatively, water electrolysis process using renewable energy can be a sustainable solution when the electric power is from the wind, solar, redundant grid power, or waste heat.

Solid oxide electrolysis cell (SOEC) operated at high temperature (ca. 600–800 °C) nowadays are receiving much attention for

Abbreviations: BZCY, $BaCe_{0.5}Zr_{0.3}Y_{0.2}O_{3-\delta}$; CFD, computational fluid dynamics; CHP, combined heat power system; CNF, carbon nanofibers; CNT, carbon nanotubes; HT-PEM, high temperature proton exchange membrane fuel cell; MH, metal hydride bed; MOF, metal organic framework; OCV, open circuit voltage; PEM, proton exchange membrane; SOEC, solid oxide electrolysis cell; SSC, $Sm_{0.5}Sr_{0.5}CoO_{3-\delta}$; TPB, triple phase boundary.

* Corresponding author at: Building Energy Research Group, Department of Building and Real Estate, The Hong Kong Polytechnic University, Hung Hom, Kowloon, Hong Kong, China.
E-mail address: bsmengni@polyu.edu.hk (M. Ni).

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Nomenclature

Letters

AV_a, AV_c	electrochemically active specific surface area, m^{-1}
$D_{eff,ij}$	effective binary diffusion coefficient of i and j, $m^2\ s^{-1}$
D_{ij}	binary diffusion coefficient of species i and j, $m^2\ s^{-1}$
E_{H_2O}	equilibrium Nernst potential of H_2O electrolysis, V
E_a	activation energy, J mol^{-1}
I_{SOEC}	current density of SOEC, A m^{-2}
L_{MH}	length of the MH bed, mm
L_{SOEC}	length of the SOEC section (cathode layer coated), mm
$Q_{H_2.ab}$	heat source due to hydrogen absorption, J $m^{-3}\ s^{-1}$
Q_{SOEC}	heat source due to electrolysis, J $m^{-3}\ s^{-1}$
$R_{H_2.ab}$	reaction rate of hydrogen absorption in MH bed, kg $m^{-3}\ s^{-1}$
$R_{i.elec}$	reaction rate of species due to electrolysis, kg $m^{-3}\ s^{-1}$
$T_{MH,av}$	average temperature of MH section, K
$T_{SOEC,av}$	average temperature of SOEC section, K
T_{airin}	inlet temperature of air flow, K
T_{fuelin}	inlet temperature of fuel flow, K
V_{op}	operating voltage, V
c_p	specific heat, J $kg^{-1}\ K^{-1}$
$i_{o.a/c}$	exchange current density, A m^{-2}
$i_{source.a}$	local current source of anode (air side), A m^{-3}
$i_{source.c}$	local current source of cathode (fuel side), A m^{-3}
k_a	reaction rate constant, 2.98×10^{-8}, s^{-1}
p_i	partial pressure of species i, Pa
r_E	outer radius of the SOEC-MH electrolyser's cooling air channel, mm
r_{MH}	radius of the MH bed, mm
r_{SOEC}	outer radius of the SOEC tube, mm
v_i	stoichiometric number of species i
w_i	mass fraction of species
w_t	gravimetric hydrogen storage capacity of the MH bed, %
w_{de}	gravimetric hydrogen storage capacity of the device, %
x_j	mole fraction of species j
η_{H_2}	H_2 storage efficiency
η_{act}	activation polarization, V
η_{ohmic}	ohmic polarization, V
$\varnothing$	potential, V
DeltaH	enthalpy change
DeltaS	entropy change
t	time, s
L	length of the SOEC-MH electrolyser, mm
M	molecular weight of Magnesium, 24.3 g/mol
M_{MH}	mass of the MH bed, kg
M_{SOEC}	mass of the SOEC, kg
R	gas constant, 8.314 J $mol^{-1}\ K^{-1}$
T	local temperature, K
U	velocity field, $m^3\ s^{-1}$
X	reacted fraction of Mg
i	local current density, A m^{-2}
p	pressure, Pa
ε	porosity
κ	permeability, m^2
κ	permeability, m^2
λ	thermal conductivity, W $m^{-1}\ K^{-1}$
μ	dynamic viscosity of fluid, Pa s
ρ	density, kg m^{-3}
σ	conductivity for ion/electron,·m^{-1}
τ	tortuosity factors

Subscripts

a	anode
ab	absorption
act	activation
airin	air flow inlet
av	average
c	cathode or cutoff
eff	effective
eq	equilibrium
g	gas phase
i	species index
l	electrolyte
op	operating
ref	reference
s	solid

water electrolysis [5,6], due to its high efficiency, and capability of recovering waste heat, which is more advantageous than the low temperature Nafion-based proton exchange membrane (PEM) electrolyser [7]. However, a lot of technical issues remain to be addressed before the commercialization of SOEC. Besides material degradation and cost issues, the hydrogen storage remains a challenge, hindering the application of SOEC in the renewable energy system.

Hydrogen, the lightest element, behaves as a low volumetric energy carrier at ambient pressure, thus requiring large compression work to improve its volumetric energy density in the case of high pressure storage (35–70 MPa) [8]. Other popular storage methods can be classified into liquefaction storage and sorption storage (adsorption/absorption). Liquefaction storage also demands large amount energy to liquefy the hydrogen (boiling point: 21.2 K at 1 atm) in the liquefaction process (eg. Linde cycle) [9]. Besides, leakage problems caused by permeation and evaporation make the liquid storage and pressure storage not energy efficient options. Differently, the sorption storage method adsorbs the hydrogen molecules/atoms onto solid surface of porous storage medium or chemically fixes the hydrogen by the reaction of hydrogen with metal to form hydrogen hydrides [10]. Thus, sorption storage shows advantages of less energy requirement, high reversibility, and low safety risk due to the moderate storage pressure and temperate. More importantly, most sorption storage media excel in the volumetric/gravimetric capacity compared to compressed H_2 gas or liquefied hydrogen. For example, pure carbon nanotube/nanofibers (CNT/CNF) can uptake hydrogen by physisorption at a theoretical capacity of 7.7 wt% [11] or even up to 20 wt% using alkali-doped CNTs at ambient pressure and moderate temperature (200–400 °C) [12]. The metal organic framework (MOF) is another kind of physisorption media, the porous cubic crystalline structure of which can uptake 1 wt% storage at room temperature and 20 bar or 4.5 wt% at 78 K and 0.8 bar [13].

Metal hydrides, which are usually solid metal-hydrogen compounds, are considered as good candidates for hydrogen storage in high mobility applications, promising to fulfill the 6.5 wt% hydrogen target set by the U.S. Department of Energy. Generally, metals (eg. Li, Na, Mg, Ti) or intermetallic compounds ($LaNi_5$, Mg_2Ni) can react with hydrogen to form metal hydrides (β-phase) when the hydrogen atoms behave like a metal element and dissolved into the metal (solid-solution, α-phase) [10]. The α-β transition process can be described by the pressure-concentration-temperature plot and Van't Hoff law [14] in Fig. 1, from which a flat charging & discharging pressure plateau can be observed. Additional heat is required to maintain the endothermic desorption process.

Presently, metal hydride has been integrated with fuel cells in energy power systems as the hydrogen desorbed from hydride is