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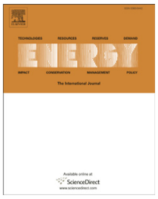

Comprehensive modeling of tubular solid oxide electrolysis cell for co-electrolysis of steam and carbon dioxide

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ABSTRACT

A two-dimensional (2D) model is developed to analyze the performance and efficiency of H_2O/CO_2 co-electrolysis in tubular SOEC (solid oxide electrolysis cell). The model fully considers the fluid flow, heat/mass transfer and electrochemical/chemical reactions in the SOEC. The results show that RWGSR (reversed water-gas shift reaction) significantly promotes CO_2 conversion ratio. The effect of important operating parameters was comprehensively studied and optimal operating condition was determined. When the inlet gas flows in parallel flow mode with the velocity of 1 m s^{-1}, TSOEC with the H_2O/CO_2 molar ratio of 1 at 700 °C at 1.4 V achieves the highest efficiency of 59.4% and the syngas conversion ratio of 43.8%. Lowering gas flow velocity decreases the syngas yield but promotes H_2O/CO_2 convert ratio and efficiency. Finally, calculation found that counter flow is superior to parallel flow.

1. Introduction

Renewable energy and hydrogen energy are regarded as promising energy forms due to sustainability and non-pollution [1–12]. SOEC (solid oxide electrolysis cell) has been studied extensively as a promising way for massive hydrogen production from renewable but unstable energy sources [1–3]. Compared with low temperature electrolyzers, the high temperature SOEC has faster reaction rate and less electrical energy consumption as a considerable fraction of required energy for electrolysis is in the form of heat [4]. To convert carbon dioxide sequestered from greenhouse gas-emitting process and produce synfuels, INL (Idaho National Laboratory) proposed the concept of co-electrolysis (i.e., electrolyzing CO_2/H_2O) in an SOEC [13]. In the SOEC, CO_2 and H_2O can be converted to H_2/CO syngas and pure O_2 via H_2O electrolysis, CO_2 electrolysis and reversible water gas shift reaction. The syngas can be further used as a feed stock for production of hydrocarbon chemicals via the Fischer–Tropsch (F–T) process [14].

A validated mechanistic model is helpful to understand the complex reacting and transport phenomena in SOEC as relevant information is hard to obtain by experiments. Currently, there are many models for describing the SOEC performance in steam electrolysis or co-electrolysis of steam and carbon dioxide [15–21]. For design optimization, a 3D model has been developed and solved with a commercial CFD (Computational Fluid Dynamic) software by Herring et al. [17] to study the planar SOEC at stack level. Ni [18,19] developed a 2D comprehensive thermal planar SOEC model to analyze the performance of co-electrolysis considering reversible WGSR (water-gas shift reaction) and DIR (direct internal reforming) reaction. This model discussed the effect of inlet temperature and gas composition and found that reversible DIR is not favored in H_2O/CO_2 co-electrolysis but the reversible WGSR can significantly influence the co-electrolysis behavior. Stempien et al. [20] studied a power plant extension system based on solid-oxide electrolyzer cell (SOEC) system and analyzed the effects of temperature, amount of exhaust gas recirculation and mole flux, a 46.2% of electricity-to-syngas efficiency was achieved. With commercial CFD software, Hawkes et al. [21] developed a 3D CFD model for H_2O/CO_2 co-electrolysis in a planar SOEC stack. Modeling results provide detailed profiles of temperature, Nernst potential, operating potential, anode-side gas composition, cathode-side gas composition,

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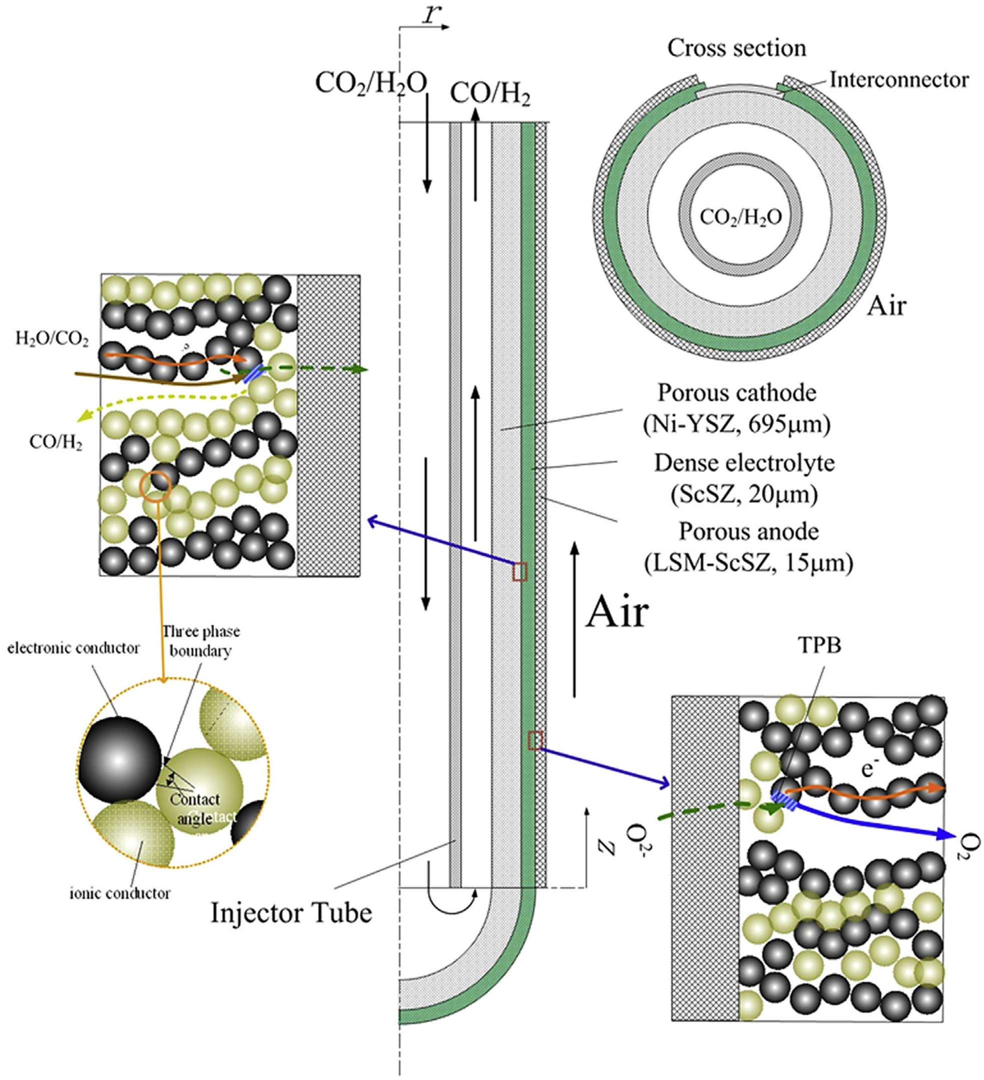

Fig. 1. TSOEC unit cell axisymmetric geometry and calculation domain.

current density and syngas production over a range of stack operating conditions, and is applied in assisting scale-up of SOEC in INL.

As mentioned above, the studies on SOEC modeling focus more on simulating button cell helpful to understand the mechanism, or developing comprehensive model of PSOEC (planar SOEC) to optimize the operating condition. PSOEC has large power density but is actually difficult to larger-scale application due to sealing problem. Among various types of SOECs, TSOEC (tubular solid oxide electrolysis cell) has the advantages of relatively more flexibility and fewer sealing problems, and is considered as one of the promising SOEC configurations for mid- to large-scale applications. Moreover, large working area can be acquired in tubes and cheaper metal is available to collect current because current collector of TSOEC is in reducing atmosphere. Many researches concentrate on modeling of tubular SOFC (solid oxide fuel cell), the inverse process of TSOEC [22–33]. However, models about TSOEC are rare. In this study, a 2D model coupling heat/mass transfer and electrochemical/chemical reactions was developed to analyze the performance and efficiency of co-electrolysis and optimize the operating condition in high temperature cathode-supported SOECs. The continuum model is adopted to simulate the porous electrode by using effective parameters related to porosity. Meanwhile, the area of TPB (three-phase boundary) is calculated by using the particle coordination number in binary random packing of spheres together with percolation theory. Therefore, a bridge connecting the micro-scale electrode model and the macro-scale cell unit model was built by extending the micro-scale electrode model to the tubular SOEC unit cell. The model can analyze not only the electrochemical process and gas species transport within the electrode, but also can provide the distributions of temperature, flow velocity and gas composition in whole reactor. Finally, the effects of temperature, cell voltage, inlet flow rate and flow mode on the performance and efficiency of SOEC unit were studied.

2. Model development

2.1. Model assumptions and calculation domain

Numerical model of tubular SOEC was developed by coupling governing equations of charge, mass, momentum, energy transport equations. The modeling geometry of the tubular SOEC unit is shown in Fig. 1. Steam and carbon dioxide are supplied to the injector tube with length 150 mm and inner diameter 5 mm. Air inflows from the bottom of tube surrounding the anode. Cathode

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