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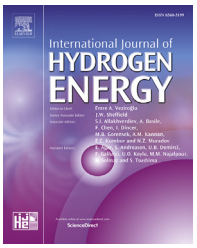

Model development and analysis of a novel high-temperature electrolyser for gas phase electrolysis of hydrogen chloride for hydrogen production

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ABSTRACT

In this study, a high temperature electrolyser for the gas phase electrolysis of hydrogen chloride for hydrogen production is proposed and assessed. A detailed electrochemical model is developed to study the J-E characteristics for the proposed electrolyser (a solid oxide electrolyser based on a proton conducting electrolyte). The developed model accounts for all major losses, namely activation, concentration and ohmic. Energy and exergy analyses are carried out, and the energy and exergy efficiencies of the proposed electrolyser are determined to be 41.1% and 39.0%, respectively. The simulation results show that at T = 1073 K, P = 100.325 kPa and J = 1000 A/m^2, 1.6 V is required to produce 1 mol of hydrogen. This is approximately 0.3 V less than the voltage required by a high temperature steam electrolyser (based on a proton conducting electrolyte) operating at same condition (T = 1073 K, P = 101.325 kPa and J = 1000 A/m^2), suggesting that the proposed electrolyser offers a new option for high temperature electrolysis for hydrogen production, potentially with a low electrical energy requirement. The proposed electrolyser may be incorporated into thermochemical cycles for hydrogen production, like Cu–Cl or chlorine cycles.

Introduction

Researchers around the globe are seeking energy sources which are environmental friendly and sustainable like renewable and nuclear energy. It is expected that, by the year 2050, the use of renewable energy in meeting energy demands is going to be double that of the year 2016 [1], suggesting that renewable energy will play a major role in meeting future energy demand. Hydrogen is considered a good energy carrier, with excellent potential to act as link between nuclear and renewable energy resources [2]. There is an increasing level of interest in the development of large-scale hydrogen production systems using nuclear energy [3].

Kondo et al. [4] have studied the gas phase electrolysis of hydrogen halide (HX) gases (such as HBr or HI) utilising an electrolyser. They report that gas phase electrolysis is superior to aqueous electrolysis in the following respects. Less theoretical voltage is required, because the gaseous phase HX molecule is at higher energy level compared to aqueous state.

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Nomenclature

B_g	permeation coefficient (m^2/s)
d	thickness of electrode (m)
D	diffusion coefficient (cm^2/s)
E	potential (V)
ex	specific exergy (kJ/kg)
F	Faraday constant (C/mol)
g	specific Gibbs free energy (kJ/mol)
J	current density (A/m^2)
k_b	Boltzmann constant (m^2kg/s^2K)
L	electrolyte thickness (m)
LHV	lower heating value (kJ/kg)
$\dot{m}$	mass flow rate (kg/s)
M	molar weight (kg/kmol)
p	partial pressure (atm)
P	total pressure (atm)
r	mean pore radius of the electrode (m)
R	universal gas constant (8.314 J/molK)
T	temperature (K)
W	work input rate (kW)

Greek Letters

ε	electrode porosity
η	efficiency
μ	dynamic viscosity (Ns/m^2)
Ω	dimensionless collision integral
ϕ	electrical resistivity of the electrolyte (Ωm)
ρ	electrical conductivity (S/m)
σ	mean characteristic length (Å)
τ	dimensionless temperature
ξ	electrode tortuosity
ε/k	Lennard-Jones potential (K)

Subscripts

a	anode
act	activation
c	cathode
conc	concentration
d	destruction
eff	effective
el	electric
elec	electrolyser
en	energy
ex	exergy
k	Knudsen
ohm	ohmic
tot	total
0	standard, exchange

Also, in the case of aqueous electrolysis it is essential to remove the product halogen (X_2) due to its solubility in the aqueous solution whereas in gas phase electrolysis, X_2 is insoluble due to presence of the electrolyte. Finally, in several thermochemical cycles, HX gases are produced (mostly in the gaseous phase), and the presence of HX in gaseous phase is favorable and efficient.

Proton conducting solid oxide electrolysers have some advantages over oxygen conducting electrolysers, such as better ionic conductivity compared to oxygen ion conductors at a moderate temperature range (773 K–973 K), and better chemical compatibility with nickel [5–7]. In addition, a proton conducting solid oxide electrolyser produces pure and dry hydrogen [8,9].

In the present study, a high temperature electrolyser (a solid oxide electrolyser based on proton conducting electrolyte) for the gas phase electrolysis of hydrogen chloride gas for hydrogen production is developed, and assessed in terms of energy, exergy and voltage efficiencies. The electrolyser incorporated has a proton conducting membrane of SCY10 ($SrCe_{0.95}Y_{0.05}O_{3-\delta}$-ZnO), which can operate with temperature range 773 K–1173 K [10]. A detailed electrochemical model is developed to study the J-E characteristics for the proposed electrolyser. The effects are evaluated of such parameters as operating temperature, current density, and hydrogen production rate on the required potential and the energy, exergy and voltage efficiencies of the proposed electrolyser.

Fig. 1 shows the working mechanism of the proposed high temperature electrolyser for the gas phase electrolysis of HCl for hydrogen production. HCl gas is fed to the porous anode where it is electrochemically split to form chlorine gas and hydrogen ions (H^+) at the anode-electrolyte interface, according to

$$2HCl \rightarrow Cl_2 + 2H^+ + 2e^- \quad (1)$$

The produced chlorine gas can be collected from the anode flow channel. The hydrogen ions pass through the electrolyte to the cathode and are reduced to form hydrogen gas in the following reaction:

$$2H^+ + 2e^- \rightarrow H_2 \quad (2)$$

Thus, the net reaction can be expressed as

$$2HCl \rightarrow H_2 + Cl_2 \quad (3)$$

Analysis

In this section, a complete electrochemical model including all major losses (activation, concentration and ohmic) for the proposed electrolyser is developed and the performance is assessed by evaluating the energy, exergy and voltage efficiencies. As with other electrochemical models [8,11] for steam electrolysers, the following reasonable assumptions and simplifications are used [12–14]:

- A one dimensional electrochemical model is adequate.
- The operation is at steady state.
- No temperature variation exists in the porous electrode layer.
- All electrochemical reactions take place at the electrode-electrolyte interface.

Electrochemical model

The electrolyser selected has a membrane SCY10 ($SrCe_{0.95}Y_{0.05}O_{3-\delta}$-ZnO), which can operate within temperature range of the electrochemical model adopted. As with a

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