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Computational fluid dynamics approach for performance evaluation of a solid oxide electrolysis cell for hydrogen production

Maria Navasa *, Jinliang Yuan, Bengt Sundén

Division of Heat Transfer, Department of Energy Sciences, Lund University, P.O. Box 118, SE-221 00 Lund, Sweden

HIGHLIGHTS

- A three-dimensional FVM based CFD model for a cathode-supported SOEC is developed.
- The effect of different operating voltages on cell performance is investigated and analyzed.
- Cross-flow and parallel-flow configurations are compared and differences are identified.

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ABSTRACT

A finite volume method based computational fluid dynamics model has been developed and applied for a cathode-supported planar solid oxide electrolysis cell (SOEC) operating in cross-flow configuration arrangement. The performance behavior, in terms of current density, temperature distribution and hydrogen production in an SOEC, has been investigated for different operating voltages and compared with a corresponding parallel-flow configuration. The predicted results show that higher current densities are obtained for higher operating voltages. The anodic current density is higher than the cathodic one. Yet, the parallel-flow configuration yields lower current density values although they remain in the same order of magnitude as those from the cross-flow arrangement. The simulation reveals various temperature profiles depending on the operating voltage emphasizing the three thermal operating modes of an SOEC, i.e., endothermic, thermo-neutral and exothermic. Per contra, the parallel-flow arrangement gives a temperature decrease along the flow direction although operating in exothermic mode. Higher hydrogen molar fractions at the outlet of the cathode channel were obtained at higher operating voltages due to the higher current densities generated and the exothermic operating mode. The parallel-flow arrangement yields lower hydrogen production due to the lower current densities revealed.

1. Introduction

Hydrogen, an ideal energy carrier, is considered to be an encouraging fuel candidate for improving the usage of renewable energy sources. Due to the increasing interest of hydrogen as a fuel, industry and governmental institutions are putting more effort to develop hydrogen-related technologies [1]. Despite the fact that nowadays the main hydrogen source is hydrocarbon reforming, hydrogen can also be obtained through green energy procedures such as water splitting (electrolysis, photolysis or thermochemical water splitting) and biomass [2–5]. At present, water electrolysis is the most viable process for hydrogen production at large scales and consists of splitting water into hydrogen and oxygen by applying electrical energy [2]. The thermal energy required for electrolysis increases with temperature while the required electrical energy decreases. Thus, high-temperature electrolysis might be a really interesting process to consider when waste heat from other processes is available [1,2]. Actually, electrolyzer cells can use the waste heat from industry and the electricity obtained from solar cells or wind turbines. Moreover, there is growing interest in integrating electrolysis cells together with nuclear energy to improve the hydrogen production efficiency [6,7].

However, the production of hydrogen via water electrolysis, especially via solid oxide electrolysis cells (SOECs), is strongly dependent upon two main factors. The first refers to the restriction of the consumption of fossil fuels, mainly by political reasons, which will lead to an increase of energy supply from renewable energy sources and a consequent increasing interest in hydrogen related energy technologies. The second factor is if the energy price for energy from non-fossil fuels sources, i.e., solar or wind energy, is lower than that of the energy from fossil fuels. Regarding the

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* Corresponding author. Tel.: +46 462228610.
E-mail address: Maria.Navasa@energy.lth.se (M. Navasa).

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Nomenclature

c_p	specific heat at constant pressure [$J\ kg^{-1}\ K^{-1}$]
D_m	mass diffusion coefficient [$m^2\ s^{-1}$]
D_T	thermal diffusion coefficient [$kg\ m^{-1}\ s^{-1}$]
F	Faraday constant [$C\ mol^{-1}$]
i_0	exchange current density [$A\ m^{-2}$]
$\mathbf{J}$	mass diffusion flux [$kg\ m^{-2}\ s^{-1}$]
j	volumetric current density [$A\ m^{-3}$]
K	permeability [m^2]
k	thermal conductivity [$W\ m^{-1}\ K^{-1}$]
N	number of species i in the gas mixture, dimensionless
n_e	number of electrons transferred per reaction, dimensionless
P	pressure [Pa]
S	entropy [$kJ\ mol^{-1}\ K^{-1}$]
S_d	source term for the momentum conservation equation [$W\ m^{-3}$]
S_m	source term for the mass conservation equation [$kg\ m^{-3}\ s^{-1}$]
S_T	source term for the energy conservation equation [$W\ m^{-3}$]
S_Φ	source term for the charge transfer equation [$A\ m^{-3}$]
T	temperature [K]
$\mathbf{U}$	velocity vector [$m\ s^{-1}$]
V	voltage [V]
Y_i	molar fraction of species i, dimensionless

Greek letters

η	polarizations [V]
μ	dynamic viscosity [Pa s]
ρ	density [$kg\ m^{-3}$]
σ	electric conductivity [$S\ m^{-1}$]
Φ	potential [V]

Subscripts and superscripts

act	activation
an	anode
cat	cathode
i	gas species *i*
j	gas species *j*
Ω	ohmic

Abbreviations

CFD	computational fluid dynamics
FVM	finite volume method
HTE	high-temperature electrolysis
SOEC	solid oxide electrolysis cell
SOFC	solid oxide fuel cell
TPB	triple-phase boundary

Chemical species compounds

CH_4	methane
CO	carbon monoxide
CO_2	carbon dioxide
e^-	electron
H_2	hydrogen
H_2O	water
O_2	oxygen
O^{2-}	oxide ion

second condition, the production cost of hydrogen and syngas will define the potential and viability of SOECs. The production cost of hydrogen and syngas by SOECs is mainly defined by the following parameters: the electricity price and the cell specifications and requirements (costs of cells and stacks, performance and durability of the device) [8]. The main part of the production cost of hydrogen and syngas is the electricity cost [2,9]. At higher operating temperatures, less electricity is required compared to low-temperature processes which can help to decrease the electricity cost. Nevertheless, if electricity at lower prices can be obtained from renewable energy sources, the production price can be lowered. Another factor that can even lower more the production price if operating at high temperatures is using the waste heat from other processes, as previously mentioned, as heat for steam generation. From a global perspective, most of the electricity produced nowadays is by fossil energy sources with relatively low efficiency compared to some renewable energy sources. For example, a SOEC operating in reversed mode, as a fuel cell, has an efficiency for electricity production of 60% compared to a 30–40% provided by conventional gas turbine power plants [9]. Another advantage that SOECs present in comparison with other electrochemical processes or hydrogen production methods is that it can be used as a device for recycling or reusing carbon dioxide from other energy systems or as a CO_2 capture device, i.e., a possibility for CO_2 storage. Although the materials used are relatively expensive for the cell production, research in this area is moving forward but a major concern is how to improve the performance and durability of the cell.

High-temperature electrolysis (HTE) of water takes place at high temperatures (700–1000 °C) and its technology is based on the high-temperature fuel cells, especially solid oxide fuel cells (SOFCs). Thus, one of the most typical devices for HTE is the solid oxide electrolysis cell (SOEC), see Fig. 1. SOECs are usually understood as SOFCs operating in reversed mode. Steam is fed into the electrolysis cell where water splitting takes place giving hydrogen and oxygen as products, as shown in Eq. (1). Thus, an SOEC is comprised of the same components as an SOFC: fuel and air channels and two electrodes (anode and cathode) separated by an electrolyte. However, it seems that the transport characteristics in SOECs differ considerably from SOFCs, especially related to kinetic reactions, and thus, results from SOFCs cannot be directly applied to SOECs, emphasizing the significant need for SOEC modeling as relatively little has been done in this field [10,11].

$$H_2O_{(g)} \rightleftharpoons H_{2(g)} + O_{2(g)} \tag{1}$$

2. Problem statement

Water steam is fed into the fuel channels on the cathode side. The water molecules diffuse through the porous cathode structure (the cathode diffusion layer in Fig. 2) to the triple phase boundary (TPB) at the cathode-electrolyte interface (the cathode TPB layer in Fig. 2) where they react with the electrons supplied by an external source to produce hydrogen gas and oxygen ions, Eq. (2). The oxide ions (O^{2-}) are transported through the electrolyte to the TPB at the anode-electrolyte interface (the anode TPB layer in Fig. 2) where the oxide ions are oxidized to oxygen gas, as shown in Eq. (3). The oxygen gas molecules produced diffuse through the porous anode structure (the anode diffusion layer in Fig. 2) to the outlet at the air channel.

$$H_2O_{(g)} + 2e^- \rightleftharpoons H_{2(g)} + O^{2-} \tag{2}$$

$$O^{2-} \rightleftharpoons 1/2O_{2(g)} + 2e^- \tag{3}$$

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