Parametric analysis of CO_2 and H_2O co-electrolysis performance of solid oxide electrolysis cell using the multi-scale model

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Introduction

Nowadays, the use of fossil fuels is facing challenges such as global warming and energy shortage. The development of alternative energy technology and carbon dioxide secondary utilization is urgent [1].

As a high-temperature electrolytic cell, solid oxide electrolysis cell (SOEC) can realize the process of co-electrolysis of H_2O and CO_2. Then, the production of synthetic fuel ($CO + H_2$) is realized by the Fischer Tropsch (F-T) process [2]. The co-electrolysis of H_2O and CO_2 using the SOEC has broad development prospects. Fig. 1 shows the schematic diagram of the process of co-electrolysis of H_2O and CO_2. In the co-electrolysis process, there are not only complex electrochemical reactions, mass transfer and charge transfer processes. Under the catalysis of nickel (Ni) electrode, complex Water-Gas Shift Reaction (WGSR) and steam reforming reaction also occur [3].

In this study, a 2D multi-scale model coupling with a mesoscale model based on the percolation theory is developed. Considering the multi-physics processes, electrochemical reactions, catalytic reactions and mesostructure of electrodes in SOEC, the effects of inlet flow rate, operating temperature and porosity of electrodes on the performance of co-electrolysis in SOEC are studied.

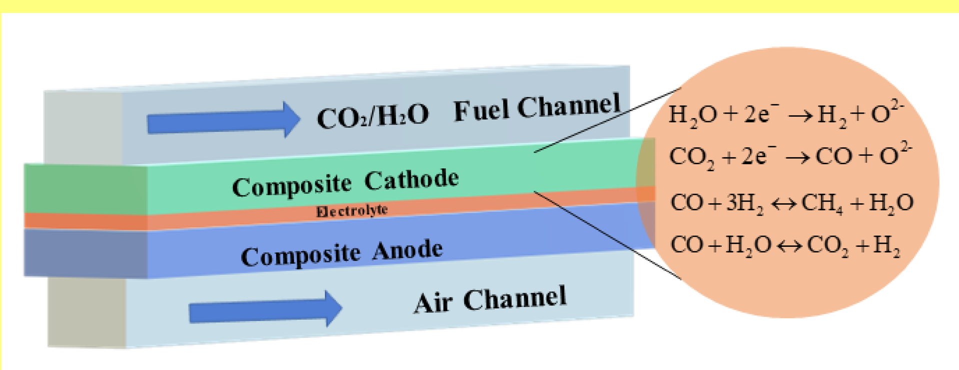

Fig. 1. Schematic diagram of co-electrolysis of H_2O and CO_2 using SOEC.

Assumptions & geometric model

In the modeling process, the following assumptions are considered:

1) Steady state.
2) All the gas species are ideal gases.
3) Chemical reactions take place inside the cathode.
4) The gas flow in the channel is a laminar flow.

The 2D multi-scale model describes a SOEC unit composed of fuel/air channel, composite cathode, electrolyte and composite anode. The corresponding geometric model is shown in Fig. 2. Table 1 lists the geometric parameters and operating parameters.

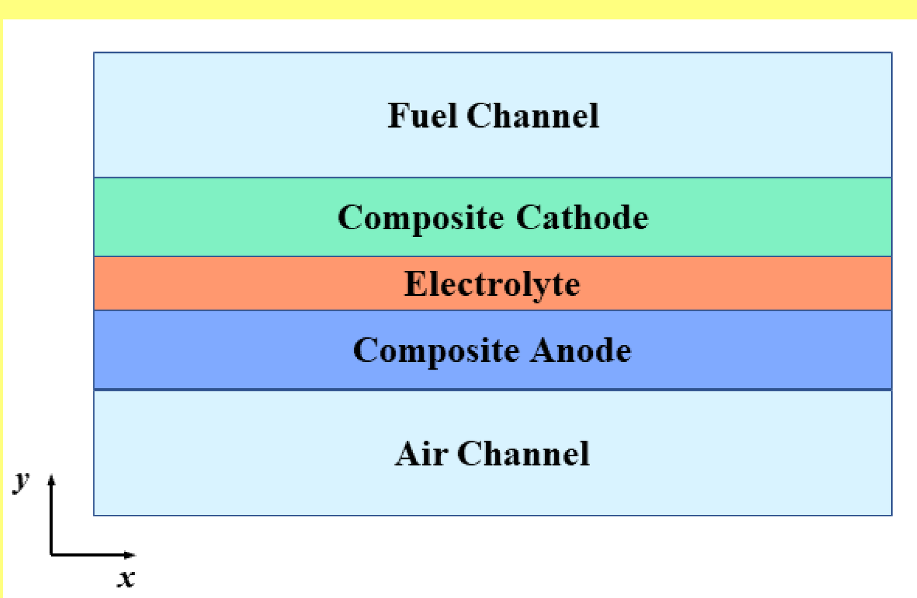

Fig. 2. Geometric model of SOEC unit.

Table 1. Geometric and operating parameters.

Parameters	Value
Channel thickness	40 μm
Cell unit length	0.6 cm
Cathode thickness	10 μm
Electrolyte thickness	10 μm
Anode thickness	15 μm
Operating pressure	1 atm
Current density	5000 A m^{-2}

Calculation methods

MATHEMATICAL MODEL

The 2D multi-scale model is solved by the finite element method using the commercial software COMSOL multiphysics 5.6. The mesoscopic model is established by directly writing a user-defined function.

BOUNDARY CONDITIONS

To solve the 2D multi-scale model, Table 2 lists some important boundary conditions. Meanwhile, the inlet components of fuel channel are 45mol% H_2O, 45 mol% CO_2 and 10 mol% H_2. The inlet components of air channel are 21 mol% O_2 and 79 mol% N_2.

Table 2. Boundary conditions.

Boundary	Boundary conditions
Inlet	Insulation, Inlet flow rate Temperature
Outlet	Insulation, Pressure, Heat flux
Cathode/Channel interface	Grounding, Continuity
Anode/Channel interface	Current density, Continuity

Results

MODEL VALIDATION

It can be seen from Fig. 3 the simulation results agree reasonably with the experimental data [4]. Thus, the accuracy of multi-scale model is validated.

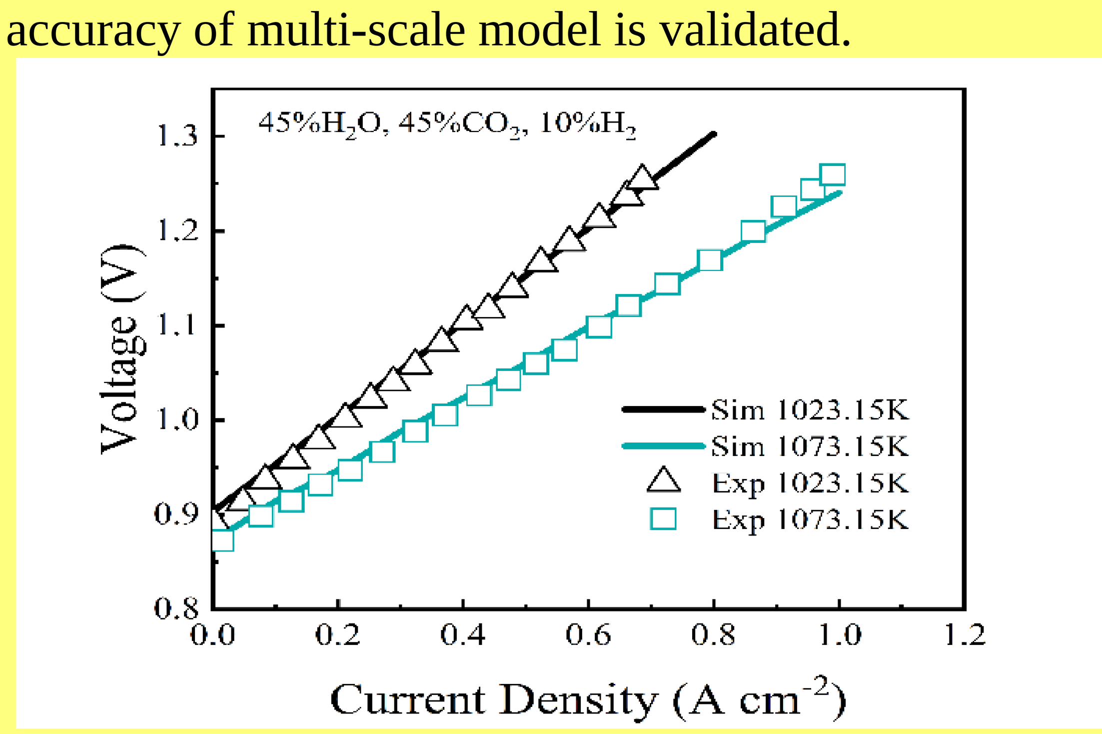

Fig. 3. Experimental and simulated polarization curves for cell at 1023.15K and 1073.15K.

EFFECTS OF INLET FLOW RATE

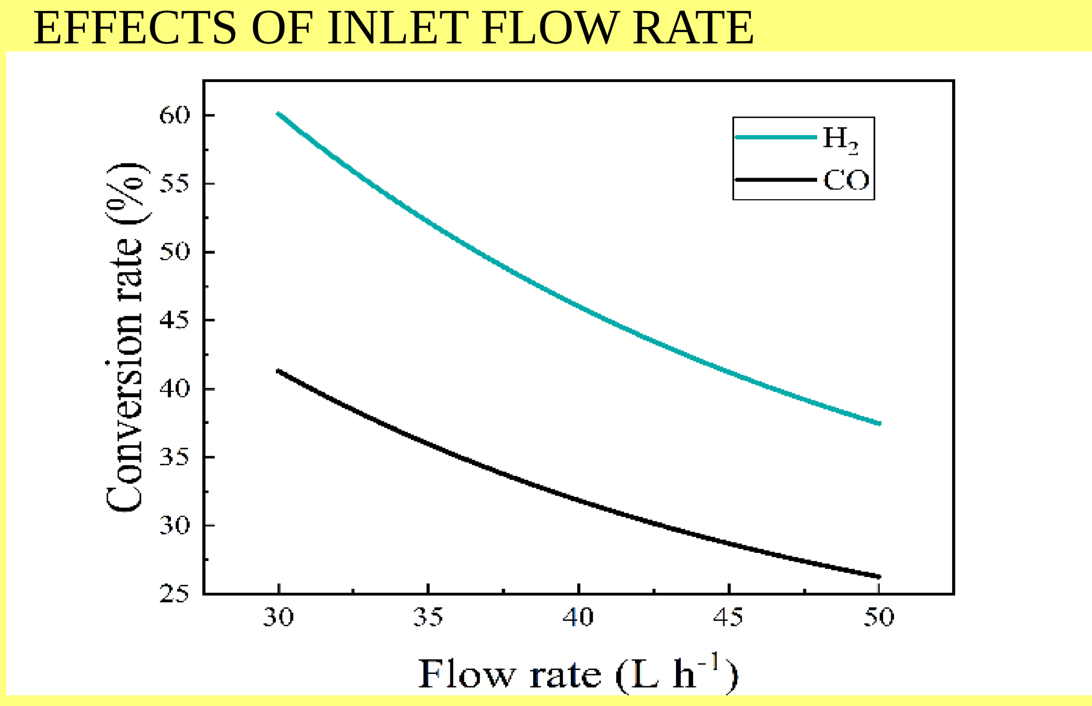

Fig. 4. The conversion rate of H_2 and CO with different inlet flow rate.

Fig. 4 shows that the conversion rate of H_2 is greater than that of CO, under certain working conditions. Meanwhile, with the increase of inlet flow rate, the conversion rate of CO and H_2 are inhibited.

Interestingly, when the inlet flow rate increased from 30L h^{-1} to 40L h^{-1}, the conversion of H_2 and CO decreased by 23.4% and 22.9% respectively. When the inlet flow rate increased from 40L h^{-1} to 50L h^{-1}, the conversion of H_2 and CO decreased by 18.6% and 17.5% respectively.

EFFECTS OF OPERATING TEMPERATURE

It can be seen from Fig. 5 that in the process of co-electrolysis, the conversion rate of H_2 and CO show an opposite trend with the increase of operating temperature. When the temperature increased from 1023.15k to 1123.15k, the conversion rate of CO increased by 11.5%, while the conversion rate of H_2 decreased by 9.8%. The reason for this phenomenon may be that the reaction rate inside the electrode is affected by operating temperature.

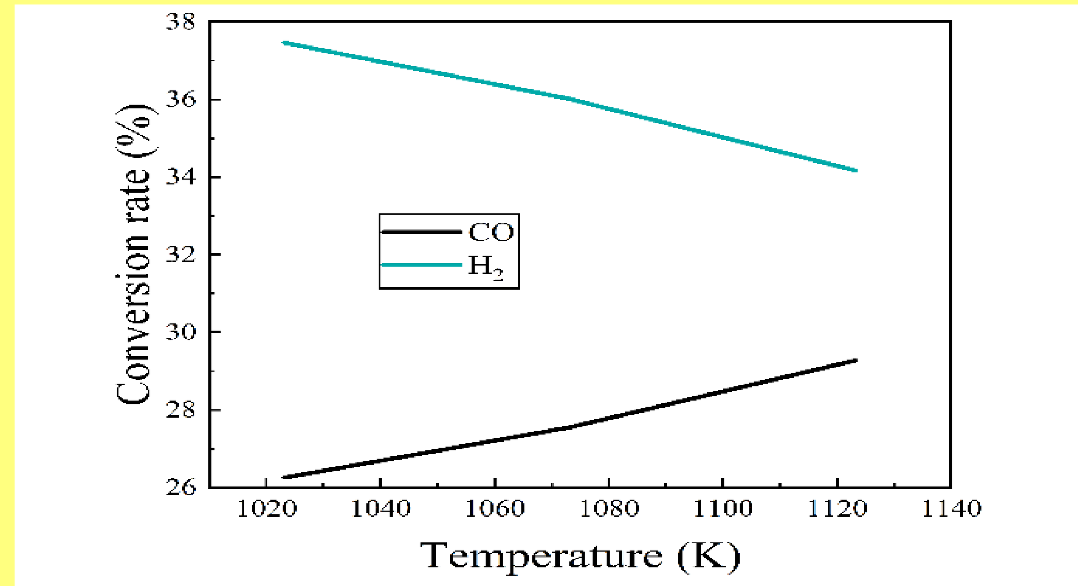

Fig. 5. The conversion rate of H2 and CO with different temperature.

EFFECTS OF POROSITY OF ELECTRODES

It can be seen from Fig. 6 and Fig. 7 that the increase of porosity improves the electrolysis reaction rate of CO_2. On the contrary, it inhibits the electrolysis reaction rate of H_2O. At the same time, increasing the porosity will also promote the reverse WGSR reaction rate.

This explains the phenomenon that the increase of porosity is beneficial to promote the conversion of CO, but it is unfavorable for the decomposition of H_2O.

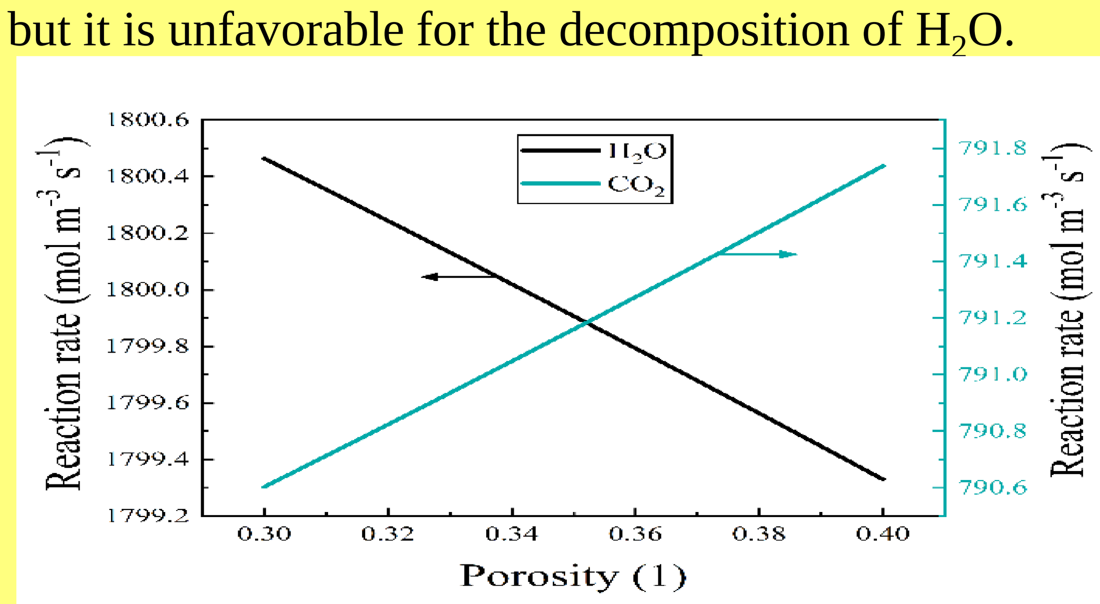

Fig. 6. The electrolysis reaction rate of H_2O and CO_2 with different porosity.

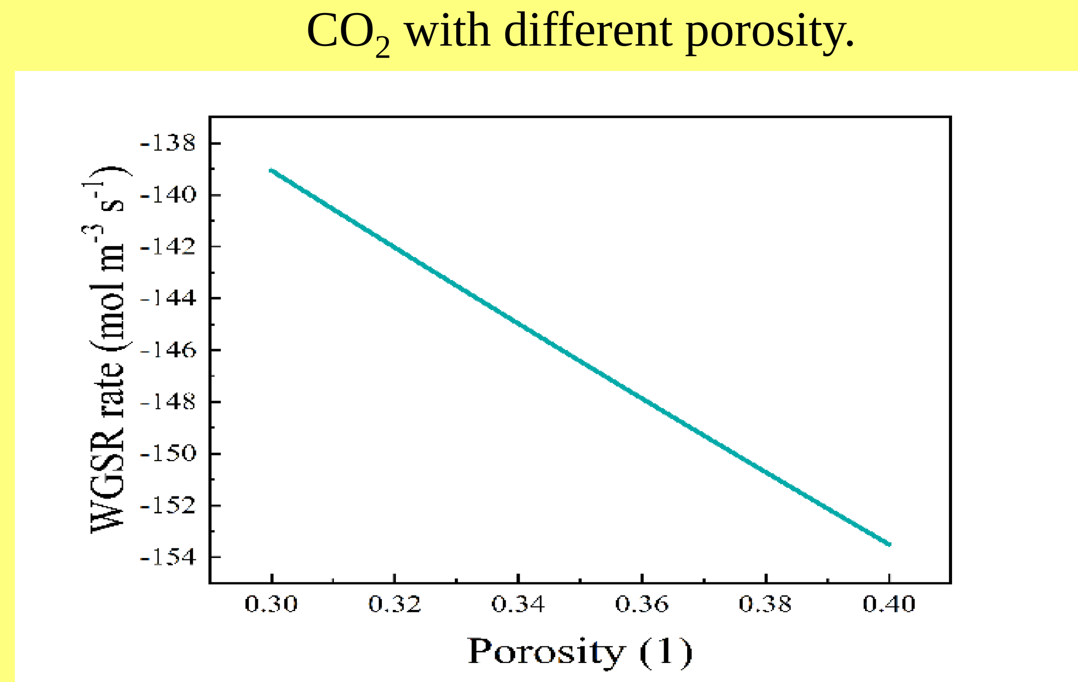

Fig. 7. The WGSR rate with different porosity.

Conclusions

The main conclusions drawn from all these work are:

- When the electrolysis conditions are fixed, increasing the flow rate is not conducive to the electrolysis of H_2O and CO_2.
- The increase of porosity will promote the conversion of CO_2 to CO, it is not conducive to the production of H_2 and the formation of effective TPB.
- The increase of operating temperature will reduce the electrolysis reaction rate of H_2O, but increase that of CO_2 and WGSR reaction rate.

References

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