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Design of Solid Oxide Fuel Cell (SOFC) Model for Flare to Power Conversion

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Abstract

This work presents an alternative approach to generating power using a Solid Oxide Fuel Cell (SOFC) based flare to power conversion model. The model utilizes pre-existing unit operating modules and other AspenPlus™ features such as a mixer, cooler, reactor, and heat exchanger. Validation of this model was performed by comparing results with the published data available in open literature. Results were obtained for induced voltage and sensitivity analyses of major operating parameters, such as operating temperature, operating pressure, and utilization factor (U_f) was performed using the developed model. The results and sensitivity analysis show the overall cell electrical voltage of 818 mV obtained at 1050°C and U_f at 0.85.

1. Introduction

The world's energy requirement has grown significantly. According to the survey, there will be a big leap in global energy consumption from 549 quadrillion BTU to 629 quadrillion BTU between years 2020 and year 2040; it is projected that this rise will continue steadily until approximately 815 quadrillion BTU by the end of year 2040 (U.S. Energy Information Administration (EIA), 2016). Figure 1 displays that the majority of the increase in energy usage took place after the industrial revolution.

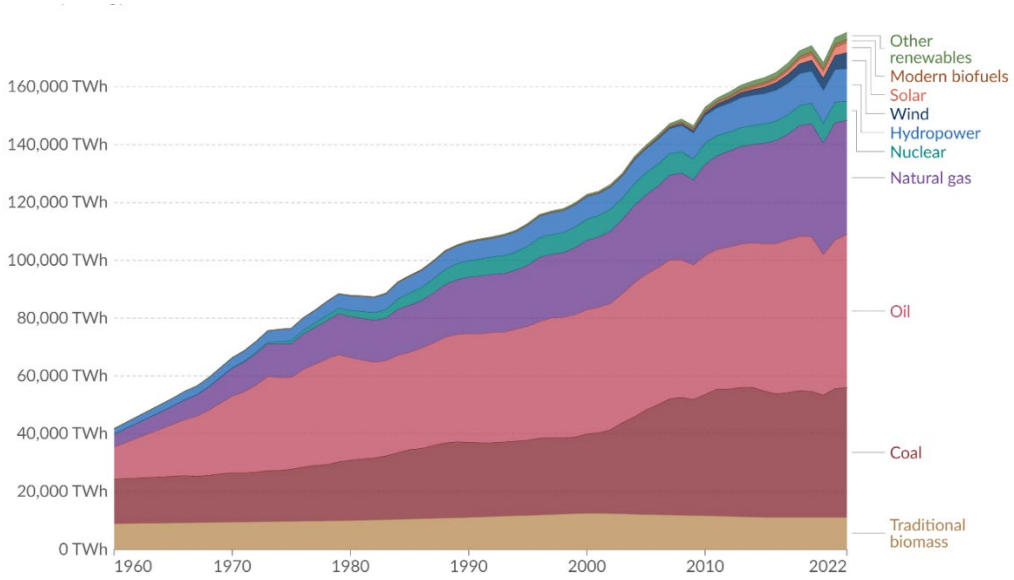

Figure 1. Increase in energy demand with time and contribution from different energy sources

The industrial revolution and population growth, both triggered a need for more energy which resulted in a negative impact on the environment because burning fossil fuels contributes greatly to emitting carbon. Therefore, it is important to find ways that can reduce the energy consumption in those nations and at the same time protect our planet. To handle the energy demand across the globe, many actions have been initiated. Burning fossil fuels emits more greenhouse gas emissions and raises concerns about environmental impact. One potential solution to address both the increasing energy demand and environmental concerns is the utilization of flare gas. The issue of increasing energy demands and environmental concerns could be addressed by the utilization of flare gas (Tahouni et al., 2016). In Oman, the utilization of flare gas can help reduce the requirement for energy and also encourage environmental preservation. By utilizing the flare gas produced during oil and gas extraction in Oman, we have the opportunity to decrease our reliance on non-renewable fuels. Proper management and utilization of flare gas can effectively reduce the release of greenhouse gases into the atmosphere. Furthermore, it has the potential to boost economic growth through the creation of new job opportunities and the promotion of technological advancements.

Several studies have been conducted to utilize flare gas for power generation, exploring various gas-to-power techniques such as gas turbines and reciprocating engines. In the petroleum industry, flare gas is a hazardous waste gas that damages the ozone layer. The presence of high methane content in the product makes burning the only effective method for preventing pressure buildup. (Dheyaa et al. 2022) reported that approximately 3.5% of flare gas globally (145 billion cubic meters) is wasted through burning or venting, resulting in significant losses of natural gases worth $16.4 billion. Figure 2 represents the statistics from 2014-2018, Oman is among the top 11 countries for flaring.

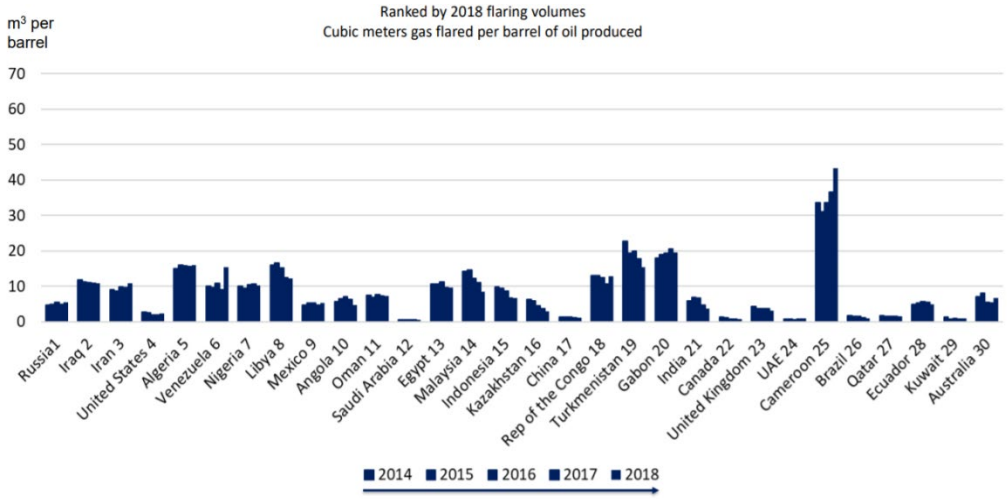

Figure 2. Contribution from different counties based on flaring intensity cubic meters of gas flared per barrel of oil produced (2014-2018) (Banco Mundial, 2023)

There has been a great deal of attention paid to the gas's substantial energy content in recent years. As a result of increasing the pressure of flare gas and managing it effectively, it can be utilized, thus aligning with petroleum production's cost-effectiveness. Using flare gas to generate electricity on the petroleum production platform can be seen as an additional resource that helps lower production costs.

The Global Gas Flaring Reduction (GGFR) aims to reduce technological and regulatory barriers to flare reduction, resulting in the development of country-specific flare reduction strategies via a public-private partnership (*Global Gas Flaring Tracker Report*, 2023). The organization was also entrusted with doing research and sharing best practices for flare reduction. GGFR had set an ambitious aim of lowering flares by 30% through this intervention.

The GGFR, which was part of the Sustainable Development Goals (SDGs), was replaced in 2015 by another effort known as Zero Routine Flaring by 2030. Despite efforts through initiatives, it was only in 2017 that there was a minor decline (5%) (United Nations Environment Programme, 2018). Currently, the methods used to recover flare gas include power generation, injection, and reinjection, feedstock for petrochemical plants, liquefying (gas to liquid (GLT)), and compression.

To choose the optimum flare gas recovery approach, operators must first understand how the flare gas is generated, transported, and used in the production plant (Emam, 2015). Attempts are being undertaken to determine the technical and economic viability of using flare gas for various uses. (Rahimpour et al., 2012a) conducted studies on the techno-economic feasibility of using flare gas in three different ways for two gas sources in Iran. The methods under consideration in the study include liquid production from flare gas, energy generation via gas turbine combustion, and compression and injection into the refinery pipeline for gas recovery. In both gas fields, they reported that liquid production is the most viable option (Rahimpour et al., 2012b; Rahimpour & Jokar, 2012). More specifically, the production of liquid methanol from flare gas was investigated by (Maroufmashat et al., 2016) for its techno-economic feasibility. Flaring and venting gas in the oil and gas industry is one of the leading causes of greenhouse gas emissions. According to (Al & Jamal, 2015) reducing flare gas is the most persistent issue in the global oil and gas business. One of the most promising reducing strategies is the utilization of flare gas for power generation via a fuel cell. (Al Waily et al., 2023; Mandhari et al., 2023) from southern oman, concluded that GHG from the flare gas could significantly be reduced by adopting six sigma continuous improvement approach alongwith management transformation. However, their study scope did not cover the direct utilization of flare gas. This particular study aims to further advance the use of flare gas for power production by incorporating solid oxide fuel cell technology. This research examines the potential of using solid oxide fuel cells to convert flare gas into electricity, as they have proven to be more efficient than traditional combustion methods in converting natural gas into power (Saidi et al., 2014). It specifically investigates Oman's current use of flare gas for power generation and explores the future possibilities associated with this approach.

2. SOFC-based Flare to Power Conversion

The SOFC is a promising technology for converting fuel gas directly into electrical energy due to its high operating temperature, making it ideal for cogeneration. Designing an efficient and cost-effective fuel cell system requires careful consideration of the auxiliary component of the plant, which impacts overall efficiency and cost. During commercialization, exploring various process designs is vital to optimizing efficiency and economics for different applications and fuel sources. Aspen Plus TM is a widely used process simulator renowned for its extensive database of thermodynamic and physical properties, saving time in chemical process studies. However, it lacks built-in models for SOFC, and integrating electrochemical reactions into it is challenging due to complexities in adapting stream mixing and transfer functions. Commercial simulation software currently lacks these capabilities. In the literature, SOFC systems are often modeled by constructing comprehensive stack models using programming languages like Fortran, Visual Basic, or C++. This method involves constructing an SOFC model in Aspen Plus TM using available functions and unit operation models, requiring minimal subroutine attachment. It facilitates analysis of SOFC power generation cycles and can be expanded to study the entire process, including the SOFC and balance of the plant. The model is based on Siemens-Westinghouse's tubular internal reforming SOFC technology, featuring a natural gas feed tubular generator with specific dimensions and performance characteristics. In this SOFC design, a tube injector introduces oxidant gas into the cells via the center while fuel gas exits through closed-end tubular cells. The injector extends toward the closed end to enable circulation of oxidant gas over the cathode surface toward the open end. Concurrently, fuel gas passes the anode on the outer part of the cell, facilitating electrochemical reactions. Cells are bundled, with in-stack reformer sections inserted between them to convert hydrocarbon fuel into hydrogen and carbon monoxide. An anode gas recycles loop supplies steam for reforming reactions in the pre-reformer. Depleted gases are expelled into a combustion plenum, generating heat to warm incoming air, some of which is used directly for reforming reactions instead of being transferred through cooling air.

2.1 AspenPlus™ model

The characteristics of the natural gas feed tubular SOFC are simulated in AspenPlus™ using standard built-in unit operation modules and functions. Figure 3 represents the simulation flow sheet which includes all components of the SOFC stack, such as ejector, pre-reformer, fuel cell (anode and cathode), and afterburner.

Recirculation and mixing of fuel in the mixer

Fresh desulfurized natural gas is mixed with recycled gas from the anode, containing electrochemical reaction products, and then fed to pre-reformers through ejectors. The ratio of recycling is determined by a specified steam/carbon (S/C) ratio required for the pre-reformers (see Table 1). This process is simulated using AspenPlus™ Mixer and Fsplitter (Figure 3).

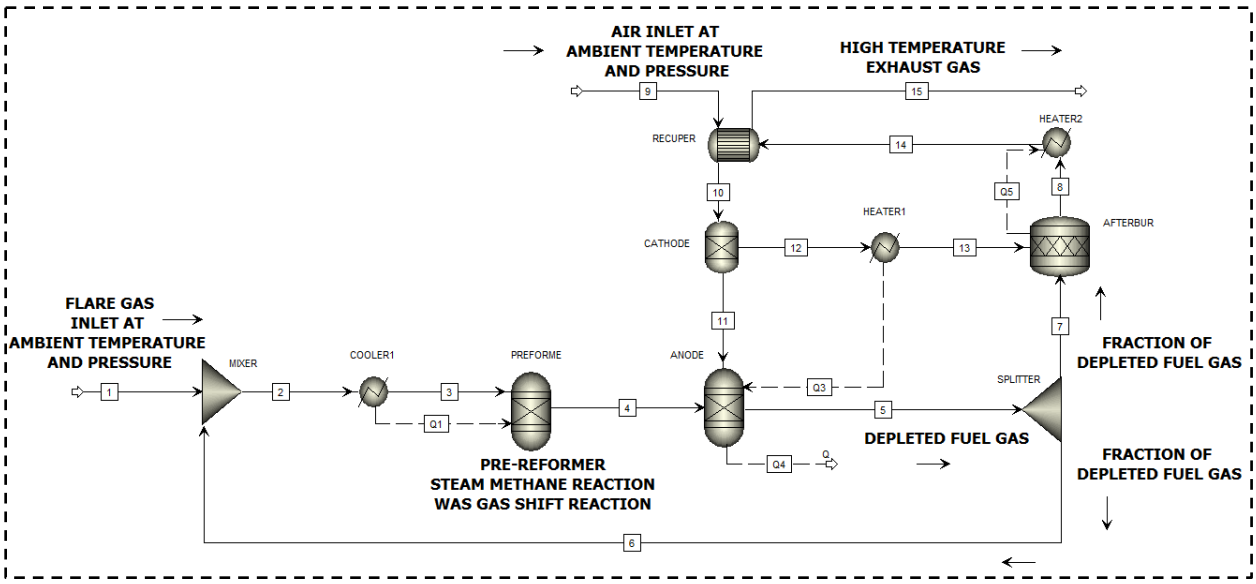

Figure 3. AspenPlus™ SOFC model flow sheet. Solid lines represent material streams and dotted lines energy streams.

Table 1. Flare gas composition and operating conditions (Zhang et al., 2005)

Fuel inlet composition	CH_4 81.3%, C_2H_6 2.9%, C_3H_8 0.4%, C_4H_{10} 0.2%, N_2 14.3%
Cell operating temperature	1000 °C
Cell operating pressure	1 atm
Power output	120 kW
Active area	96.1 m^2 (1152 cells)
Cell exhaust temperature (streams 5 and 13)	910 °C
Inlet air temperature (stream 9)	630 °C
Inlet fuel temperature (stream 1)	200 °C
Afterburn efficiency	100%
Overall fuel utilization factor	85%
Steam/Carbon ratio	2.5
Mixer fresh fuel pressure ratio	3
Pressure drop inside the SOFC	0

Feed stream 1 represents the fresh natural gas fuel feed into the SOFC, which is directed to the Mixer block named "MIXER". A fraction of recycled gas is splitted from stream 5 using the Fsplitter block named "SPLITTER" and goes back to the “MIXER”. The split fraction is determined to meet the desired steam/carbon (S/C) ratio value using the AspenPlusTM Design-spec function. Another Design-spec function is used to calculate the required inlet fresh fuel pressure (P_{fresh}) to drive the recycling of the anode gas, based on an assumed ejector fresh fuel pressure ratio (P_{fresh}/P_{cell}).

Pre-reforming of mixed fuel

To prevent carbon formation and mitigate temperature gradients in the SOFC, a pre-reformer is included in the design. It converts higher hydrocarbons and a small amount of methane into natural gas through steam reforming reactions, decreasing the fuel gas temperature. AspenPlus™ is utilized with a reactor module named "PREFORME" to simulate the reforming reactions within the pre-reformer. Additionally, an AspenPlus™ Heater module named "COOLER1" is employed to simulate the temperature decrease due to the endothermic reactions and predict the fuel gas outlet temperature. The chemical reactions specified in the pre-reformer block are:

Steam reforming reactions: $C_nH_{2n+2} + nH_2O \rightleftharpoons (2n + 1)\ H_2 + n\ CO$ (R1)
Water–gas shift reaction: $CO + H_2O \rightleftharpoons CO_2 + H_2$ (R2)
As shown in Fig. 3, the fuel gas entering "COOLER1" (stream 2) corresponds to input to the PREFORME. The temperature of the stream leaving "COOLER1" (stream 3) indicates the fuel gas temperature at the exit. The "PREFORME" is set to operate at this temperature, with all reactions reaching thermodynamic equilibrium. To ensure adiabatic conditions, a heat stream (Q1) from "COOLER1" to "PREFORME" is introduced, with the help of Design-spec in AspenPlus™ setting the net heat duty of the "PREFORME" to zero. Thus, the fuel gas leaving the "PREFORME" (stream 4) represents the output of the adiabatic pre-reformer, with its temperature matching the "REFORMER" operating temperature, usually above 500°C to avoid large temperature gradients in the stack.

Internal reforming and electrochemical reaction at the anode
At 1000°C, direct oxidation of CO and CH_4 in the pre-reformed fuel (stream 4) is feasible in the SOFC without a catalyst but is less favored compared to the water gas shift of CO to H_2 and reforming of CH_4 to H_2. It's commonly assumed in system analysis that only H_2, being more readily oxidized, electrochemically reacts as fuel. This simplifies analysis while accurately predicting the fuel cell's electrochemical behavior. To simulate reactions within the cell, an equilibrium reactor module Rgibbs (named "ANODE") is utilized. The stoichiometry of the electrochemical reaction is based on hydrogen reacting with oxygen. The reactions considered in the block are:

Electrochemical reaction: $H_2 + \frac{1}{2}O_2 \rightarrow H_2O$ (R3)
Methane steam reforming: $CH_4 + H_2O \rightleftharpoons CO + 3H_2$ (R4)
Water-gas shift reaction: $CO + H_2O \rightleftharpoons CO_2 + H_2$ (R2)

The three specified reactions reach thermodynamic equilibrium at a given temperature to simplify the simulation. Despite the electrochemical reaction not being represented as reversible, the simulation closely approximates electrochemical conversion due to high-temperature conditions, resulting in a large equilibrium constant (K) for reaction (R3). The equilibrium and exhaust temperature are set at 910°C, where the steam reforming reaction is nearly complete. The hydrogen involved in the electrochemical reaction (R3) comprises hydrogen from reactions (R2) and (R4) along with any hydrogen in stream 4.

Air stream preheating and oxygen supply
In the simulation, the SOFC stack's inlet air (stream 9) is preheated by the hot exhaust from the afterburner (stream 14) before entering the cell cathode to provide oxygen for the electrochemical reaction. AspenPlus™ implements this process using the rigorous heat exchanger module "Heatx" (named "RECUPER"), separator module "Sep" (named "CATHODE"), and temperature changer module "Heater" (named "HEATER1"). In the "RECUPER" block, the inlet air stream exchanges heat with the exhaust before entering the "CATHODE" block. Within the "CATHODE" block, a portion of oxygen (stream 11) is separated to enter the "ANODE" block for oxidizing the fuel, simulating oxygen ion crossover to the anode side. An AspenPlus™ Calculator calculates the molar flow rate of stream 11 ($n_{o_2\ required}$) based on the anode fuel equivalent hydrogen molar flow rate ($n_{H_2\ equivalent}$) and the expected fuel utilization factor (u_f) as

$$n_{o_2\ required} = \frac{1}{2}(u_f)(n_{H_2\ equivalent}) \quad (1)$$

The $n_{H_2\ equivalent}$ is the equivalent hydrogen contained in fresh fuel. It can be calculated as

$$n_{H_2\ equivalent} = n_{H_2\ in} + 1\ x\ n_{CO\ in} + 4\ x\ n_{CH_4\ in} + 7\ x\ n_{C_2H_6\ in} + \cdots \quad (2)$$

Afterburn

Depleted fuel gases undergo electrochemical and chemical reactions, with a portion recycled to mix with fresh fuel for pre-reforming reactions and the rest entering the combustion plenum. In the plenum, remaining H_2 and CO in the fuel react with depleted air's oxygen, releasing heat transferred to exhaust gases and incoming air. AspenPlus™ utilizes a reactor module R_{stoic} (named "AFTERBUR") to simulate combustion, suitable when reaction stoichiometry and conversion are known. Reactions specified in the "AFTERBUR" block are considered to reach completion (100% conversion) and include:

Hydrogen oxidation: $H_2 + \frac{1}{2} O_2 \rightarrow H_2O$ (R5)

Carbon monoxide oxidation: $CO + \frac{1}{2} O_2 \rightarrow CO_2$ (R6)

Calculation of cell voltage required fresh fuel and cell efficiency

The cell voltage calculation in the proposed model relies on a performance curve obtained by interpolating experimental data at standard operating conditions, followed by predicting cell voltage using semi-empirical correlations. This approach simplifies the model by avoiding detailed analysis of the cell's physical structure, making calibration easier. Empirical correlations are particularly useful in SOFC systems models due to continuous technological development. The method allows for predicting cell performance and can be implemented in AspenPlus™ using a Design-Spec. The model adopts an experimental curve from the (Energy, 2000) Fuel Cell Handbook as the reference curve and incorporates four semi-empirical equations to adjust for operating pressure, temperature, current density, and fuel/air composition effects on actual voltage.

- Operating pressure

  $\Delta V_P\,(mV) = 76\,x\,log\,\frac{P}{P_{ref}}$ (3)

  where P is the operating pressure (bar) and P_{ref} is the reference operating pressure (here P_{ref} = 1 bar).
- Operating temperature and current density

  $\Delta V_T(mV) = 0.008\,x\,\left(T - T_{ref}\right)(℃)\,x\,I_c(\frac{mA}{cm^2})$ (4)

  where T is the operating temperature and T_{ref} is the reference operating temperature (T_{ref} = 1000 °C).
- Fue composition

  $\Delta V_{anode}(mV) = 172\,x \log\left[\frac{{}^{P_{H_2}}/_{P_{H_2O}}}{\left({}^{P_{H_2}}/_{P_{H_2O}}\right)_{ref}}\right]$ (5)

  where ${}^{P_{H_2}}/_{P_{H_2O}}$ is the ratio of H_2 and steam partial pressures in the system and $(P_{H_2} / P_{H_2O})_{ref}$ is the ratio of H_2 and steam partial pressures in the system under reference conditions, $(P_{H_2} / P_{H_2O})_{ref}$ = 0.15).

- Oxidant composition

  $\Delta V_{cathode}(mV) = 92\ \times \log\left[\frac{P_{O_2}}{(P_{O_2})_{ref}}\right]$ (6)

  where P_{O_2} and $\left(P_{O_2}\right)_{ref}$ are the average oxygen partial pressures at the cathode for the actual case and the reference case, respectively here $\left(P_{O_2}\right)_{ref}$ = 0.164.

By summing the four correlations, the actual voltage V can be calculated as

$V = V_{ref} + \Delta V_P + \Delta V_T + \Delta V_{anode} + \Delta V_{cathode}$ (7)

3. Results analysis

This section discusses results obtained from Aspen plus simulation. The discussion includes simulation validation from the literature (Zhang et al., 2005). Additionally, sensitivity analysis was conducted to investigate the overall voltage of the cell by varying different parameters i.e., operating temperature, operating pressure, and overall fuel utilization factor.

Model Validation

The proposed model conducted a complete simulation based on a 120kW class atmosphere SOFC stack (1152 cells) detailed in the literature. Major calculation results and comparisons between simulation results and literature data are listed in Table 2. The SOFC model utilizing AspenPlus™ built-in unit operation modules demonstrates the predictive capability of the fuel cell stack performance successfully.

Table 2. SOFC model simulation results (120 kW DC output)

	Reference Data (Zhang et al, 2005)	Model simulation data
Voltage (V)	0.70	0.73
Current density (A/m^2)	178	176
Pre-reformer outlet temperature (°C)	536	537
Anode outlet composition (stream 5)	50.9% H_2O, 24.9% CO_2, 11.6% H_2, 7.4% CO, 5.1% N_2	50.6% H_2O, 24.8% CO_2, 11.8% H_2, 7.5% CO, 5.1% N_2
Stack exhaust composition (stream 15)	77.3% N_2, 15.9% O_2, 4.5% H_2O, 2.3% CO_2	77.2% N_2, 15.8% O_2, 4.5% H_2O, 2.3% CO_2
Stack exhaust temperature (°C)	834	837

The performance estimation for the stack is based on experimental data collected under specific fuel conditions. These conditions include 67% hydrogen (H_2), 22% carbon monoxide (CO), and 11% water (H_2O) in the inlet fuel mixture. Additionally, the simulation considers 85% utilization factor (U_f). A summary of the simulation assumptions and simulated stream properties can be found in Table 1 and Table 3.

The simulation reveals the overall cell potential of the SOFC stack is 0.73mV at 1000°C and 1 atm pressure. This result aligns closely with the (Zhang et al., 2005) which proves the reliability of the model simulation .

Table. 3. A property for the AspenPlus™ SOFC model

Stream no.	Temperature (K)	Pressure (atm)	Mole flow (kmol/hr)	Gas composition (mol%)						
				H_2	CH_4	H_2O	CO	CO_2	O_2	N_2
1	308.13	3	1.07	-	87.2	0.12	-	-	-	3.6
2	965.18	1	5.76	20.0	16.2	32.4	12.4	15.5	-	1.6
3	835.0	1.08	5.76	20.0	16.2	32.4	12.4	15.5	-	1.6
4	835.3	1	6.27	33.8	14.7	20.1	9.8	19.9	-	1.4
5	1183.15	1	8.11	24.6	-	39.8	15.2	19.1	-	1.1
6	1183.15	1	4.69	24.6	-	39.8	15.2	19.1	-	1.1
7	1183.15	1	3.42	24.6	-	39.8	15.2	19.1	-	1.1
8	1183.15	1	41.2	-	-	5.3	-	2.8	14.8	76.9
9	308.13	1	40.1	-	-	-	-	-	21	79
10	1094.47	1	40.1	-	-	-	-	-	21	79
11	1094.47	1	1.6	-	-	-	-	-	100	-
12	1094.47	1	38.5	-	-	-	-	-	17.7	82.3
13	1183.15	1	38.5	-	-	-	-	-	17.7	82.3
14	1426.38	1	41.24	-	-	5.3	-	2.8	14.8	76.9
15	732.06	1	41.24	-	-	5.3	-	2.8	14.8	76.9

Sensitivity analysis

The AspenPlus™ SOFC model allows for convenient and time-efficient sensitivity analyses, facilitating a deeper understanding of how changes in operating parameters affect the SOFC's performance. The subsequent section presents the outcomes of multiple sensitivity analyses conducted using AspenPlus™. Importantly, the assumptions utilized for validating the stack model (as listed in Table 1) remain consistent throughout these analyses.

Effect of operating temperature

The performance of a SOFC is substantially influenced by its operating temperature. A key characteristic of SOFC is its high operating temperature, typically ranging from 800 to 1000°C (Kundu & Jang, 2009).

The simulation results in this work have provided valuable insights into the relationship between operating temperature and performance. Specifically, the simulations indicate that the overall voltage of the SOFC increases as the operating temperature rises. Figure 4 shows that higher temperature enhances the electrochemical reactions occurring within the fuel cell, thereby improving its performance.

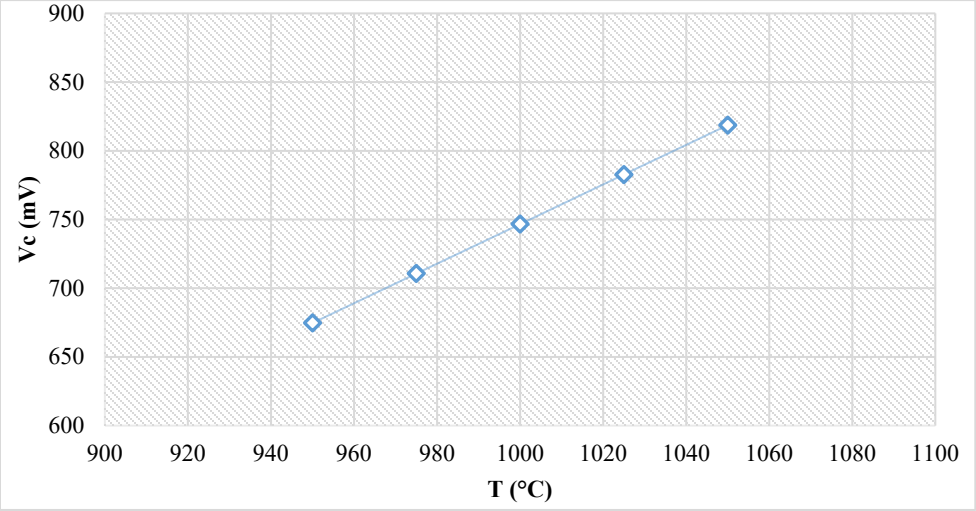

Figure 4. Effect of operating temperature on voltage

Effect of operating pressure

The operating pressure of a SOFC is closely related to its performance. This relationship has been established by simulation results, which show a logarithmic association between the SOFC's total voltage and operating pressure (Figure 5).

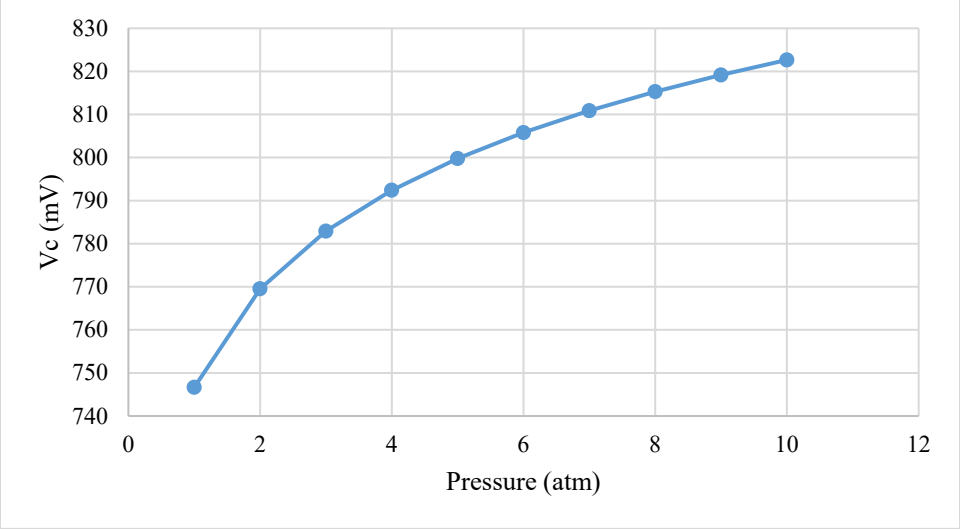

Figure 5. Effect of operating pressure on voltage

Effect of overall utilization factor (U_f) and current density (I_c)

The utilization factor of a Solid Oxide Fuel Cell (SOFC) has a direct impact on its output and efficiency. According to the simulation results, the overall voltage of the SOFC decreases as the utilization factor increases. It can be seen in the Figure 6 that a high utilization factor can result in a more efficient use of the fuel.

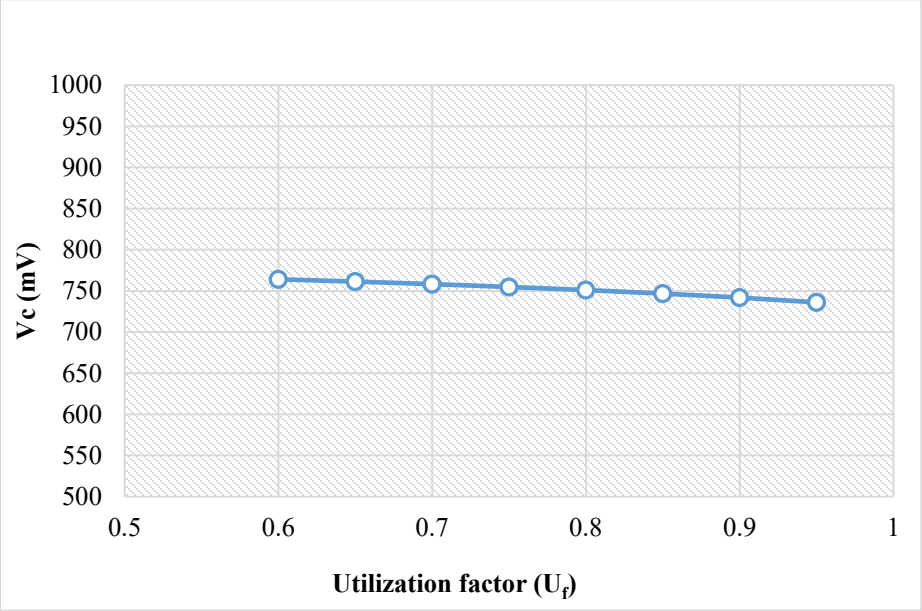

Figure 6. Variation of induced voltage (V_c) with the change in Utilization factor (U_f)

4. Conclusions and Future work

The simulation in current research work utilizes existing AspenPlus™ functions and unit operation models to allow for thorough thermodynamic and parametric analysis of SOFC operations. It can also be expanded to study the entire process, including both the SOFC stack and the auxiliary component of the plant.

The model was calibrated with published data. Sensitivity analyses revealed that the cell's electrical voltage reaches a maximum value of 818 mV at 1050℃ and U_f at 0.85. Also, cell electrical voltage increased from 746 to 822 mV as operating pressure increased from 1 to 10 atm.

However, the accuracy and flexibility of the model are limited by the methods and correlations used to calculate cell voltage, which rely heavily on semi-empirical relationships. To address this limitation, ongoing efforts are focused on developing a model grounded in fundamental phenomena rather than empirical relationships. This updated model is currently in development, with plans to refine the correlations based on its outputs.

Acknowledgment

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