

Article

Multi-Physics Coupling Simulation of H₂O–CO₂ Co-Electrolysis Using Flat Tubular Solid Oxide Electrolysis Cells

Chaolong Cheng ^{1,2,†}, Wen Ding ^{3,†}, Junfeng Shen ¹, Penghui Liao ³, Chengrong Yu ³, Bin Miao ⁴, Yexin Zhou ^{3,*}, Hui Li ⁵, Hongying Zhang ^{5,*} and Zheng Zhong ³

¹ Shenzhen Energy Group Co., Ltd., No. 2026 Jintian Rd., Shenzhen 518031, China

² Shenzhen Energy Innovation Technology Co., Ltd., Fubao Street, Shenzhen 518048, China

³ School of Science, Harbin Institute of Technology, Shenzhen 518055, China

⁴ Energy Research Institute at NTU (ERI@N), Nanyang Technological University, 1 CleanTech Loop #06-04, Singapore 637141, Singapore

⁵ Qingpeng Hydrogen Technology (Shenzhen) Co., Ltd., No. 5 Gongye 5th Road, Shenzhen 518067, China

* Correspondence: zhouyexin@hit.edu.cn (Y.Z.); hyzhang-2008@163.com (H.Z.)

† These authors contributed equally to this work.

Abstract

Solid oxide electrolysis cells (SOECs) have emerged as a promising technology for efficient energy storage and CO₂ utilization via H₂O–CO₂ co-electrolysis. While most previous studies focused on planar or tubular configurations, this work investigated a novel flat, tubular SOEC design using a comprehensive 3D multi-physics model developed in COMSOL Multiphysics 5.6. This model integrates charge transfer, gas flow, heat transfer, chemical/electrochemical reactions, and structural mechanics to analyze operational behavior and thermo-mechanical stress under different voltages and pressures. Simulation results indicate that increasing operating voltage leads to significant temperature and current density inhomogeneity. Furthermore, elevated pressure improves electrochemical performance, possibly due to increased reactant concentrations and reduced mass transfer limitations; however, it also increases temperature gradients and the maximum first principal stress. These findings underscore that the design and optimization of flat tubular SOECs in H₂O–CO₂ co-electrolysis should take the trade-off between performance and durability into consideration.

Keywords: solid oxide electrolysis cell (SOEC); flat tubular; H₂O–CO₂ co-electrolysis; multi-physics modeling; thermal stress



Academic Editors: Michael C. Georgiadis and Mohd Azlan Hussain

Received: 25 August 2025

Revised: 24 September 2025

Accepted: 4 October 2025

Published: 8 October 2025

Citation: Cheng, C.; Ding, W.; Shen, J.; Liao, P.; Yu, C.; Miao, B.; Zhou, Y.; Li, H.; Zhang, H.; Zhong, Z. Multi-Physics Coupling Simulation of H₂O–CO₂ Co-Electrolysis Using Flat Tubular Solid Oxide Electrolysis Cells. *Processes* **2025**, *13*, 3192. <https://doi.org/10.3390/pr13103192>

Copyright: © 2025 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (<https://creativecommons.org/licenses/by/4.0/>).

1. Introduction

In this era of rapid technological advancement, the energy crisis has emerged as one of the most critical challenges impeding the progress of human society. Traditional fossil fuels release substantial amounts of CO₂ and other greenhouse gases during combustion, significantly contributing to global warming and severely disrupting the ecological balance of nature. Reducing atmospheric CO₂ levels and mitigating the pace of global climate change have become imperative issues that humanity must address to achieve sustainable development. Therefore, a rising trend in the widespread adoption of renewable energy is observed. Nevertheless, the inherent intermittency and variability of renewable energies demand effective energy storage solutions to ensure grid stability and reliable power supply.

Solid oxide electrolysis cells (SOECs) are a high-temperature water electrolysis technology [1–5]. Table 1 compares the characteristics of three types of water electrolyzers, including alkaline electrolysis cells (AECs), proton exchange membrane electrolysis cells (PEMECs), and SOECs. Compared to low-temperature water-electrolysis technologies, such as AECs and PEMECs, SOECs exhibit higher electrolysis efficiency due to reduced activation loss. Therefore, a long-term, large-scale energy storage solution can be achieved by converting surplus renewable electricity into H₂ using SOECs. H₂ is an extensively utilized chemical product in traditional industrial applications, such as ammonia and methanol synthesis. With a wide availability of H₂ enabled by renewable energy, the potential of H₂ as an energy carrier can be further explored owing to its advantages, such as high gravimetric energy density (120 MJ/kg) and negligible environmental impact, during utilization [6,7]. Beyond water electrolysis for H₂ production, SOECs can also co-electrolyze H₂O and CO₂ to produce CO and H₂ (Figure 1) [8], or even CH₄ with an in situ methanation reaction [9]. This process not only yields valuable synthetic gas fuels, but also enables CO₂ utilization and contribution to carbon neutrality efforts. Figure 1 gives a typical *I*–*V* curve of SOEC and the three characteristic voltage losses, including activation loss, ohmic loss, and concentration loss.

Table 1. Comparison of characteristics between different electrolyzers.

Technology	AECs	PEMECs	SOECs
Electrolyte	Potassium hydroxide	Proton exchange membrane	Solid oxide
Operating temperature	70–90 °C	80–150 °C	600–1000 °C
Charge carrier	OH [−]	H ⁺	O ^{2−}
Electrolyte state	Immobilized liquid	Hydrated solid	Solid
Electrodes	Transition metals	Carbon	Ceramic/Metal cermet
Catalyst	Platinum	Platinum	Ni-Cermet
Reactant	Pure H ₂ O	Pure H ₂ O	H ₂ O _(g) , CO ₂
Efficiency (% LHV of H ₂)	56–69	56–83	>80
References	[10–12]	[12–14]	[12,15]

In H₂O–CO₂ co-electrolysis via SOECs, multiple processes are coupled, such as the transport of gases and charged ions, electrochemical reactions, chemical reactions, and the generation/consumption and transfer of heat. In contrast to being capable of only characterizing the overall electrochemical performance by experiments, multi-physics coupling simulations are effective in probing the distribution of various physical fields. These simulations thereby provide useful information on the underlying physical mechanisms responsible for performance variations resulting from a change in materials and the structure of SOECs. Luo et al. [16] developed a two-dimensional (2D) model to analyze the performance and efficiency of H₂O–CO₂ co-electrolysis in tubular SOECs. Their calculations demonstrated that counter-flow configuration outperforms parallel-flow. Building upon this work, Luo et al. [17] found that tubular electrolysis cells, without additional hydrogen supply, cannot produce sufficient CH₄ solely from H₂ generated through H₂O electrolysis. This limitation arises from the temperature difference between the optimal reaction rates of the water–gas shift reaction (WGSR) and methanation reaction (MR). They proposed that increasing hydrogen content in the inlet gas and elevating the electrolysis current could enhance CH₄ production.

Chen et al. [18] reported that elevated pressure could improve CH₄ conversion rates, with 3 bar identified as the optimal pressure. Beyond this threshold, no further conversion rate improvement was observed (achieving 2.5 times the conversion rate at 1 bar), suggesting that lower temperatures would be required for additional

CH_4 yield enhancement. Chi et al. [1] conducted a comparative study of various water electrolysis technologies, including alkaline water electrolysis, proton exchange membrane electrolysis, solid oxide electrolysis, and alkaline anion exchange membrane electrolysis. Their work examined ion transport mechanisms, operational characteristics, energy consumption, and process outputs, while also discussing the prospects of water electrolysis technologies.

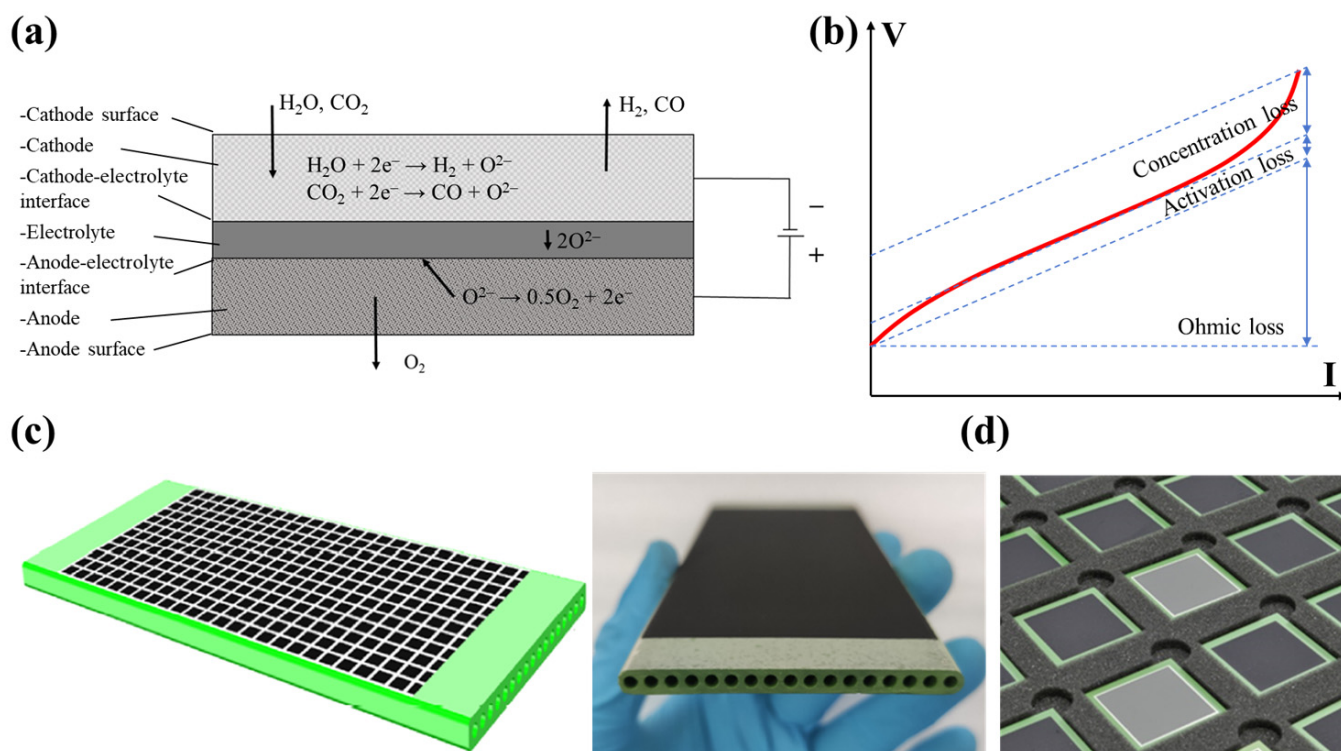


Figure 1. (a) Schematic diagram of co-electrolysis by SOEC; (b) schematic illustration of a typical I - V curve of SOEC and corresponding losses; (c) schematic image and photograph of flat tubular SOECs; (d) photograph of planar SOECs.

Beyond electrochemical performance, researchers have also explored the mechanical properties of SOECs through multi-physical modeling. Cui et al. [19] calculated the thermal stress in an SOEC unit, evaluating the effects of voltage, flow direction, water mole fraction, and pressure. Their results indicate that the maximum principal stress occurs in the electrolyte layer. Fan et al. [20] observed that thinner electrolytes and thicker anodes lead to lower residual stresses in the PEN (Positive electrode–Electrolyte–Negative electrode) structure. They noted that tensile stresses in the electrolyte increase at higher SOFC operating temperatures, potentially causing anode cracking. Consequently, they recommended employing smaller operational temperature gradients, carefully matched coefficient of thermal expansion (CTE) materials, and thinner electrolyte layers.

The above studies focused on either planar or tubular SOECs. Recently, a novel flat tubular structure with a symmetrical double cathode was proposed, combining the advantages of both planar and tubular configurations [21]. In this work, based on the flat tubular SOEC, a three-dimensional multi-physics coupling model was built in the COMSOL Multiphysics simulation platform. The model took into account the complex chemical reactions, electrochemical reactions, gas diffusion, and internal thermal stress in the H_2O – CO_2 co-electrolysis process. The current density, gas distribution, reaction

rate, temperature, and stress distribution of a single cell under different voltages were analyzed and are discussed herein.

2. Numerical Model

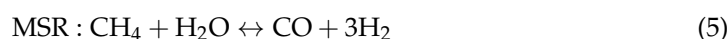
2.1. Governing Equations

2.1.1. Electrochemical Reaction

In the co-electrolysis model, the gas in the cathode flow channel diffuses in the porous cathode and enters the three-phase interface through porous electrodes to enable electrochemical reactions, including the reduction of H_2O and CO_2 to H_2 and CO , respectively, and the oxidation of O^{2-} to O_2 [22]:



As the commonly used Ni catalyst in the cathode, the water–gas shift reaction (WGS) and methane steam reforming reaction (MSR) also take place catalyzed by Ni [18,23].



Owing to various potential losses, including activation overpotential (η_{act}), ohmic overpotential (η_{ohm}), and concentration overpotential (η_{conc}), the working voltage (V) of an SOEC is higher than the open circuit voltage (E^{OCV}) [24]:

$$V = E^{\text{OCV}} + \eta_{\text{act,a}} + \eta_{\text{act,c}} + \eta_{\text{ohmic}} + \eta_{\text{conc,a}} + \eta_{\text{conc,c}} \quad (6)$$

Subscripts a and c denote anode and cathode, respectively.

During H_2O – CO_2 co-electrolysis, E^{OCV} can be calculated based on the Nernst equation of thermodynamic reversible potential [25]:

$$E_{\text{H}_2}^{\text{OCV}} = 1.253 - 0.00024516T + \frac{RT}{2F} \ln \left[\frac{P_{\text{H}_2}^{\text{b}} (P_{\text{O}_2}^{\text{b}})^{\frac{1}{2}}}{P_{\text{H}_2\text{O}}^{\text{b}}} \right] \quad (7)$$

$$E_{\text{CO}}^{\text{OCV}} = 1.46713 - 0.0004527T + \frac{RT}{2F} \ln \left[\frac{P_{\text{CO}}^{\text{b}} (P_{\text{O}_2}^{\text{b}})^{\frac{1}{2}}}{P_{\text{CO}_2}^{\text{b}}} \right] \quad (8)$$

where R is the gas constant ($8.3145 \text{ J} \cdot \text{mol}^{-1} \cdot \text{K}^{-1}$), T represents the reaction temperature (K), F is the Faraday constant ($96,485 \text{ C} \cdot \text{mol}^{-1}$), and P_{H_2} , P_{O_2} , $P_{\text{H}_2\text{O}}$, P_{CO} , and P_{CO_2} are the partial pressures of H_2 , O_2 , H_2O , CO , and CO_2 , respectively. The superscript L indicates the electrolyte–electrode interface, while b indicates the electrode surface.

The relationship between η_{act} and current density can be obtained through the Butler–Volmer equation [24]:

$$i_{\text{a,O}_2} = AV_{\text{a}} \cdot i_{0,\text{O}_2} \left(\exp \left(\frac{0.5F \cdot \eta_{\text{act,a}}}{RT} \right) - \exp \left(\frac{-0.5F \cdot \eta_{\text{act,a}}}{RT} \right) \right) \quad (9)$$

$$i_{c,H_2} = AV_c \cdot i_{0,H_2} \left(\frac{P_{H_2}}{P_{H_2}^b} \exp\left(\frac{0.5F \cdot \eta_{act,c}}{RT}\right) - \frac{P_{H_2O}}{P_{H_2O}^b} \exp\left(\frac{-0.5F \cdot \eta_{act,c}}{RT}\right) \right) \quad (10)$$

$$i_{c,CO} = AV_c \cdot i_{0,CO} \left(\frac{P_{CO}}{P_{CO}^b} \exp\left(\frac{0.5F \cdot \eta_{act,c}}{RT}\right) - \frac{P_{CO_2}}{P_{CO_2}^b} \exp\left(\frac{-0.5F \cdot \eta_{act,c}}{RT}\right) \right) \quad (11)$$

where AV_a and AV_c are the surface area of the anode and cathode electrochemical reaction interface and i_0 is the exchange current density of the reaction.

The η_{ohm} can be easily obtained via ohmic law.

The η_{conc} is caused by the slow mass transfer of gas species in the electrodes, leading to concentration differences between the electrode surface and the electrode–electrolyte interface. Thus, η_{conc} can be calculated with respect to these concentration differences with a Nernst-type expression [26]:

$$\eta_{conc,a} = \frac{RT}{2F} \ln\left(\frac{p_{H_2O}^L p_{H_2}^b}{p_{H_2O}^b p_{H_2}^L}\right) + \frac{RT}{2F} \ln\left(\frac{p_{CO_2}^L p_{CO}^b}{p_{CO_2}^b p_{CO}^L}\right) \quad (12)$$

$$\eta_{conc,c} = \frac{RT}{2F} \ln\left(\frac{p_{O_2}^b}{p_{O_2}^L}\right) \quad (13)$$

The relevant parameters used in this section are shown in Table 2.

Table 2. Model parameter table.

Parameters	Value	Unit
Ionic conductivity of cathode [27]	$\frac{9.5 \times 10^7}{T} \exp\left(-\frac{1150}{T}\right)$	$S \cdot m^{-1}$
Ionic conductivity of anode [27]	$\frac{4.2 \times 10^7}{T} \exp\left(-\frac{1200}{T}\right)$	$S \cdot m^{-1}$
Ionic conductivity of electrolyte [27]	$33.4 \times 10^3 \exp\left(-\frac{10300}{T}\right)$	$S \cdot m^{-1}$
Electronic conductivity of anode [28]	30,300	$S \cdot m^{-1}$
Electronic conductivity of cathode [29]	17,000	$S \cdot m^{-1}$
Electronic conductivity of interconnect [28]	769,000	$S \cdot m^{-1}$
AV_a [30]	2.14×10^5	m^{-2}
AV_c [30]	2.14×10^5	m^{-2}

2.1.2. Gas Flow

Gas flow in the flow channels and in the porous electrodes is described by the Navier–Stokes equation modified with the Darcy term [31,32]:

$$\nabla \cdot (\rho \mathbf{v}) = S_{mass} \quad (14)$$

$$\rho \mathbf{v} \cdot \nabla \mathbf{v} = -\nabla p + \nabla \cdot \left[\mu (\nabla \mathbf{v} + \mathbf{v} \nabla) - \frac{2}{3} \mu \nabla \mathbf{v} \right] - \frac{\varepsilon \mu \mathbf{v}}{k} \quad (15)$$

$$\text{anode :} \quad S_{mass} = \frac{(M_{H_2O} - M_{H_2})i}{2F} \quad (16)$$

$$\text{cathode :} \quad S_{mass} = -\frac{M_{O_2}i}{4F} \quad (17)$$

In the formula, ρ is the density of the mixed gas; $\mathbf{v}$ is the velocity vector; S_{mass} is the external quality source term; μ is the dynamic viscosity; ε and k are the permeability and porosity of the electrode structure of the electrolytic cell, respectively; and M_i is the relative molecular mass of i gas.

Gas diffusion in the porous electrodes is expressed using the Maxwell–Stefan model, modified with Knudsen diffusion:

$$j_i = -\rho D_i^{mK} \nabla \omega_i - \rho \omega_i D_i^{mK} \frac{\nabla M}{M} + \rho \omega_i \sum_k \frac{M_i}{M} D_i^{mK} \nabla x_i \quad (18)$$

$$D_i^{mk} = \frac{\varepsilon}{\tau} \left(\frac{1}{D_i^m} + \frac{1}{D_i^k} \right)^{-1} \quad (19)$$

$$M = \left(\sum_i \frac{\omega_i}{M_i} \right)^{-1} \quad (20)$$

where j_i and ω_i are the flow rate and mass fraction of component i , respectively; τ is the tortuosity factor; and D^{mK} is the total diffusion coefficient, which is determined by Fick diffusion coefficient D^m and Knudsen diffusion coefficient D^K .

2.1.3. Heat Transfer

The heat transfer in the whole cell is based on the classical heat transfer and energy conservation equation:

$$\nabla \left(-\lambda_{eff} \nabla T \right) + \rho C_p v \cdot \nabla T = Q \quad (21)$$

where λ_{eff} represents effective thermal conductivity, and results are determined by the thermal conductivity of solid materials and fluid materials. The detailed material and structure parameters required for the simulation were extracted from the literature [33,34] and are shown in Table 3.

Table 3. Material properties used in the model [33].

Component	Porosity	Permeability (m ²)	Thermal Conductivity (W·m ⁻¹ ·K ⁻¹)	Thermal Capacity (J·Kg ⁻¹ ·K ⁻¹)
Anode functional layer	0.23	1×10^{-12}	11	450
Anode support layer	0.46	1×10^{-10}	11	450
Electrolyte	-	-	2.7	550
Cathode layer	0.3	1×10^{-12}	6	430
Interconnect	-	-	20	550

As the physical fields in the multi-physical field model are coupled, the thermal strain in the whole cell calculation formula can be transformed into:

$$\varepsilon_{th} = \alpha (T - T_{ref}) \mathbf{I} \quad (22)$$

The thermal expansion coefficient of the material is affected by the type of material. T_{ref} is the reference temperature without stress, which is 1023 K; $\mathbf{I}$ is a second-order unit tensor.

The equations of mechanics used are [35]:

$$\varepsilon = (\nabla \mathbf{u} + \mathbf{u} \nabla) / 2 \quad (23)$$

$$\nabla \cdot \sigma + \mathbf{f} = 0 \quad (24)$$

$$\sigma = \mathbf{C} : \varepsilon \quad (25)$$

where $\mathbf{u}$ represents displacement; σ is stress; $\mathbf{f}$ is physical strength; and $\mathbf{C}$ is the fourth-order elastic coefficient tensor. Each component in SOECs is assumed to be isotropic, and thus the material constitutive equation can be simplified into:

$$\begin{Bmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \sigma_{zz} \\ \tau_{xy} \\ \tau_{xz} \\ \tau_{yz} \end{Bmatrix} = \frac{E}{(1+\nu)(1-2\nu)} \begin{bmatrix} 1-\nu & \nu & \nu & 0 & 0 & 0 \\ \nu & 1-\nu & \nu & 0 & 0 & 0 \\ \nu & \nu & 1-\nu & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1-2\nu}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1-2\nu}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1-2\nu}{2} \end{bmatrix} \begin{Bmatrix} \varepsilon_{xx} - \varepsilon_{th} \\ \varepsilon_{yy} - \varepsilon_{th} \\ \varepsilon_{zz} - \varepsilon_{th} \\ \gamma_{xy} \\ \gamma_{xz} \\ \gamma_{yz} \end{Bmatrix} \quad (26)$$

where E is Young's modulus and ν is Poisson's ratio. Mechanical parameters are shown in Table 4.

Table 4. Mechanical property parameters of solid mechanics in SOEC [36].

Component	E (GPa)	ν (-)	CET ($10^{-6} \cdot \text{K}^{-1}$)
Anode functional layer	213	0.3	11.4
Anode	220	0.3	12.5
Electrolyte	205	0.3	10.3
Cathode	160	0.3	11.4

2.1.4. Chemical Reaction

In the cathode of SOECs, due to the presence of Ni catalyst, chemical reactions such as the reverse WGS and reverse MSR take place, as confirmed by Haberman and Young [37]. The reaction rates are calculated by:

$$R_{WGS} = K_{sf} \left(p_{H_2O} p_{CO} - \frac{p_{H_2} p_{CO_2}}{K_{ps}} \right) (\text{mol} \cdot \text{m}^{-3} \cdot \text{s}^{-1}) \quad (27)$$

$$K_{sf} = 0.0171 \times \exp\left(\frac{-103191}{RT}\right) (\text{mol} \cdot \text{m}^{-3} \cdot \text{Pa}^{-2} \cdot \text{s}^{-1}) \quad (28)$$

$$K_{ps} = \exp\left(-0.2935Z^3 + 0.6351Z^2 + 4.1788Z + 0.3169\right) \quad (29)$$

$$R_{MSR} = K_{rf} \left(p_{CH_4} p_{H_2O} - \frac{p_{CO} (p_{H_2})^3}{K_{pr}} \right) (\text{mol} \cdot \text{m}^{-3} \cdot \text{s}^{-1}) \quad (30)$$

$$K_{rf} = 2395 \times \exp\left(\frac{-231266}{RT}\right) (\text{mol} \cdot \text{m}^{-3} \cdot \text{Pa}^{-2} \cdot \text{s}^{-1}) \quad (31)$$

$$K_{ps} = 1.0267 \times 10^{10} \times \exp\left(-0.2513Z^4 + 0.36651Z^3 + 0.5810Z^2 - 27.134Z + 3.277\right) \quad (32)$$

$$Z = \frac{1000}{T(\text{K})} - 1 \quad (33)$$

2.2. Geometric Model and Boundary Conditions

Figure 2 shows the geometry of the flat tubular SOEC. As the SOEC is symmetric, a semi-structure of the cell is used in the model. The 3D multi-physical model is solved across the whole body of the geometry. Geometric parameters are shown in Table 5.

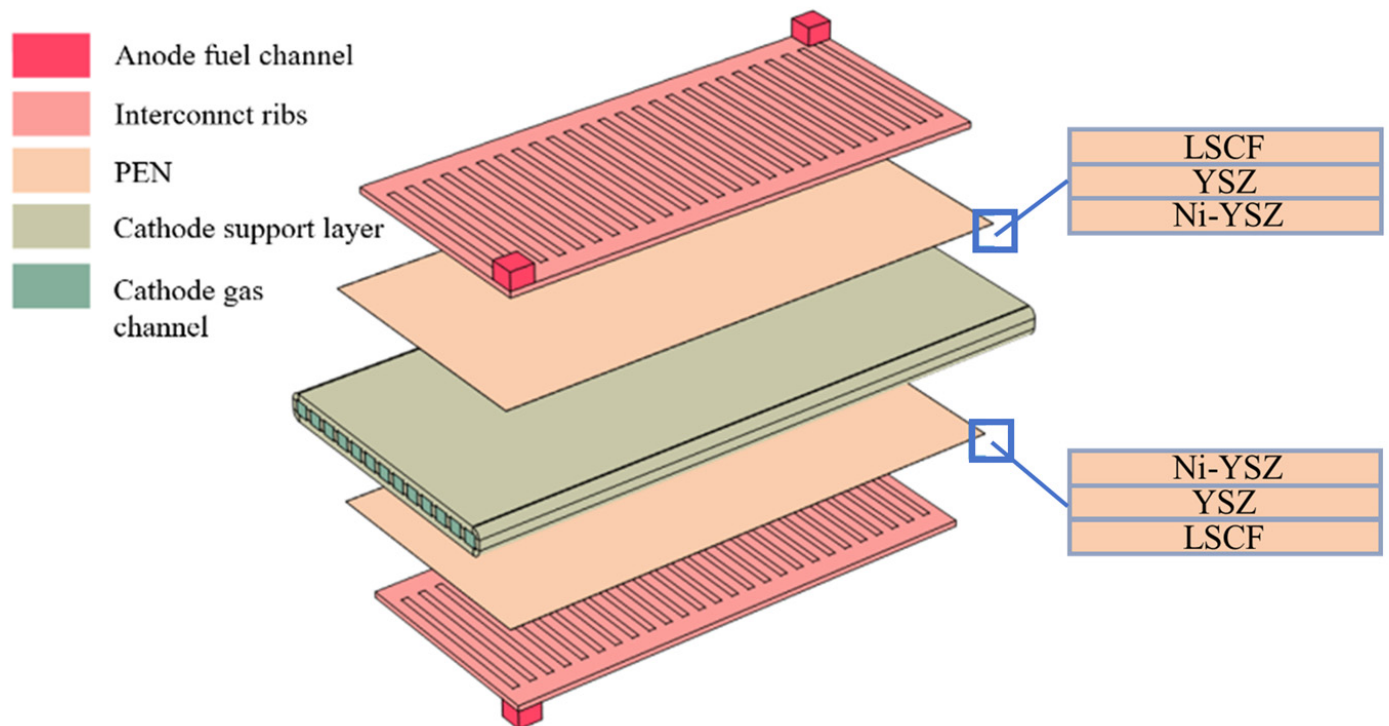


Figure 2. SOEC structure diagram.

Table 5. Geometric parameters of solid oxide electrolytic cell.

	SOFC_S
Ni-3YSZ supporting layer (mm ³)	98.6 × 46 × 4.7
NiO + 8YSZ anode functional layer (mm ³)	85.5 × 41 × 0.02
YSZ electrolyte layer (mm ³)	85.5 × 41 × 0.01
LSCF perovskite cathode layer (mm ³)	85.5 × 41 × 0.02
Number of steam channels	13
Number of metallic alloy interconnect ribs	26

The boundary conditions of the model are as follows: the cathode inlet gas is 0.4 H₂O, 0.4 CO₂, and 0.2 H₂; the flow rate is 0.3 m·s^{−1}; the anode inlet gas is air (0.79 N₂ and 0.21 O₂); the gas flow rate is 1 m·s^{−1}; and the outlet gas conditions of both are an atmospheric pressure of 1 atm. The external temperature is 1023 K. The voltage is 0 V on the surface of the supporting cathode. The model is solved with COMSOL Multiphysics 5.6 (COMSOL, Sweden).

3. Results and Discussion

3.1. Model Validation

Figure 3 compares *I–V* curves from simulation and from experimental results extracted from a previously published report [38]. These simulation results are in good agreement at operating temperatures of both 700 °C and 750 °C, validating the as-developed model.

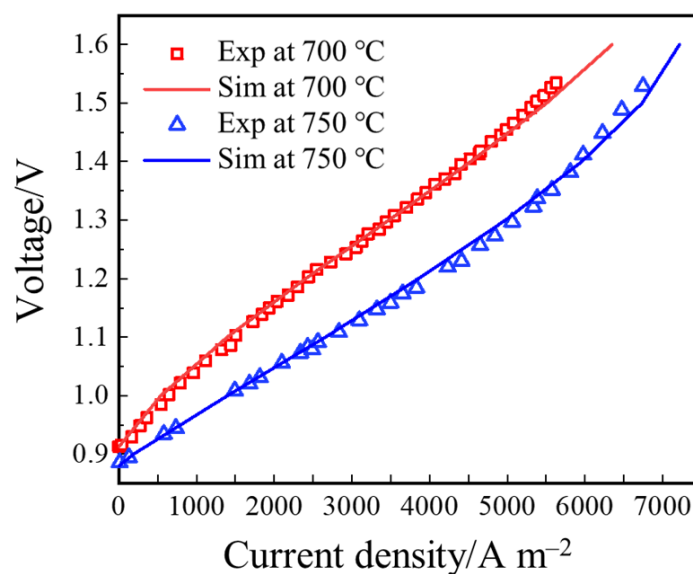


Figure 3. *I*-*V* curves of H_2O - CO_2 co-electrolysis using flat tubular SOEC.

3.2. Physical Field Distributions

3.2.1. Current Density Distribution

The current density distributions of the electrolyte at different voltages are shown in Figure 4. It can be clearly seen from the figure that as the operating voltage increases, the electrolyte current density gradually increases, and the distribution of the current density at the inlet and outlet gradually becomes uneven. This is because the electrolysis reaction rate at the entrance is accelerated, which consumes a large amount of H_2O and CO_2 , resulting in insufficient reactant concentration in the middle and exit parts of the electrolytic cell.

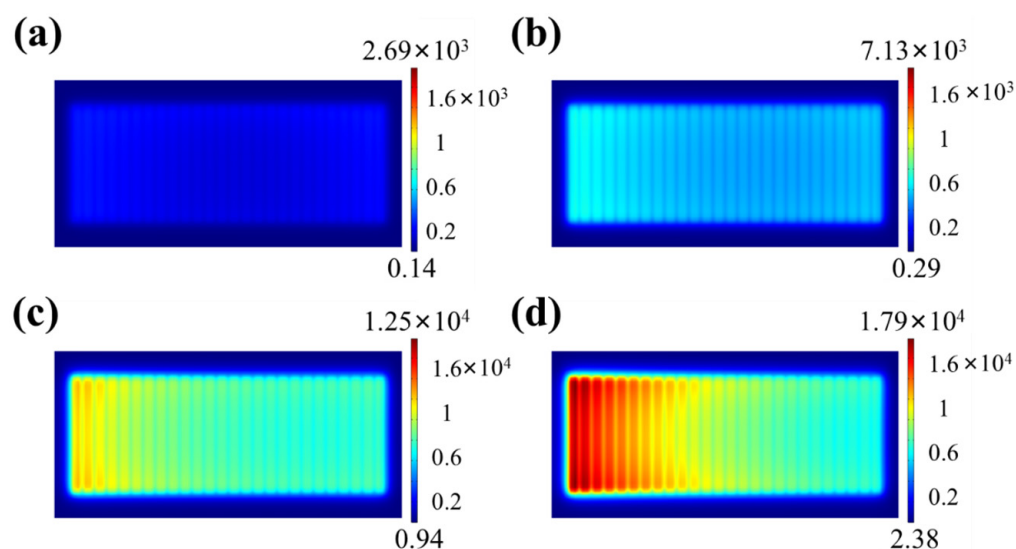


Figure 4. Current density distribution of electrolyte at different voltages of (a) 1 V; (b) 1.2 V; (c) 1.4 V; and (d) 1.6 V.

3.2.2. Gas Composition Distribution

Figures 5 and 6 show the distributions of H_2 and CO concentrations at different voltages. Obviously, H_2 and CO concentrations increase with an increase in applied voltage, due to the progress of electrochemical reactions. When the applied voltage is 1.2 V, the average H_2 concentration reaches 0.27, corresponding to a conversion ratio of H_2O of

2.5%. As the voltage continues to increase, the conversion ratio increases to 82.5% at an applied voltage of 1.6 V. Simultaneously, the conversion of CO₂ also enhances. However, contributions to the CO₂ reduction from the direct CO₂ electrochemical reduction and reverse WGS reaction need to be further investigated. Furthermore, at the investigated temperature of 750 °C, the amount of CH₄ production is minimal [39]. Thus, the impact of MSR on the overall performance can be considered negligible.

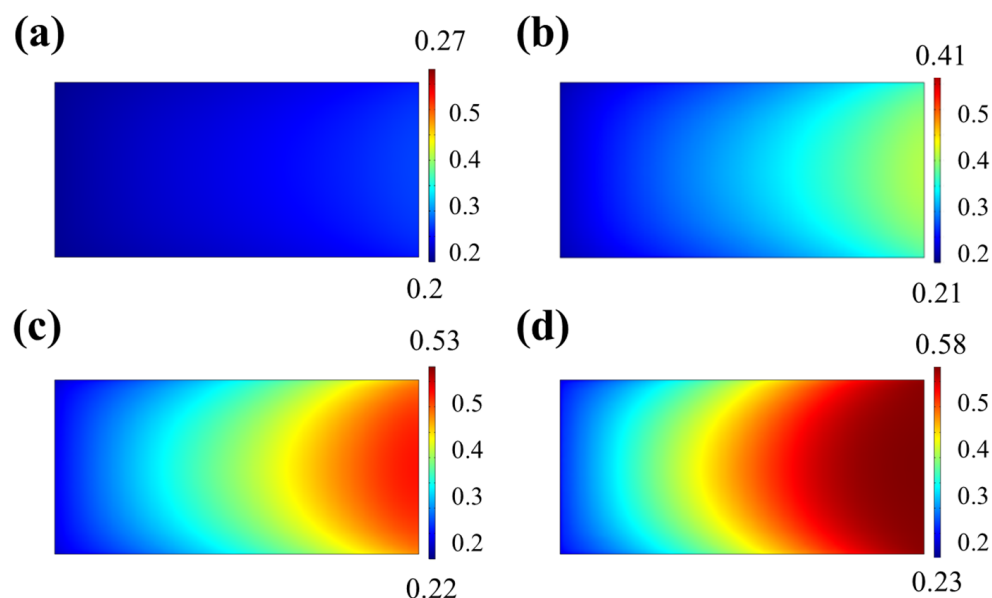


Figure 5. H₂ distribution at different voltages of (a) 1 V; (b) 1.2 V; (c) 1.4 V; and (d) 1.6 V.

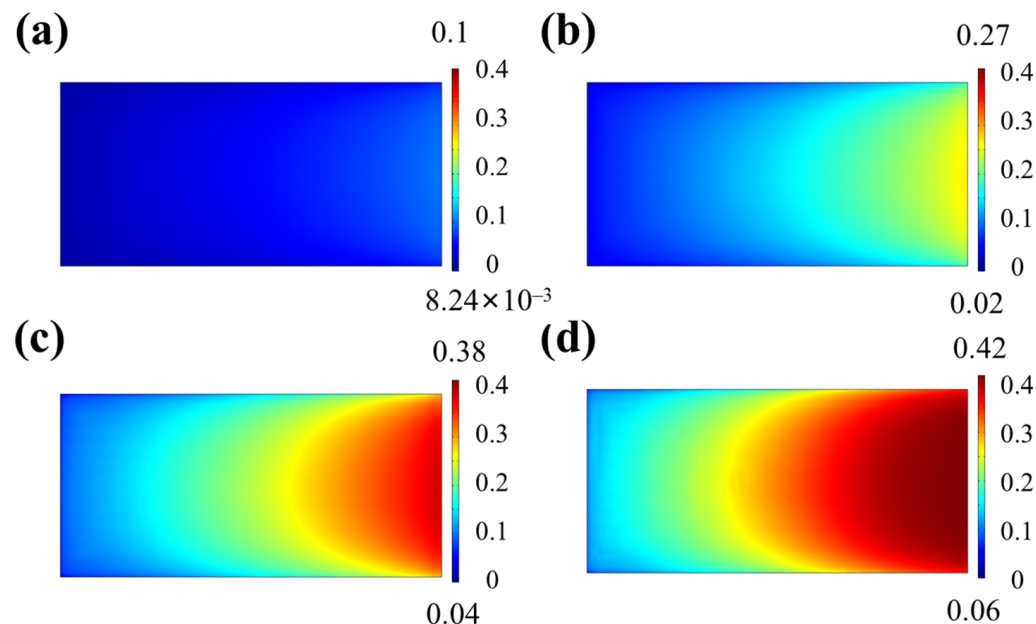


Figure 6. CO distribution at different voltages of (a) 1 V; (b) 1.2 V; (c) 1.4 V; and (d) 1.6 V.

3.2.3. Temperature Distribution

Figure 7 shows the temperature distribution in the flat tubular SOEC under different voltages. It can be seen from the figure that with an increase in operating voltage, the average temperature increases and the distribution becomes more uneven. Inside the SOEC, a few electrochemical and chemical reactions take place simultaneously, including the water–gas shift reaction, methanation reaction, and the electrochemical

reduction of H_2O and CO_2 . Among these, the electrochemical reduction reactions are both endothermic processes, while the two chemical reactions are both exothermic reactions. Thus, the temperature distribution in the SOEC is a combined result of the interplay of these competing thermal effects. At low voltages of 1.0 V and 1.2 V, concentrations of H_2 and CO are relatively low, as shown in Figures 5 and 6. Thus, WGS and MR reactions are hindered due to the lack of reactants and the existence of a high concentration of products. As a result, the temperature of SOEC is low, close to the boundary temperature of 1023 K. In contrast, with applied voltages increasing to 1.4 V and 1.6 V, chemical reactions are dominant and more heat is released, increasing the SOEC temperature. Furthermore, it can be noted that the highest temperature is observed at the middle part of the SOEC.

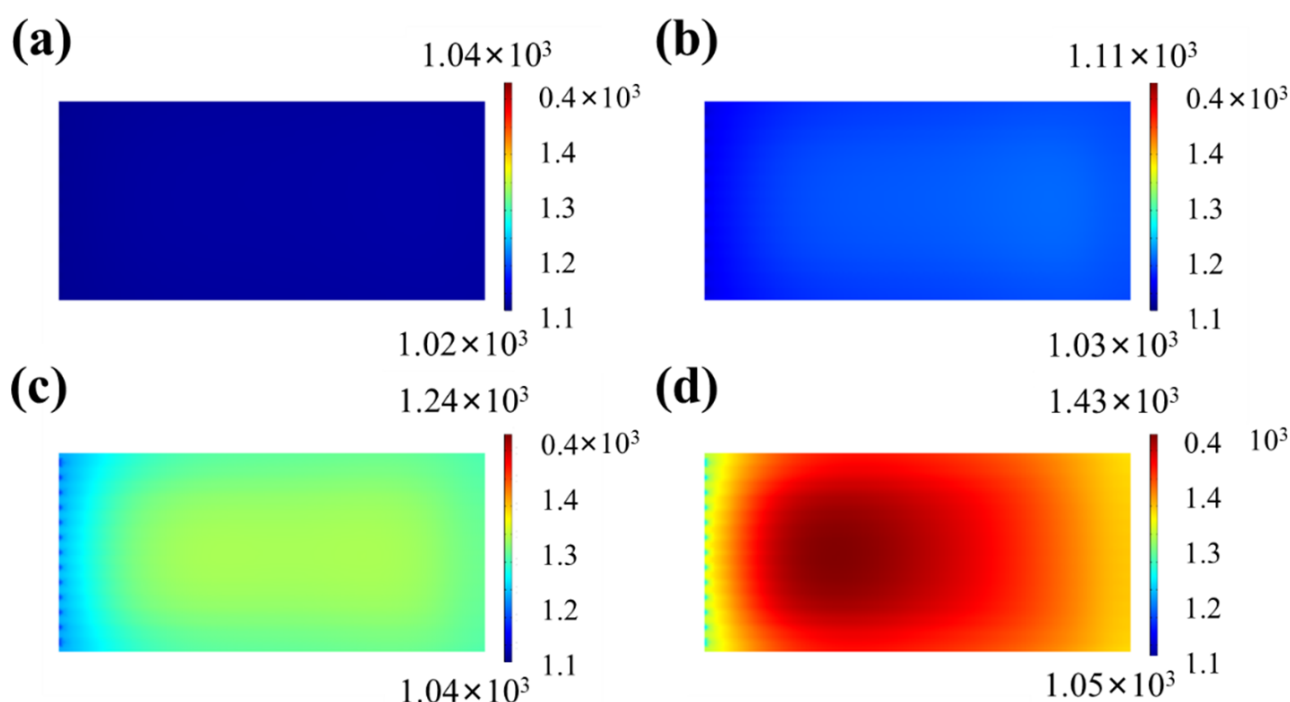


Figure 7. Temperature distribution under different voltages of (a) 1 V; (b) 1.2 V; (c) 1.4 V; and (d) 1.6 V.

3.2.4. Stress Distribution

The distribution of the first principal stress inside the SOEC at different voltages is shown in Figure 8. The first principal stress can be used to predict the crack and fail of brittle materials such as ceramic along planes perpendicular to the direction of maximum tensile stress. Thus, in this work, the larger the first principal stress, the higher the failure probability of an SOEC. The main origin of the stress is thermal stress due to the temperature gradient, shown in Figure 7, generated inside the SOEC during operation. Therefore, with an increase in the applied voltage, the maximum first principal stress also increases, from 0.19 MPa at an applied voltage of 1 V to 301 MPa at an applied voltage of 1.6 V. The compressive strength of YSZ is around 1.6 GPa [40]. Considering that the anode is highly porous and the electrolyte layer is very thin ($\sim 10\text{--}20\text{ }\mu\text{m}$), a higher stress increases the failure probability. In addition, at 1.6 V, the first principal stress is higher near both inlet and outlet regions, while the central section presents a lower stress level. This distribution corresponds to the fact that the highest temperature occurs in the middle part, leading to the highest temperature gradients near the inlet and outlet areas.

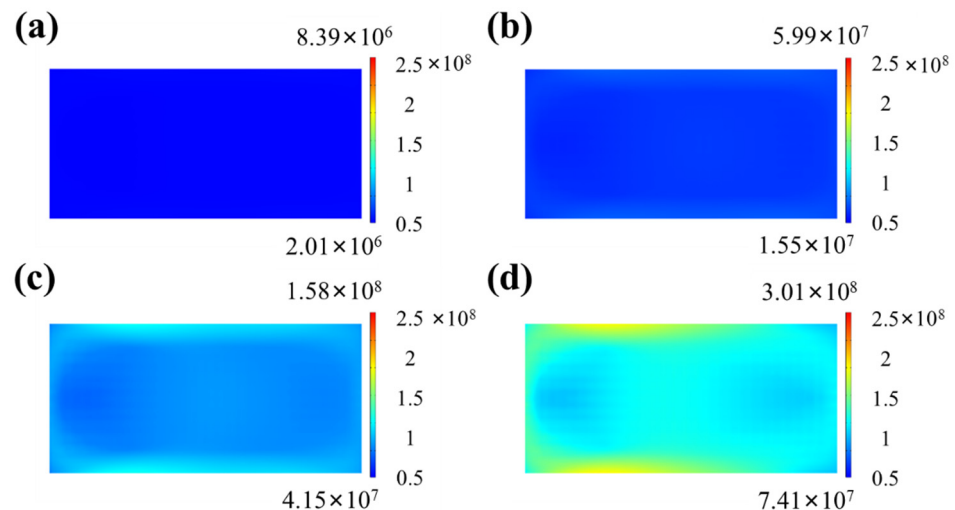


Figure 8. First principal stress distribution at different voltages of (a) 1 V; (b) 1.2 V; (c) 1.4 V; and (d) 1.6 V.

3.2.5. Effect of Operating Pressure

In this section, the effect of operating pressure on SOEC performance and physical field distributions are presented. Figure 9 gives the variation in I - V curves with the operating temperature. Clearly, a high operating pressure is beneficial to electrochemical performance; the higher the operating pressure, the higher the current density at the same applied voltage. With an operating pressure of 1 atm, the average current density is 7116 A/m^2 at an applied voltage of 1.6 V; the value increases to 9817 A/m^2 under an operating pressure of 2 atm, and further reaches $12,586 \text{ A/m}^2$ under 10 atm. This trend is in accordance with the previous modeling study on a planar SOEC stack [41,42] and the experimental study [43]. The high operating pressure could improve cell performance through the following two mechanisms. First, a high operating pressure improves the reactant volumetric concentration. Thus, especially in regions near the outlet, the increased concentration of reactants could improve electrochemical reaction rates. Second, the higher operating pressure may also promote the transport of gas molecules, and thus lower the concentration overpotential. This is demonstrated by the more substantial performance improvement observed at higher current densities.

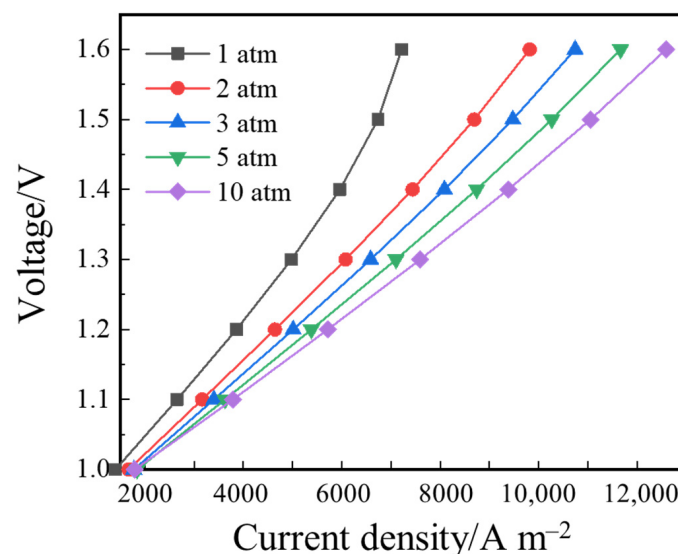


Figure 9. Variation in I - V curves with operating pressure.

Figure 10 gives temperature distributions at different operating pressures. Evidently, with an increase in operating pressure, the temperature distribution becomes more uneven. Figure 11 summarizes the highest and lowest temperatures at each operating pressure. At 1 atm, the temperature difference between the highest and the lowest is 380 K, while at 10 atm, the difference increases to 490 K. Furthermore, a shift in the peak temperature region from near the inlet to near the outlet can also be observed. As mentioned above, the electrochemical reactions are endothermic and the chemical reactions are exothermic. The shift in temperature distribution implies a shift in the distributions of sites where the various reactions take place.

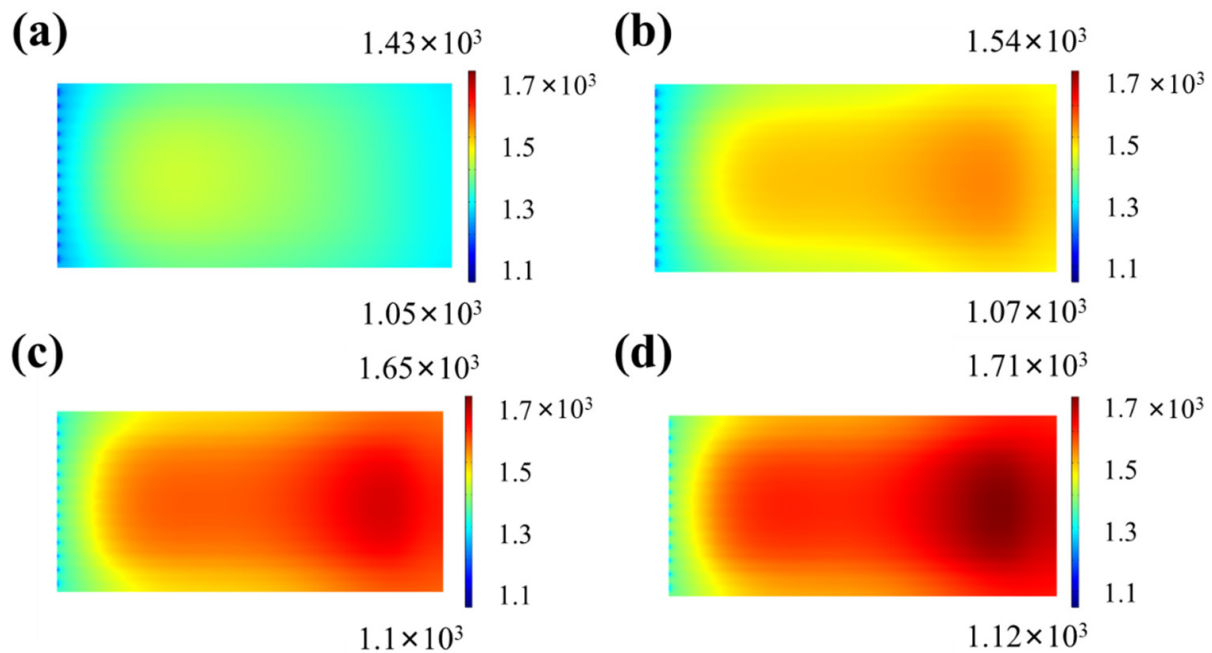


Figure 10. Temperature distributions under different operating pressures of (a) 1 atm; (b) 2 atm; (c) 5 atm; and (d) 10 atm.

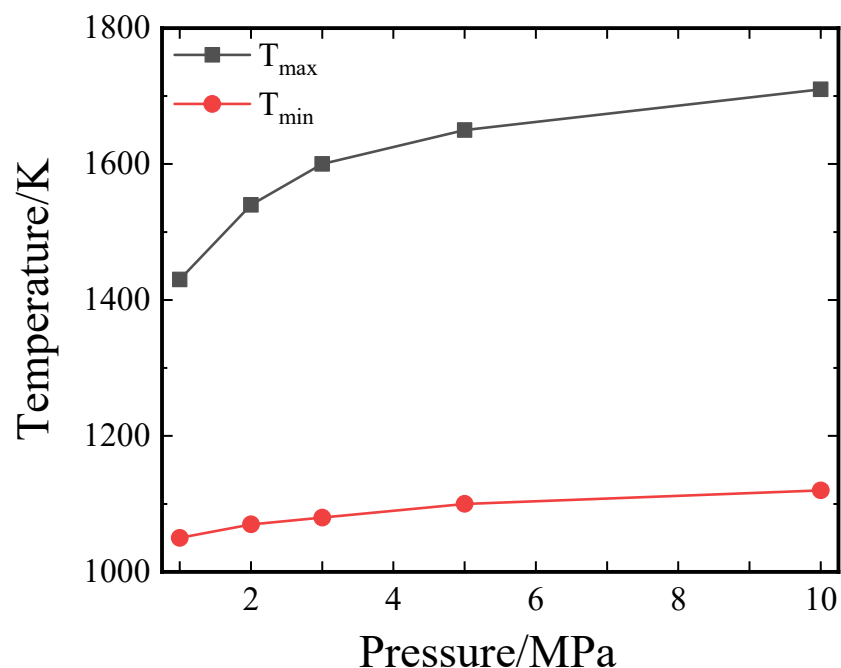


Figure 11. Temperature variation with a change in operating pressure.

Correspondingly, increasing uneven distribution leads to higher maximum first principal stress, as shown by Figure 12. At 1.6 V, the maximum first principal stress increases from 301 MPa at an operating pressure of 1 atm to 465 MPa at an operating pressure of 10 atm. Thus, when aiming to achieve higher performance by operating the SOEC at elevated pressures, the potential cell degradation caused by the higher first principal stresses should also be taken into consideration.

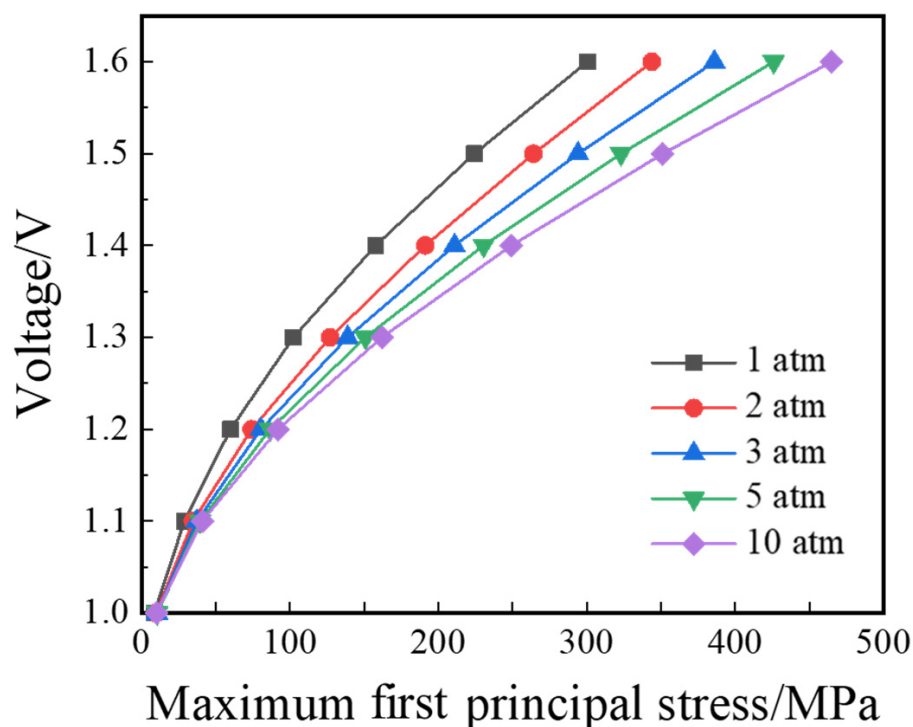


Figure 12. Variation in maximum first principal stress along operating pressure.

4. Conclusions

This study established a multi-physics model to evaluate the performance and mechanical behavior of a flat tubular SOEC during H₂O–CO₂ co-electrolysis. Results reveal that higher operating voltages cause more uneven distributions of current density and temperature. Furthermore, the highest temperature shifts toward the middle region, leading to increased temperature gradients near the inlet and outlet, and thus the first principal stress. Elevated operating pressure is beneficial to enhancing electrochemical performance, while simultaneously increasing the maximum first principal stress from 300 MPa to 465 MPa as pressure rises from 1 atm to 10 atm, potentially compromising cell stability. In the future, a more detailed optimization should be performed considering the trade-offs between performance and stability.

Author Contributions: Conceptualization, C.C., Y.Z., H.Z. and Z.Z.; methodology, C.C., P.L., C.Y. and Z.Z.; validation, W.D., J.S., C.Y., B.M. and Y.Z.; formal analysis, C.C., W.D. and J.S.; investigation, C.C., W.D., P.L., C.Y. and H.L.; resources, Y.Z., H.Z. and Z.Z.; data curation, C.C., P.L. and H.Z.; writing—original draft preparation, C.C., W.D., J.S., P.L. and C.Y.; writing—review and editing, B.M., Y.Z., H.Z. and Z.Z.; visualization, P.L. and C.Y.; supervision, Y.Z. and Z.Z.; project administration, H.Z.; funding acquisition, Y.Z. and Z.Z. All authors have read and agreed to the published version of the manuscript.

Funding: This research received funding from Shenzhen Energy Group Co., Ltd.

Data Availability Statement: Original contributions presented in this study are included in this article. Further inquiries can be directed to the corresponding authors.

Acknowledgments: The authors acknowledge the management and research facilities of the Harbin Institute of Technology, Shenzhen.

Conflicts of Interest: Chaolong Cheng was employed by the Shenzhen Energy Group Co., Ltd. and Shenzhen Energy Innovation Technology Co., Ltd. Junfeng Shen was employed by the Shenzhen Energy Group Co., Ltd. Hui Li was employed by the Qingpeng Hydrogen Technology (Shenzhen) Co., Ltd. Hongying Zhang was employed by the Qingpeng Hydrogen Technology (Shenzhen) Co., Ltd. The remaining authors declare that this research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest. The authors declare that this study received funding from the Shenzhen Energy Group Co., Ltd. The funder was not involved in this study's design, the collection, analysis, or interpretation of data, the writing of this article, or the decision to submit it for publication.

References

- Chi, J.; Yu, H. Water electrolysis based on renewable energy for hydrogen production. *Chin. J. Catal.* **2018**, *39*, 390–394.
- Kang, S.; Pan, Z.; Guo, J.; Zhou, Y.; Wang, J.; Fan, L.; Zheng, C.; Cha, S.W.; Zhong, Z. Scientometric analysis of research trends on solid oxide electrolysis cells for green hydrogen and syngas production. *Front. Energy* **2024**, *18*, 583–611. [\[CrossRef\]](#)
- Yuan, B.; Zhang, X.; Tang, C.; Wang, N.; Ye, S. How AI guided the development of green hydrogen production: In the case of solid oxide electrolysis cell? *J. Mater. Inform.* **2025**, *5*, 25. [\[CrossRef\]](#)
- Ferrete, F.; Molina, A.; Cabello González, G.M.; Moreno-Racero, Á.; Olmedo, H.; Iranzo, A. Solid Oxide Electrolyzers Process Integration: A Comprehensive Review. *Processes* **2025**, *13*, 2656. [\[CrossRef\]](#)
- Pan, Z.; Liu, Q.; Ni, M.; Lyu, R.; Li, P.; Chan, S.H. Activation and failure mechanism of La_{0.6}Sr_{0.4}Co_{0.2}Fe_{0.8}O_{3-δ} air electrode in solid oxide electrolyzer cells under high-current electrolysis. *Int. J. Hydrogen Energy* **2018**, *43*, 5437–5450. [\[CrossRef\]](#)
- Cunjin, Z.; Shuaibo, Q.; Hui, G.; Peng, J. High hydrogen evolution activities of dual-metal atoms incorporated N-doped graphenes achieved by coordination regulation. *J. Mater. Inform.* **2024**, *4*, 1.
- Wang, S.; Chen, H.; Hu, S.; Zhao, W.; Chen, M.; Chen, D.; Xu, X. Characterization of Hydrogen-in-Oxygen Changes in Alkaline Electrolysis Hydrogen Production System and Analysis of Influencing Factors. *Processes* **2025**, *13*, 2517. [\[CrossRef\]](#)
- Dogu, D.; Gunduz, S.; Meyer, K.E.; Deka, D.J.; Co, A.C.; Ozkan, U.S. CO₂ and H₂O electrolysis using solid oxide electrolyzer cell (SOEC) with La and Cl-doped strontium titanate cathode. *Catal. Lett.* **2019**, *149*, 1743–1752. [\[CrossRef\]](#)
- Pan, Z.; Duan, C.; Pritchard, T.; Thatte, A.; White, E.; Braun, R.; O'hAyre, R.; Sullivan, N.P. High-yield electrochemical upgrading of CO₂ into CH₄ using large-area protonic ceramic electrolysis cells. *Appl. Catal. B* **2022**, *307*, 121196. [\[CrossRef\]](#)
- Cifrain, M.; Kordesch, K.V. Advances, aging mechanism and lifetime in AFCs with circulating electrolytes. *J. Power Sources* **2004**, *127*, 234–242. [\[CrossRef\]](#)
- Gülzow, E. Alkaline fuel cells: A critical view. *J. Power Sources* **1996**, *61*, 99–104. [\[CrossRef\]](#)
- International Energy Agency. *2014 Annual Report*; International Energy Agency: Paris, France, 2014.
- Litster, S.; McLean, G. PEM fuel cell electrodes. *J. Power Sources* **2004**, *130*, 61–76. [\[CrossRef\]](#)
- Sishtla, C.; Koncar, G.; Platon, R.; Gamburzev, S.; Appleby, A.J.; Velez, O.A. Performance and endurance of a PEMFC operated with synthetic reformat fuel feed. *J. Power Sources* **1998**, *71*, 249–255. [\[CrossRef\]](#)
- Gardner, F.J.; Day, M.J.; Brandon, N.P.; Pashley, M.N.; Cassidy, M. SOFC technology development at Rolls-Royce. *J. Power Sources* **2000**, *86*, 122–129. [\[CrossRef\]](#)
- Luo, Y.; Shi, Y.; Li, W.; Cai, N. Comprehensive modeling of tubular solid oxide electrolysis cell for co-electrolysis of steam and carbon dioxide. *Energy* **2014**, *70*, 420–434. [\[CrossRef\]](#)
- Luo, Y.; Li, W.; Shi, Y.; Cao, T.; Ye, X.; Wang, S.; Cai, N. Experimental characterization and theoretical modeling of methane production by H₂O/CO₂ co-electrolysis in a tubular solid oxide electrolysis cell. *J. Electrochem. Soc.* **2015**, *162*, F1129. [\[CrossRef\]](#)
- Chen, B.; Xu, H.; Ni, M. Modelling of SOEC-FT reactor: Pressure effects on methanation process. *Appl. Energy* **2017**, *185*, 814–824. [\[CrossRef\]](#)
- Cui, T.; Xiao, G.; Yan, H.; Zhang, Y.; Wang, J.-Q. Numerical simulation and analysis of the thermal stresses of a planar solid oxide electrolysis cell. *Int. J. Green Energy* **2023**, *20*, 432–444. [\[CrossRef\]](#)
- Fan, P.; Li, G.; Zeng, Y.; Zhang, X. Numerical study on thermal stresses of a planar solid oxide fuel cell. *Int. J. Therm. Sci.* **2014**, *77*, 1–10. [\[CrossRef\]](#)
- Guan, W.; Du, Z.; Wang, J.; Jiang, L.; Yang, J.; Zhou, X.-D. Mechanisms of performance degradation induced by thermal cycling in solid oxide fuel cell stacks with flat-tube anode-supported cells based on double-sided cathodes. *Int. J. Hydrogen Energy* **2020**, *45*, 19840–19846. [\[CrossRef\]](#)
- Zheng, Y.; Chen, Z.; Zhang, J. Solid oxide electrolysis of H₂O and CO₂ to produce hydrogen and low-carbon fuels. *Electrochem. Energy Rev.* **2021**, *4*, 508–517. [\[CrossRef\]](#)

23. Sun, X.; Chen, M.; Jensen, S.H.; Ebbesen, S.D.; Graves, C.; Mogensen, M. Thermodynamic analysis of synthetic hydrocarbon fuel production in pressurized solid oxide electrolysis cells. *Int. J. Hydrogen Energy* **2012**, *37*, 17101–17110. [\[CrossRef\]](#)
24. Yu, C.; Pan, Z.; Zhang, H.; Chen, B.; Guan, W.; Miao, B.; Chan, S.H.; Zhong, Z.; Zhou, Y. Numerical multi-physical optimization of operating condition and current collecting setup for large-area solid oxide fuel cells. *Front. Energy* **2024**, *18*, 356–368. [\[CrossRef\]](#)
25. Xu, H.; Chen, B.; Irvine, J.; Ni, M. Modeling of CH₄-assisted SOEC for H₂O/CO₂ co-electrolysis. *Int. J. Hydrogen Energy* **2016**, *41*, 21839–21849. [\[CrossRef\]](#)
26. Xiong, X.; Liang, K.; Ma, G.; Ba, L. Three-dimensional multi-physics modelling and structural optimization of SOFC large-scale stack and stack tower. *Int. J. Hydrogen Energy* **2023**, *48*, 2742–2761. [\[CrossRef\]](#)
27. Kim, Y.J.; Lee, M.C. Numerical investigation of flow/heat transfer and structural stress in a planar solid oxide fuel cell. *Int. J. Hydrogen Energy* **2017**, *42*, 18504–18513. [\[CrossRef\]](#)
28. Pianko-Oprych, P.; Zinko, T.; Jaworski, Z. A Numerical Investigation of the Thermal Stresses of a Planar Solid Oxide Fuel Cell. *Materials* **2016**, *9*, 814. [\[CrossRef\]](#) [\[PubMed\]](#)
29. Stevenson, J.W.; Armstrong, T.R.; Carneim, R.D.; Pederson, L.R.; Weber, W.J. Electrochemical properties of mixed conducting perovskites La(1-x)M(x)Co(1-y)Fe(y)O(3-delta) (M = Sr, Ba, Ca). *J. Electrochem. Soc.* **1996**, *143*, 2722–2729. [\[CrossRef\]](#)
30. Xu, H.R.; Chen, B.; Liu, J.; Ni, M. Modeling of direct carbon solid oxide fuel cell for CO and electricity cogeneration. *Appl. Energy* **2016**, *178*, 353–362. [\[CrossRef\]](#)
31. Ali, S.; Sørensen, K.; Nielsen, M.P. Modeling a novel combined solid oxide electrolysis cell (SOEC)-Biomass gasification renewable methanol production system. *Renew. Energy* **2020**, *154*, 1025–1034. [\[CrossRef\]](#)
32. Baxter, S.J.; Rine, M.; Min, B.; Liu, Y.; Yao, J. Near 100% CO₂ conversion and CH₄ selectivity in a solid oxide electrolysis cell with integrated catalyst operating at 450 °C. *J. CO₂ Util.* **2022**, *59*, 101954. [\[CrossRef\]](#)
33. Zhang, Z.; Yue, D.; Yang, G.; Chen, J.; Zheng, Y.; Miao, H.; Wang, W.; Yuan, J.; Huang, N. Three-dimensional CFD modeling of transport phenomena in multi-channel anode-supported planar SOFCs. *Int. J. Heat Mass Transf.* **2015**, *84*, 942–954. [\[CrossRef\]](#)
34. Rui, W.; Lucas, R.P.; Yu, Z. Sulfur poisoning mechanism of LSCF cathode material in the presence of SO₂: A computational and experimental study. *J. Mater. Inform.* **2023**, *3*, 3.
35. Yu, C.; Guo, Z.; Pan, Z.; Zhou, Y.; Zhang, H.; Chen, B.; Tan, P.; Guan, W.; Zhong, Z. Performance and stress analysis of flat-tubular solid oxide fuel cells fueled with methane and hydrogen. *Acta Mech. Solida Sin.* **2024**, *38*, 402–414. [\[CrossRef\]](#)
36. Jiang, C.; Gu, Y.; Guan, W.; Ni, M.; Sang, J.; Zhong, Z.; Singhal, S.C. Thermal Stress Analysis of Solid Oxide Fuel Cell with Z-type and Serpentine-Type Channels Considering Pressure Drop. *J. Electrochem. Soc.* **2020**, *167*, 044517. [\[CrossRef\]](#)
37. Haberman, B.; Young, J. Three-dimensional simulation of chemically reacting gas flows in the porous support structure of an integrated-planar solid oxide fuel cell. *Int. J. Heat Mass Transf.* **2004**, *47*, 3617–3629. [\[CrossRef\]](#)
38. Xi, C.; Sang, J.; Wu, A.; Yang, J.; Qi, X.; Guan, W.; Wang, J.; Singhal, S.C. Electrochemical performance and durability of flat-tube solid oxide electrolysis cells for H₂O/CO₂ co-electrolysis. *Int. J. Hydrogen Energy* **2022**, *47*, 10166–10174. [\[CrossRef\]](#)
39. Xie, K.; Zhang, Y.; Meng, G.; Irvine, J.T.S. Direct synthesis of methane from CO₂/H₂O in an oxygen-ion conducting solid oxide electrolyser. *Energy Environ. Sci.* **2011**, *4*, 2218. [\[CrossRef\]](#)
40. Shimonosono, T.; Ueno, T.; Hirata, Y. Mechanical and thermal properties of porous yttria-stabilized zirconia. *J. Asian Ceram. Soc.* **2019**, *7*, 20–30. [\[CrossRef\]](#)
41. Du, Y.; Qin, Y.; Zhang, G.; Yin, Y.; Jiao, K.; Du, Q. Modelling of effect of pressure on co-electrolysis of water and carbon dioxide in solid oxide electrolysis cell. *Int. J. Hydrogen Energy* **2019**, *44*, 3456–3469. [\[CrossRef\]](#)
42. Henke, M.; Willich, C.; Kallo, J.; Friedrich, K.A. Theoretical study on pressurized operation of solid oxide electrolysis cells. *Int. J. Hydrogen Energy* **2014**, *39*, 12434–12439. [\[CrossRef\]](#)
43. Bernadet, L.; Gousseau, G.; Chatroux, A.; Laurencin, J.; Mauvy, F.; Reytier, M. Influence of pressure on solid oxide electrolysis cells investigated by experimental and modeling approach. *Int. J. Hydrogen Energy* **2015**, *40*, 12918–12928. [\[CrossRef\]](#)

Disclaimer/Publisher’s Note: The statements, opinions and data contained in all publications are solely those of the individual author(s) and contributor(s) and not of MDPI and/or the editor(s). MDPI and/or the editor(s) disclaim responsibility for any injury to people or property resulting from any ideas, methods, instructions or products referred to in the content.