Bio-syngas fueled operation of a Solid Oxide Fuel Cell-Numerical simulations in COMSOL and experimental validation

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Abstract

The motivation for this study arises from the growing interest in clean and efficient energy conversion technologies. This study focuses on modeling and analysis of an SOFC of flat tubular cell geometry with specific focus on comparison between air and oxygen as cathode fuels with two different bio-syngas compositions being used as the anode gas. COMSOL Multiphysics is employed in this study owing to its capability of integrating various physical phenomena such as mass transport, charge-transfer kinetics, flow distribution in gas channels/porous electrodes, electrochemical reactions and heat transfer within a single simulation platform. This integrated approach is essential for accurately capturing the intricate interactions occurring within a SOFC system. By comparing the performance of SOFCs operated with air and oxygen on cathodes, it is observed that syngas/producer gas operated with oxygen as cathode fuel resulted in a maximum current and power values than air as cathode fuel. The current and power values of syngas and producer gas fueled SOFCs in an oxygen environment are 5724 A/m^2 and 1789 W/m^2 (syngas) and 3737 A/m^2 and 1369 W/cm^2 (producer gas), respectively. Whereas, in the case of air environment, the current and power values of syngas and producer gas fueled SOFCs are 3625 A/m^2 and 1365 W/m^2 (syngas) and 2858 A/m^2 and 1174 W/cm^2 (producer gas), respectively. This is consistent considering that with air as the Oxidizing media, the cathode side experience dilution effects due to Nitrogen. Polarization traces showed negligible activation loss, ohmic losses and very small mass transport losses. Moreover, the mass distribution of each species of syngas and producer gas along with velocity and pressure profile is also simulated to understand the properties of modelled flat tubular SOFC. The distribution of CO, CO_2, CH_4 and H_2 is higher near the anode inlet and very low near the anode outlet which shows that the current density is decreasing along the flow channel due to the depletion of fuels. The current study contributes to the understanding of syngas-fueled and producer gas-fueled SOFCs and the influence of cathode fuel selection on their performance.

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Keywords: Solid Oxide Fuel cell, Syngas, Producer gas, Performance optimization

Introduction

The fuel cell is one of the most efficient and promising energy conversion technologies in this regard because it directly converts the chemical energy or calorific value of a fuel (hydrogen, hydrocarbons, etc.) into electrical energy without any conversion steps. Depending on the electrolytes and fuels employed, fuel cells come in distinct types, including proton-exchange or polymer-electrolyte membrane fuel cells (PEMFC), solid-oxide fuels cells (SOFC), alkaline fuel cells (AFC), molten-carbonate fuel cells (MCFC), direct-methanol fuel cells (DMFC), and phosphoric-acid fuel cells (PAFC), respectively [1].

Amongst various fuel cells, Solid Oxide Fuel Cells (SOFCs) have gained prominence due to their ability to directly convert a variety of fuels into electricity with high conversion efficiency and produces significantly lower emissions compared to traditional combustion-based power generation [2]. The concept of SOFCs has been explored extensively over the past few decades, and these electrochemical devices have demonstrated remarkable potential in various applications, including stationary power generation, distributed energy systems, and even transportation. SOFCs operate at high temperatures, typically between 500°C and 1000°C, allowing for efficient conversion of a wide range of fuels, including hydrogen, natural gas, and, importantly, syngas [2]. The ability to tolerate substantially high levels of contaminants is a critical selling point for SOFCs. Among the wide array of fuels available, bio-syngas has garnered significant attention due to its renewable nature and potential as a sustainable energy source [3]. Bio-syngas, a mixture of hydrogen and carbon monoxide, is produced through the gasification of biomass. Biomass gasification is a sustainable approach that can utilize various organic materials, including agricultural residues, forestry waste, and dedicated energy crops [4]. This process offers a carbon-neutral or even carbon-negative energy source,

making it a key player in the transition towards a greener and more sustainable energy future. Numerous studies have investigated the operation of SOFCs with syngas as a fuel source.

These investigations have explored various aspects, including electrochemical performance, thermal management, and fuel reforming within the cell. However, several critical research gaps persist in this domain, encompassing the need for fine-tuning operational parameters and the absence of comprehensive numerical and experimental investigations elucidating the intricate processes taking place within SOFCs.

Therefore, in order to comprehend the complex interplay of various physical phenomena, including electrochemical reactions, ion and heat transfer, and fluid dynamics within SOFCs, this study seeks to fill the gaps previously mentioned in the existing literature. It aims to achieve this by employing advanced numerical simulations in COMSOL to acquire a more profound insight into the operation of FT-SOFCs fueled by bio-syngas. Moreover, experimental verification will be undertaken to validate the simulation outcomes and offer valuable data for practical implementation.

Additionally, our research has also delved into the utilization of oxygen and air as fuel sources for the solid oxide fuel cell (SOFC) cathode. This aspect is crucial as it can boost efficiency, streamline compatibility, and enhance environmental sustainability within the SOFC technology. Simultaneously, it helps mitigate the adverse effects of impurities on membrane electrode assembly (MEA) degradation, ultimately facilitating the wider adoption of SOFCs across diverse applications.

Methodology

Flat-Tubular SOFC (FT-SOFC) Modelling Methods and Details

This study utilizes COMSOL Multiphysics version 6.0 to create an all-encompassing numerical model for a Flat Tubular Solid Oxide Fuel Cell (FT-SOFC) (Figure 1). This comprehensive FT-SOFC model is designed with a three-dimensional (3D) domain, which includes various components such as the anode flow channel, anode Gas Diffusion Electrode (GDE), Ni-YSZ membrane, cathode GDE, and cathode flow channel.

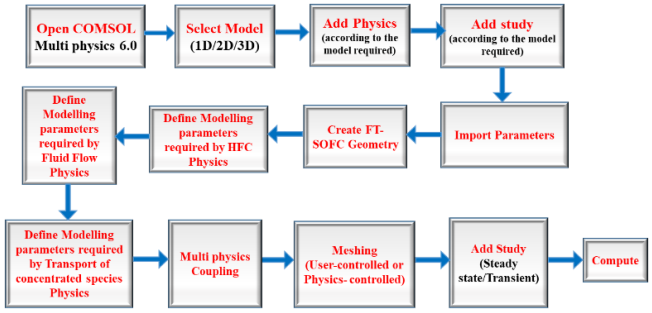

Figure 1. Fuel cell modelling steps in COMSOL Multiphysics.

Visualization of the geometric representation of a 2D and 3D FT-SOFC model showcasing the intricate spatial details and domain structures are illustrated in Figure 2.

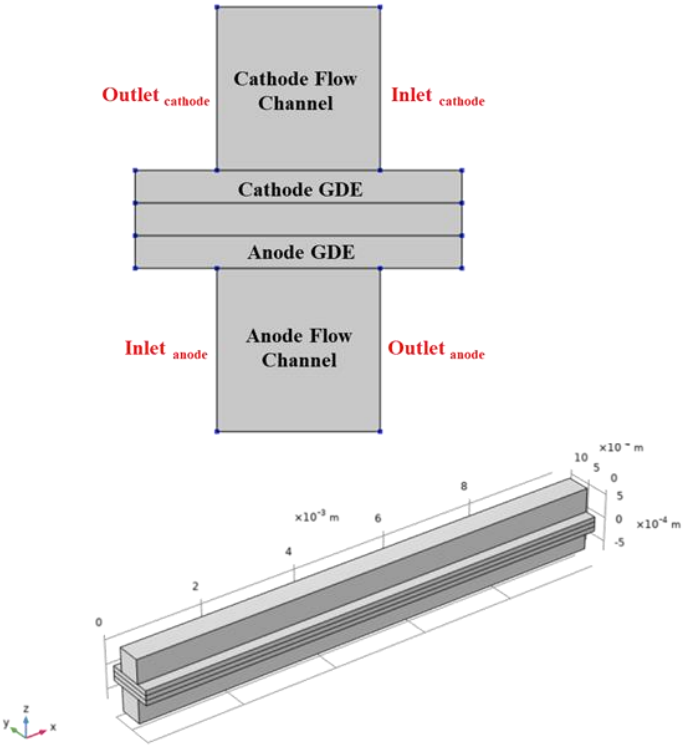

Figure 2. Geometric representation of FT-SOFC Constructed employing COMSOL Multiphysics in 2D and 3D.

Further, the performance of the modelled FT-SOFC is studied employing simulated bio-syngas of two different composition (Table 1) in an oxygen and air environment (Table 2). To maintain clarity, we have provided the dimensions of the modeled FT-SOFC and specific cell parameters used to study its performance in Tables 3 and Table 4. We manually input all other definitions and equations as prescribed variables into the model.

Table 1. Composition of simulated Bio-syngas employed as anode fuel feed in a Flat-tubular SOFC model.

Composition (%)	Syngas 1	Syngas 2
H_2	50	42.5
CO_2	32.5	26.5
CO	12.5	17.5
CH_4	5	3.5
N_2	0	10

To simulate the FT-SOFC model, we initially create a 2D layout of each component. Subsequently, we expand this layout into a 3D domain for in-depth analysis through extrusion option.

Table 2. Anode and Cathode fuel flow conditions adopted to study the performance of Flat-tubular SOFC model.

Case	Anode Fuel	Cathode Fuel
I	Syngas 1	Oxygen
II	**Syngas 1**	**Air**
III	Syngas 2	Oxygen
IV	**Syngas 2**	**Air**

Table 3. Cell dimensions of simulated FT-SOFC model

Cell Dimensions	
Cathode Flow channel Width	0.5 mm
Cathode Flow channel Height	0.5 mm
Anode Flow channel Width	0.5 mm
Anode Flow channel Height	0.5 mm
Anode Gas Diffusion Electrode thickness	0.1 mm
Cathode Gas Diffusion Electrode thickness	0.1 mm
Electrolyte/Membrane thickness	0.1 mm
Flow channel length	10 mm

Table 4. Physical parameters adapted to study the performance of FT-SOFC model in COMSOL

Cell Parameters	
Pressure	1 atm.
Temperature	1073.2 K
GDL permeability	1.18E-11 m²
Permeability (porous electrodes)	1E-10 m²
Pressure drop (Anode/Cathode)	2 Pa/6 Pa
Membrane	Ni-YSZ
Exchange current density, anode	0.1 A/m²
Exchange current density, Cathode	0.01 A/m²
Porosity	0.4
Solid effective conductivity (electrode)	1000 (S/m)
Electrolyte conductivity	5 (S/m)

We comprehensively assessed the fuel cell's performance through polarization and power curves, the distribution of various species within the fuel cell, velocity profiles, pressure distribution, and the electrochemical behavior of the FT-SOFC model. We achieve this through the use of predefined modules and physics offered by the COMSOL Multiphysics software, including the Hydrogen fuel cell module and the Free and Porous Media Flow module.

Constructed FT-SOFC model comprises of five discrete domains, featuring 30 faces, 56 edges with 9744 elements, each with a minimum element quality of 1.0 (Figure 2). The current FT-SOFC model adopted a segmented step-by-step approach, utilizing the PARDISO solver with a general relative tolerance of 0.001.

Further, the model used a steady state approach to solve the electronic and ionic potentials, mass distribution of each species along with velocity and pressure profile. To generate polarization curves, we executed a parametric procedure involving voltage steps, with 0.05V increments, ranging from 0.95V to 0.1V.

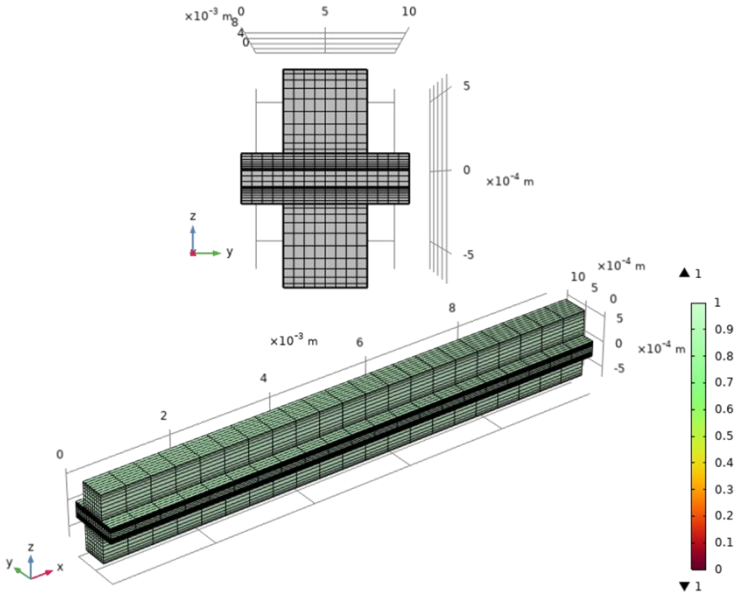

Figure 2. Mesh quality distribution of FT-SOFC Model (2D & 3D).

The central focus of this research centers on assessing the performance of a bio-syngas-fueled Flat Tubular Solid Oxide Fuel Cell (FT-SOFC) in both oxygen and air environments. To achieve this, we conduct simulations using two distinct syngas compositions, supplying them as anode fuel, while separately utilizing air and oxygen as cathode fuel sources (Table 2). We then compare performance metrics, including current and power density values, for each scenario. The results of these comparative analyses are presented in the subsequent section.

In order to ensure the accuracy and reliability of our model, it undergoes validation against experimental data. This validation process provides confirmation that the model effectively simulates the behavior and performance of Solid Oxide Fuel Cells (SOFCs), lending further credibility to our findings.

Governing Equations

The three-dimensional solid oxide fuel Cell (FT-SOFC) model we have developed comprises various key components, including the anode flow channel, anode Gas Diffusion Electrode (GDE), the Ni-YSZ membrane, cathode GDE, and cathode flow channel. This comprehensive model is designed to encapsulate a wide array of physical phenomena, encompassing mass transport, momentum transfer, electrochemical reactions, and fluid dynamics (Table 5). These facets collectively enable us to capture the intricate interactions taking place within the solid oxide fuel cell structure.

Table 4. List of intricate processes taking place within the FT-SOFC model with corresponding medium and physics interfaces employed in COMSOL.

Process	Medium	Physics Interface
Mass Transfer	Fuel & air channels, Gas diffusion layers (GDLs), Catalyst layers (CLs) and Membrane	Hydrogen Fuel cell
Momentum Transfer (Fluid Flow)	Fuel & air channels, GDLs and CLs	Fluid flow in porous media, Brinkman equation
Species Transfer	Fuel & air channels, GDLs, CLs and membranes	Transport of concentrated species
Heat Transfer	Everywhere	Heat Transfer
Electronic and Ionic Charge transfer	Bipolar plates, GDLs, CLs, Membrane	Ohm's Law, Conservation & Continuity equations and Butler- Volmer Equation

Within this model, the electrochemical reactions are mathematically represented using appropriate charge transfer kinetics, specifically employing the Butler-Volmer equation, while ensuring thermodynamic consistency. Additionally, the transport processes are described using the Maxwell-Stefan diffusion equations and convection equations, which account for the complex movement of various species within the fuel cell.

Concurrently, we address the distribution of fluid flow within the PEMFC model comprehensively. This is achieved through the incorporation of continuity equations, Navier-Stokes equations for anode and cathode flow fields, and the Brinkmann equations for the porous electrodes. These equations collectively consider the intricate fluid dynamics within the fuel cell structure.

Regarding boundary conditions, we impose no-slip conditions along the walls, necessitating zero velocity gradients. Additionally, we set prescribed inlet velocities and account for pressure drops at both the anode and cathode, ensuring a complete and realistic representation of the model's behavior.

Results and Discussion

Figure 3a and 3b shows the polarization and power curve simulated at two different syngas compositions (Table 1) in an oxygen and air environment. In an oxygen-rich environment, the Solid Oxide Fuel Cells (SOFCs) fueled with two different syngas compositions, referred to as "Syngas-1" and "Syngas-2" exhibit specific current and power values.

For "Syngas-1", the current and power values are recorded at 5724 A/m² and 1789.8 W/m², respectively. For "Syngas-2", these values are slightly lower, with a current of 5378 A/m² and power of 1735.7 W/m².

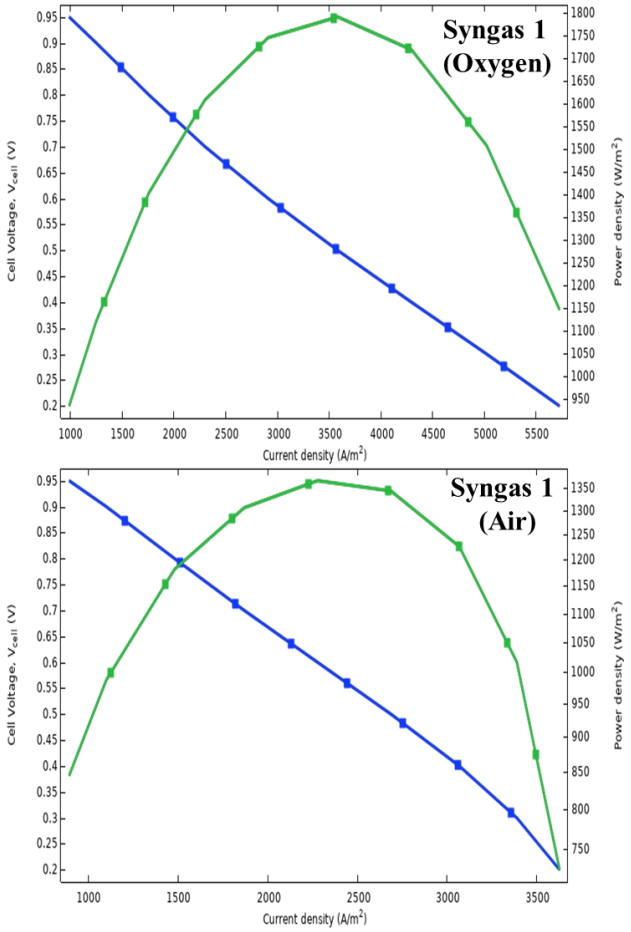

Figure 3a. Polarization and Power Curves of Modeled FT-SOFC at syngas-1 composition in an Oxygen and air environment.

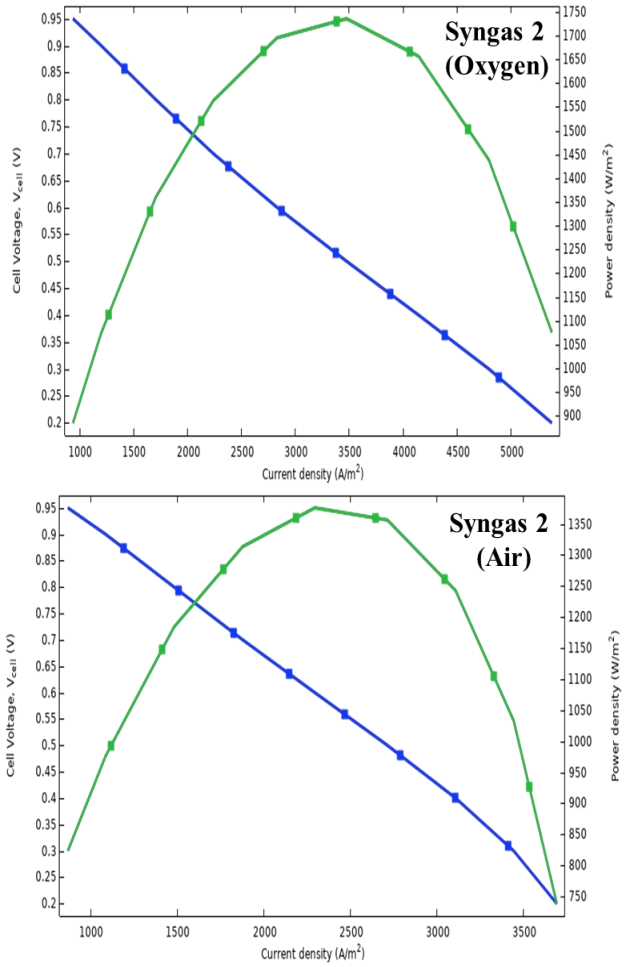

Figure 3b. Polarization and Power Curves of Modeled FT-SOFC at syngas-2 composition in an Oxygen and air environment.

Conversely, when these same SOFCs are operating in an air environment, the recorded current and power values vary. For "Syngas-1", the current and power are measured at 3625 A/m² and 1365 W/m², respectively. Meanwhile, "Syngas-2" demonstrates slightly higher values in this context, with a current of 3691 A/m² and power of 1376 W/m². This data indicates how the choice of fuel source and environment significantly impacts the performance of the SOFCs. This consistency in results can be attributed to the presence of air as the oxidizing medium, which introduces dilution effects due to the presence of nitrogen in the cathode side. Examination of polarization traces revealed minimal activation loss, negligible ohmic losses, and only minor mass transport losses.

In essence, these findings suggest that the use of air as the oxidizing medium in the cathode side has a specific impact on the various factors influencing SOFC performance, particularly activation, ohmic, and mass transport processes and electrochemical performance.

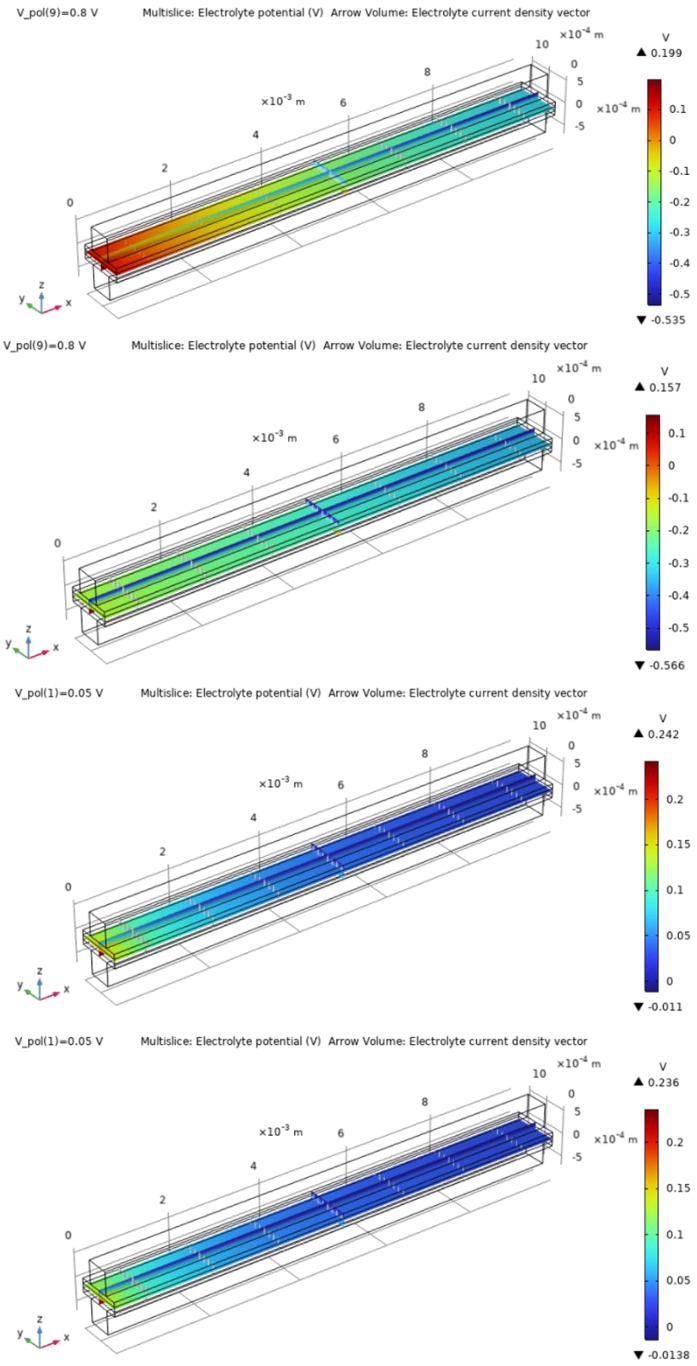

Figure 4. Distribution of electrolyte potential and electrolyte current density vector of syngas-1 in an air and oxygen environment simulated at 0.05 V & 0.8 V. Multislice: Electrolyte potential (V) & Arrow volume: Electrolyte current density vector

Figure 4 illustrates the distribution of electrolyte potential and electrolyte current density in a FT-SOFC model employing syngas-1 as anode fuel in an oxygen and air environment. It is discerned from the results that the electrolyte potential of FT-SOFC in an oxygen rich environment is higher than an air environment. This may be due to the high oxide ion mobility as a result of availability of oxygen rich fuel for electrochemical reactions to takes place.

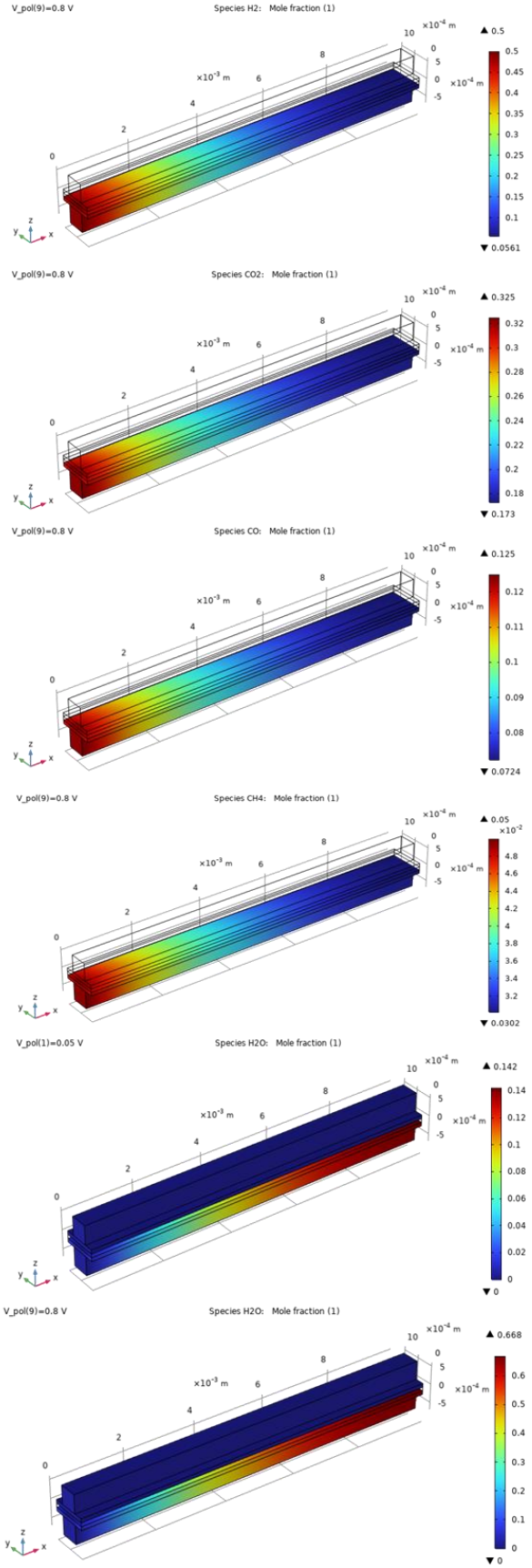

Figure 5a. Mass distribution of H_2, CO_2, CO, CH_4 and H_2O of Syngas-1 at 0.8 V in an oxygen environment.

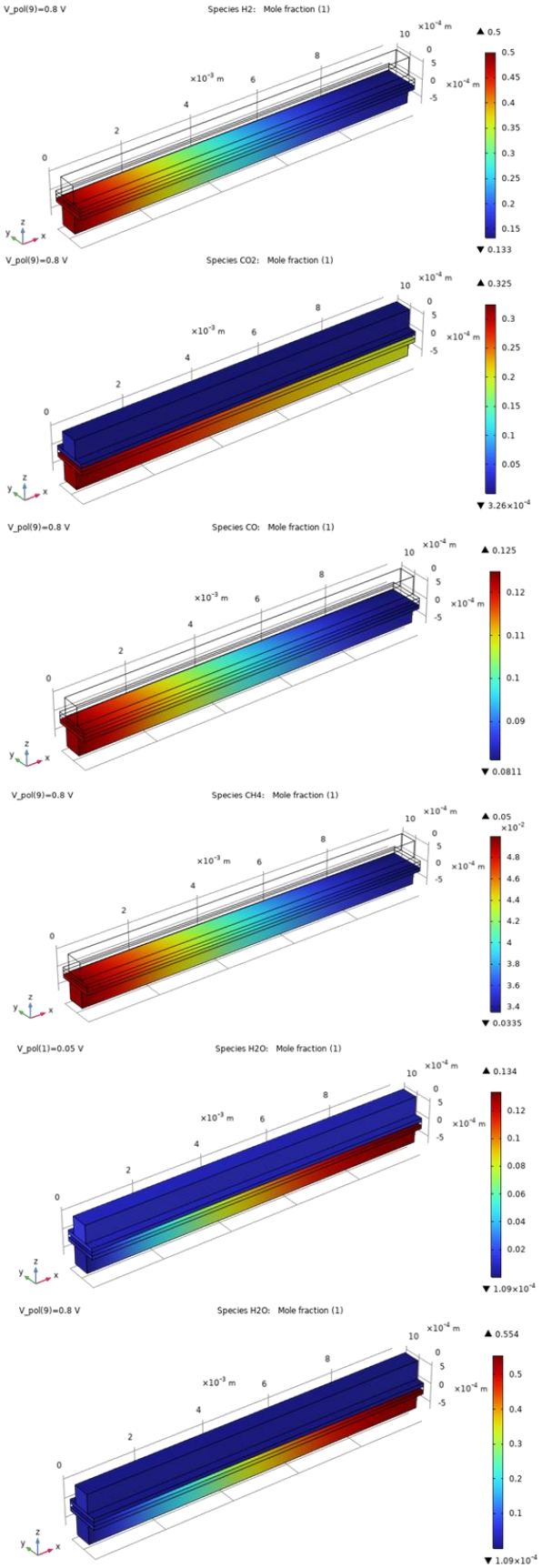

Figure 5b. Mass distribution of H_2, CO_2, CO, CH_4 and H_2O of Syngas-1 at 0.8 V in an air environment.

Furthermore, we conducted simulations to analyze the mass distribution of each syngas (Figure 5a & 5b) and producer gas species, as well as examined the velocity and pressure profiles to gain insights into the characteristics of the modeled flat tubular SOFC. The findings reveal that the initial concentrations of CO, CO_2, CH_4, and H_2 are at their peak near the anode inlet but decline notably as we progress towards the anode outlet. This trend signifies a decrease in current density within the flow channel, primarily due to fuel depletion.

On the other hand, the analysis of H_2O mass distribution illustrates a significant increase in H_2O concentration as we move across the fuel cell from the anode inlet to the anode outlet, correlating with cell voltage (Figure 5a). This H_2O mass distribution pattern further corroborates that water formation is more pronounced in syngas-fueled SOFCs in an oxygen environment compared to an air environment (Figure 5b).

This particular insight gained from our study significantly enriches our understanding of SOFCs powered by syngas and producer gas. It sheds light on how the choice of cathode fuel influences overall performance, demonstrating a complex interplay between fuel distribution, velocity, pressure, and the underlying electrochemical processes occurring within the fuel cell. Moreover, the experimental validation of the current study is in progress and will include in the subsequent publication.

Conclusions

This extensive study systematically explored the utilization of bio-syngas and producer gas as fuel sources for Flat Tubular Solid Oxide Fuel Cells (FT-SOFCs) with two distinct syngas compositions in both oxygen and air environments. The investigation employed a dual approach, combining numerical simulations using COMSOL Multiphysics software with experimental validation. In an oxygen-rich environment, FT-SOFCs powered by "Syngas-1" exhibited specific current and power values of 5724 A/m² and 1789.8 W/m², respectively. For "Syngas-2," slightly lower values were recorded, with a current of 5378 A/m² and power of 1735.7 W/m². When the same FT-SOFCs operated in an air environment, different current and power values emerged. "Syngas-1" yielded 3625 A/m² and 1365 W/m², while "Syngas-2" showed slightly higher values of 3691 A/m² and 1376 W/m². These results underscore how the choice of fuel and environment substantially influences SOFC performance.

Consistency in these results can be attributed to the presence of air as the oxidizing medium, introducing dilution effects due to nitrogen on the cathode side. Polarization traces further confirmed minimal activation loss, negligible ohmic losses, and minor mass transport losses.

Moreover, the study examined the distribution of various gas species and velocity and pressure profiles within the FT-SOFC model. Concentrations of CO, CO_2, CH_4, and H_2 were highest near the anode inlet and decreased toward the anode outlet, reflecting a decrease in current density due to fuel depletion. In contrast, the analysis of H_2O distribution indicated a substantial increase in concentration from the anode inlet to the anode outlet, corresponding to cell voltage. This pattern also highlighted that water formation is more prominent in syngas-fueled SOFCs in an oxygen-rich environment compared to an air environment.

In summary, this study provides valuable insights into the performance of FT-SOFCs fueled by different gas compositions in varying environments. It underscores the multifaceted interplay of fuel choice, oxidizing medium, and electrochemical processes within the fuel cell, shedding light on their complex dynamics.

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