INVESTIGATION OF MICROALGAE GASIFICATION IN A BUBBLING BED GASIFIER WITH INTEGRATED SOLID OXIDE FUEL CELL USING ASPEN PLUS

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ABSTRACT

High-temperature solid oxide fuel cells (SOFCs) provide sustainable and highly efficient distributed and modular energy conversion systems when combined with biomass gasification. Biomass gasification is an efficient alternative to the use of fossil fuels for the production of syngas containing mainly H₂, CO, and CH₄. Compared to inland biomass sources, microalgae are considered a promising source due to their more flexible cultivation methods, higher growth rate, and lower land requirements. They can be grown in the ocean, freshwater, or wastewater without requiring land for agriculture. By using steam as a gasification agent, the gasifier produces a higher hydrogen content in the syngas, resulting in a suitable fuel for SOFC. This study was conducted in Aspen Plus simulation to investigate the gasification with integrated SOFC system using microalgae as biomass source. A bubbling fluidized bed gasifier was selected and integrated into the SOFC after cleaning of the syngas. As a result, the influence of various key parameters such as energy efficiency, voltage and current density depending on the operating temperature of the gasifier and anode, and the ratio of steam to biomass of the gasifier in an integrated biomass gasification and SOFC is investigated. The results show that the efficiency of the system increases dramatically as the concentration of H₂ increases, but it decreases considerably when the concentrations of CO and CO₂ increase.

Keywords: Biomass, SOFC, Syngas, Gasifier, Energy Efficiency

1. Introduction

In the following decades, global energy consumption will continue to climb at a quick rate (Indrawan, 2018). With a considerable rise in population, there will be a proportional increase in demand for trustworthy and sustainable energy supplies. Fossil fuel depletion is posing a serious danger to economic development and energy security (Celaya et al., 2015). As a result, the use of alternative energy sources to replace traditional fuels is gaining popularity. Biomass is an attractive alternative from an environmental standpoint because of its CO₂ neutrality and low nitrogen and sulfur content. Biomass, unlike fossil fuels, is rapidly replenished and contains a diverse range of waste products obtained from animals and plants (Shayan et al., 2018).

Microalgae have more flexible culture methods, faster growth rates and need less area than terrestrial plants (Chen et al., 2011). Furthermore, since crops and algae do not compete, algae production will have no detrimental influence on food costs or other human activities. Algae might be treated thermochemically to create energy or biofuel in addition to biological conversion (López-González et al., 2014). Microalgal biomass has lower decomposition temperatures during the thermal conversion process than lignocellulosic biomass, resulting in better reactivity and reduced operating costs. The changes in composition are the primary cause. Proteins, lipids, and carbohydrates are the key components of microalgae, which are less thermally resistant than hemicellulose, cellulose and notably lignin, which are the main components of lignocellulosic biomass (Chisti, 2007). One of the thermochemical methods for algae to create value added products is via gasification.

Through partial oxidation with air, steam, or CO₂, gasification of algae might produce a syngas consisting of CO₂, CH₄, H₂, and CO (Safarian et al., 2020). Gasification is a successful approach because it increases energy recovery, provides less CO₂ emissions, and reduces tar and char content in the finished product.

The operating and design characteristics of the gasification, like heat source, gasifier type, gasification agent, and pressure, are the most important variables for achieving the proper syngas composition. For more effective syngas production, selecting the appropriate gasifier type is crucial. Fluidized bed is favoured over entrained flow and fixed bed gasifiers because of its improved heat transfer and mass transfer, higher carbon conversion efficiency, and ability to utilize a broad range of particle sizes (Gómez-Barea & Leckner, 2010). Fluidized bed gasifiers may either

circulate the gas or bubble up through the bed. The BFBG is a very simple machine for producing syngas. When using a different oxidizing agent, the exit gas will have different chemical and physical properties. When steam is applied as an gasifying agent, it creates a syngas with a greater H₂ content.

Electricity and heat might be produced directly in an steam turbine, gas turbine, or fuel cells using syngas (Segurado et al., 2019). It is widely agreed that fuel cell-based systems are among the most viable of the many possible combined process systems for producing electricity from syngas. Electrochemical machines known as fuel cells convert chemical energy into electricity with great efficiency and little pollution. One form of fuel cell that can be run at high temperature than others is the solid oxide fuel cell (SOFC). Since a higher processing temperature helps to fuel adaptability and contaminant tolerance, this kind is also considered the most practicable for biomass-derived fuels.

Although the combined gasification and SOFC system has the potential to be more efficient than competing heat and power technologies, more research and optimization are required to address issues with the system's design and operation. To define the influence of the operational parameters on the integrated system, more time and money are needed for experiments. As such, gasification and SOFC unit modeling is a dependable method for determining the best setup and optimal values for operating circumstances (Ahmed et al., 2012; Hauck et al., 2017). The thermodynamic (zero-dimensional) approach is often used in modeling-related research withouth to need gasifier design (Basu, 2018; Silva et al., 2019). Thermodynamic modeling is the most straightforward approach to making such estimates (Patra & Sheth, 2015). The gasification process and the SOFC are shown as a sequence of complicated chemical processes.

Aspen Plus is commonly used as the modeling tool of choice for designing systems based on mass balance and energy balance (Ramos et al., 2019). Since the integrated gasification and SOFC model was developed with thermodynamic principles in mind, it is possible to acquire the output parameters with ease and precision, including cell power, cell voltage, efficiency, syngas composition, and so on. A thermodynamic equilibrium-based approach might be either stoichiometric or non-stoichiometric. The stoichiometric model is based on the mass-action law and the equilibrium constants. For a simulation model to be run using the stoichiometric approach, the conversion rates of chemical processes and the stoichiometric coefficients of each component

must be specified. Conversely, the non-stoichiometric approach based on Gibbs free energy reduction is applicable in every situation because of its generality (Basu, 2018; Żogała, 2014). Another benefit of the non-stoichiometric approach is that it may be used to carry out chemical reactions using simply the chemical formula of the reactants, without the need of knowing anything about reaction kinetics, conversion values or stoichiometric coefficients (Baruah & Baruah, 2014).

Some research has simulated biomass gasification and integrated systems via Aspen Plus using the Gibbs free energy minimization concept. Lopes-Motta et al., (Motta et al., 2019) studied the impact of operating parameters and gasifying agent (steam and oxygen) on syngas composition and process performance using Aspen Plus. Numerous scenarios of biomass gasification in diverse fluidized bed configurations were simulated based on Gibbs free energy minimization approach. Faraji and Saidi (Faraji & Saidi, 2021) used Aspen Plus to create a steady-state model of algal biomass gasification. Algal waste, Rhizoclonium sp, Chlorella vulgaris and Spirogyra were chosen as the algal biomass feedstock, and a sensitivity analysis was conducted to determine the effect of gasifier pressure, gasifier temperature and air flow rate on the composition of syngas. The results of this research were utilized to make predictions about the behavior of the process at commercial and industrial sizes, allowing for its efficient and economical industrialisation. Lan et al. (Lan et al., 2018) built a model of the gasification-gas turbine system based on Gibbs free energy minimization using the ASPEN PLUS simulation environment to forecast the gasifier's performance and power generating capacity under different operating circumstances. The developed model successfully validated and model run with high accuracy. Palomba et al. (Palomba et al., 2017) obtained the syngas from the gasification of lignocellulosic biomass and used it for heating and electricity production in Aspen Plus simulation environment. They validated all components and developed the gasification-SOFC model to obtain CHP and plant gross electrical and efficiencies.

Even though there is a lot of work related to gasification, microalgae gasification, combined gasification and power processes, there is no model developed for the gasification with integrated SOFC process using algal biomass as fuel using Aspen Plus simulation. In this study, for the first time, a developed bubbling fluidized bed gasifier-SOFC model from literature was used to conduct an integrated microalgae gasification and SOFC process. The model was validated with experimental work and the effects of operating parameters such as gasifier temperature, steam to

biomass ratio of the gasifier and anode temperature were discussed in terms of electrical efficiency (E), voltage (V) and current density (I).

2. Methodology

2.1. Material Characterization

In this work, microalgae were selected as a marine biomass sample to use as a feedstock, and their physicochemical parameters were gathered from the existing literature. Microalgae, unlike land plants, may develop without a soil base, a central stem, or leaves. Microalgae samples with an LHV (dry basis) of 14.75 MJ/kg were selected for the gasification process due to their favorable energy properties. Table 1 displays the findings of both the proximate and ultimate analyses performed on the microalgae. Microalgae's hydrogen, carbon, sulphur, and nitrogen levels were measured experimentally, while oxygen was found by a difference calculation.

Table 1. Proximate and ultimate analyses of Hapalosiphon sp. microalgae (Liu et al., 2012).

| (wt.%) | Volatile Matter | 74.29 |
|---------------------------|-----------------|-------|
| Proximate Analysis (wt.%) | Ash | 13.98 |
| nate An | Moisture | 3.97 |
| Proxin | Fixed Carbon | 11.73 |
| (%: | Oxygen | 37.59 |
| Ultimate Analysis (wt.%) | Nitrogen | 6.45 |
| Analys | Hydrogen | 7.44 |
| mate / | Carbon | 47.94 |
| Ulti | Sulfur | 0.58 |

As seen in Table 1. Hapalosiphon sp. microalgae has exceptable amount of C, H and O content for gasification with integrated SOFC system.

2.2. Model Discription

This section details the work done using the Aspen Plus simulation tool to create a model of a gasification with integrated SOFC. In order to mimic complicated systems in Aspen Plus, they are often divided into smaller subprocesses. It's important to depict each individual process step to be as realistic as desirable. To clear away each step, we use a sequential modular strategy. It is challenging to describe the gasification with integrated SOFC system because of the many specific types of chemical reactions that occur throughout the process (exothermic and endothermic, homogeneous and heterogeneous).

The equilibrium model is a basic tool for modeling and predicting a system's output. The gasification with integrated SOFC system was modeled in the literature using the thermodynamic equilibrium model in Aspen Plus program (V11 aspenONE Engineering Suite) (Sezer et al., 2022). The following assumptions were taken into account throughout the simulation of the process in order to create a reliable model:

- The procedure has developed in steady state conditions.
- There are zero pressure and heat losses.
- The fuel devolatilizes instantly.
- Char is entirely made of carbon.
- Ash is nonreactive because of its presumed inertness.
- Chemical equilibrium is attained within a practical amount of time.
- H₂, CO₂, CO, H₂O, CH₄ and some of the heavyhydrocarbons are found in syngas.
- Chlorine (Cl) and sulfur (S) found in biomass combine to generate hydrogen chloride (HCl) and hydrogen sulfide (H₂S), respectively.
- Gases are thought to be ideal.
- Only nitrogen (N_2) and oxygen (O_2) make up the air.

Figure 1 shows the Aspen Plus flow diagram for the gasification with integrated SOFC model

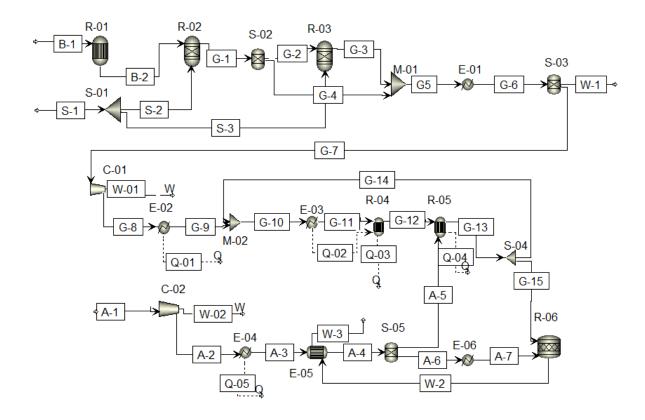


Figure 1. Process flow diagram of the gasification with integrated SOFC system (Sezer et al., 2022).

From receiving the fuel until completing the syngas generation, the whole gasification process was shown. In addition, the syngas from the gasifier was used as the fuel for SOFC, which then used Fortran subroutine computations to generate power. Using distinct reactors and building components, we were able to describe in great detail each stage of the process. Due to the rapid and complicated nature of the gasification processes and the intricate configuration of SOFC, equilibrium-based models were favored to be simplify matters and developed using by minimization of the Gibbs free energy (non-stoichiometric).

2.2.1. Bubbling Fluidized Bed Gasifier Part

Drying, pyrolysis, combustion, and reduction are the four cornerstone steps of the gasification process; they are modeled by connecting unit operation blocks in a sequential manner. Inputs for the fuel's thermodynamic characteristics and flow rate were made after the sample was defined as a nonconventional component based on findings from both ultimate and proximate analyses. The biomass must be transformed into a conventional form in a yield reactor called "R-01". The

following "R-02" block's (RGIBBS reactor) purpose is carrying out the drying and pyrolysis steps. The temperature at this stage is typically set about 200 and 500 °C. Here, pyrolysis, the second stage of thermal degradation, was initiated by setting the temperature to 300 °C. Because water and other volatiles may be released throughout the pyrolysis process, it was unnecessary to model drying as a distinct step.

Compared to other gasifying agents, steam produces a syngas with a higher H₂ content, hence it was favored. Pure steam flow "S-1" was first implemented in the "S-01" block, operating at 250 °C and atmospheric pressure. The entering steam flow was split into two streams at a predetermined ratio to provide a steam environment inside the pyrolysis and gasification reactors. The thermodynamic conditions of the "S-1" were not altered when it was sent "R-02" reactor. Gas and solid phase processes of the "R-02" reactor produced the output stream "G-1", which mostly consisted of CH₄, H₂O, CO₂ and tiny amounts of CO, C₂H₆ and C₂H₂. It was decided to split some of the CH₄ and put in the "S-02" block so that it wouldn't all be used up. The CH₄ achieves a chemical equilibrium and is not detectable in the syngas because of the high temperature in the "R-03" reactor. Additionally, the "S-02" block was used to separate gases that do not participate in the gasification operations. The gasification processes were carried out in "R-03" reactor. The G-4 that was collected was piped directly into the exhaust stream, bypassing the gasification unit entirely.

The key gasification and oxidation reactions—the water—gas shift, steam—methane reforming and Boudouard —occur in the gasification section. After passing through the "G-2" stream, the "R-03" reactor heats up to well over 700 °C to carry out the reactions in accordance with the concept of minimization of Gibbs free energy. Using the secondary "S-3" stream, pure steam at the identical thermodynamic values as the intake steam (atmospheric pressure and 250 °C) was injected into the "R-03" reactor.

At the equal temperature as the "R-03" reactor, syngas was generated together with water and other by-products. The "G-3" outflow stream was mixed with the "G-4" stream after being separated from "G-1" in the pyrolysis process using the "M-01" mixer. The gas mixture at 500 °C was obtained by passing "G-6" through a "E-01" block. Moisture and undesirable byproducts (H₂S, N₂, ash, etc.) should be cleaned from this flow. To do this, we employed the "S-03" block's

separation procedure to generate the "G-7" stream, which consisted only of the gases H₂, CH₄, CO and CO₂. Table 2 details the various building components and reactors in this part.

Table 2. Definition of reactors and blocks in the gasification part.

| Name | Block | Description |
|------------|--------|---|
| R-01 | RYIELD | Biomass is converted into conventional form. |
| R-02, R-03 | RGIBBS | Pyrolysis and gasification steps occur in these reactors. |
| S-01 | FSPLIT | Steam is divided between the two reactors. |
| M-01 | MIXER | G3 and S-GAS streams are mixed. |
| E-01 | HEATER | Cools the gas to desired temperature |
| E-05 | HEATX | Temperature is maintained as 500 °C |
| S-02, S-03 | SEP | Predetermined amount of gases is separated. |

2.2.2. SOFC Part

Aspen Plus with Fortran subroutines were used to conduct the SOFC model and calculate the desired parameters such as voltage, current density and energy efficiency. When taking into account its cutting-edge technology and its potential for commercialisation, the tubular SOFC system stands out as the most promising. For the purposes of this research, a Siemens Power Generation Inc.-developed 120 kW tubular SOFC unit was chosen for analysis. Many authors have cited this method's usage in their work (Doherty et al., 2010; Özveren, 2013; Zhang et al., 2005).

For the purpose of maintaining a constant pressure in the fuel supply, the "G-7" stream was sent through the "C-01" compressor block. Discharge pressure was determined by setting the design specification block "D-1" to a P_{SYNGAS}/P_{SOFC} ratio of 3. The "G-7" temperature, composition and pressure were defined, but the starting flow rate was adjusted according to the obtaining desired stack power using design specification block "D-5".

Compressed stream (G-8) was preheated by block "E-02", supplied to "M-02", and mixed with "G-14", the recycle from the "ANODE (G-13)" output. The "R-04" and "E-03" worked together to depict the SOFC stack's pre-reformer. The primary objective of "E-03" is to provide the

necessary heat for carrying out the reforming reactions in "R-04", and this is accomplished by using the heat emitted during the cooling process. When the net heat duty of the "R-04" is being equal zero value, as it is when run adiabatically, the discharge stream temperature of the "G-11" is adjusted using "E-03".

It is expected that only H_2 may participate in electrochemical processes, the "R-04" reactor converts CO into H_2 (CO + H_2 O \leftrightarrow CO₂ + H_2) and other heavier hydrocarbons and CH₄ into H_2 (C_xH_z + xH₂O \leftrightarrow (z/2 + x) H_2 + xCO). At that point, "G-12" stream combines with the O₂ flow coming from the "S-05" as it runs along the "R-05" reactor. Since ion transfer cannot be simulated with the existing model, just a single full reaction was carried out for the oxidant and fuel streams (H_2 + 0.5O₂ \rightarrow H_2 O).

The air was introduced into the system through the "C-02" block, which is a kind of air compressor. The air discharge pressure was adjusted to be somewhat greater than the surrounding atmosphere. Its composition, as well as its pressure and temperature, were entered. The design specification block "D-4" was used to set the air molar flow rate at a value that would result in an air utilization factor named as U_a of 0.19. The "E-05" heat exchanger block was used to bring the "A-2" stream from compressor stream up to the preheating temperature of air. The combustion processes in the "R-06" reactor produced hot products that provided the necessary heat. The required temperature and pressure of air is introduced into the "S-05" block. The "S-05" module filters out the O_2 in the air. The calculator block partitioned the O_2 fraction and organized it is obtaining a desired amount O_2 by using following equations:

$$nH_{2,in} = nH_{2,syngas} + 1 (nCO_{syngas}) + 4 (nCH_{4,syngas}) + ...$$
 (1)

$$Uf = \frac{nH_{2,cons}}{nH_{2,in}} \tag{2}$$

$$nO2,cons=0.5nH2,cons$$
 (3)

$$O_{2,split} = \frac{nO_{2,cons}}{nO_{2,in}} \tag{4}$$

Using the value of 0.85 for the fuel utilization factor (U_f), we can get the total molar flow rate of $H_{2,cons}$.

A fixed quantity of O₂ from the cathode was used to complete the reaction in the anode reactor. Then, utilizing design-spec "D-2" a fraction of the "R-05" gas was recycled, with the ratio being set at 1.8 with regard to the steam to carbon ratio. The stoichiometric reactor "R-06" burned any remaining "R-05" fuel with any extra "S-05" oxidant. The air was preheated by the combustion products in the "E-05" before it entered the "S-05" block. Furthermore, the exhaust stream temperature from the stack was defined.

Table 3 provides the operation blocks.

Table 3. Outlined of components in the SOFC.

| Block Name | Block Type | Description |
|---------------------------|---------------|---|
| C-01, C-02 | COMPR | Sets the operational pressure of streams. |
| E-02, E-03, E-04, E-06 | HEATER | Sets the temperature in streams. |
| M-02 | MIXER | Mixes the streams. |
| R-04, R-05 | RGIBBS | Reforms the other hydrocarbons and methane to H_2 , represents the electrochemical parts. |
| S-05 | SEP | Separates the O_2 . |
| S-04 | FSPLIT | Splits the stream to acquire the required steam to carbon ratio. |
| R-06 | RSTOIC | Represents the combustion processes. |
| E-05 | HEATX | Heats the air stream. |

2.2.2.1. Calculations of SOFC Parameters

The voltage calculation begins with an assumption of ideal performance. Next, the real voltage is determined by calculating the voltage losses in light of the non-ideal behavior. The expression of the standard potential when the voltage present in standard pressure is the ideal voltage value (V_{ideal}) (O'Hayre et al., 2009):

$$V_{id} = \frac{-\Delta \overline{g_f}}{2F} \tag{5}$$

Maximum electrical energy produced by a fuel cell without losses is represented by the Gibbs free energy of formation ($\Delta \bar{g}_f$) (Song, 2002). The anode half-reaction releases 2 moles of electrons, where F is the Faraday constant (96485 C/mol). Cell voltage is found to be most closely approximating the Nernst voltage (V_{Nernst}), sometimes called the reversible or equilibrium potential. The V_{Nernst} is calculated using the Nernst equation as seen in below:

$$V_{Nr} = V_{id} + \frac{RT}{2F} ln \frac{P_{H_2} P_{O_2}^{0.5}}{P_{H_2O}}$$
 (6)

The equations in Table 4 may be used to determine the activation, concentration and ohmic losses that contribute to the overall voltage drop.

Table 4. Calculation of voltage losses.

| Activation (Vactivation) | | |
|--------------------------|--|------|
| Cathode | $\frac{1}{R_{A,Cathode}} = \frac{4F}{R_g T_{OP}} k_{CA} \left(\frac{P_{O_2}}{P^0}\right)^m exp\left(\frac{-E_{CA}}{R_g T_{OP}}\right)$ | (7) |
| Anode | $\frac{1}{R_{A,Anode}} = \frac{2F}{R_g T_{OP}} k_{AN} \left(\frac{P_{H_2}}{P^0}\right)^m exp\left(\frac{-E_{AN}}{R_g T_{OP}}\right)$ | (8) |
| | Ohmic (Vohmic) | |
| Electrolyte | $V_{O,Elect} = j ho_E t_E$ | (9) |
| Interconnection | $V_{O,Inter} = j \rho_{Int} rac{t_{Int}}{w_{Int}} (\pi D_{mA})$ | (10) |
| Cathode | $V_{o,Cathode} = \frac{j\rho_{CA}(\pi D_{mA})^2}{8t_C}A[A + 2(1 - A - B)]$ | (11) |
| Anode | $V_{O,Anode} = rac{j ho_{AN}(A\pi D_{mA})^2}{8t_A}$ | (12) |
| | Concentration (V _{conc}) | |
| Cathode | $V_{C,cathode} = \frac{R_g T_{OP}}{4F} ln \left[\frac{\left(P_{SOFC} / \delta_{O_2} \right) - \left[\left(P_{SOFC} / \delta_{O_2} \right) - y_{O_2}^0 P_{SOFC} \right] exp \left[\left(R_g T_{OP} / 4F \right) (\delta_{O_2} t_C / D_{C,eff} P_{SOFC}) j \right]}{y_{O_2}^0 P_{SOFC}} \right]$ | (13) |
| Anode | $V_{C,anode} = \frac{R_g T_{OP}}{2F} ln \left[\frac{1 - (R_g T_{OP}/2F)(t_A/D_{A,eff} y_{H_2}^0 P_{SOFC})j}{1 + (R_g T_{OP}/2F)(t_A/D_{A,eff} y_{H_2}^0 P_{SOFC})j} \right]$ | (14) |

The all terms related to voltage losses and cell geometry and material characteristics are presented in Table 5 and 6, respectively.

 Table 5. Model parameters related to voltage losses.

| Activation | |
|------------------------------------|-----------------------|
| m (slope) | 0.25 |
| k _A (A/m ²) | 2.13×10 ⁸ |
| k _B (A/m ²) | 1.49×10 ¹⁰ |
| E _C (J/mol) | 160000 |
| E _A (J/mol) | 110000 |
| Ohmic | |
| A | 0.804 |
| В | 0.13 |
| Concentration | |
| ε | 0.5 |
| r (m) | 5×10 ⁻⁷ |
| В | 5.9 |

Table 6. Model geometry and material parameters.

| Geometry | |
|--|--|
| Cell Length (m) | 1.5 |
| Cell Diameter (m) | 0.022 |
| WInt (m) | 0.009 |
| $t_{\text{Int}}, t_{\text{A}}, t_{\text{E}}, t_{\text{C}} (m)$ | 0.000085, 0.0001, 0.00004, 0.0022 |
| | |
| Material Characteristics | |
| $ ho_{Anode} \left(\Omega \right. $ m $)$ | $2.98 \times 10^{-5} \exp(-1392/T_{OP})$ |
| $ ho_{Int} \left(\Omega \right. m ight)$ | 0.025 |
| $ ho_E \ (\Omega \ \mathrm{m})$ | $2.94\times10^{-5} \exp(10350/T_{OP})$ |
| $ ho_{Cathode} (\Omega m)$ | $8.114 \times 10^{-5} \exp(600/T_{OP})$ |

Concentration loss (V_{conc}) occurs in porous electrodes due to limitations in mass transport. We assumed diffusion and convection in the electrodes, and used the corresponding equations in Table 7 to get the relevant values.

Table 7. Diffusion calculations

| Parameters | Eq. |
|---|------|
| $D_{K,eff} = D_K(\varepsilon/\exists)$ | (15) |
| $D_K = 97r \left(T_{OP}/M_i\right)^{0.5}$ | (16) |
| $D_{ik} = \frac{1 \times 10^{-7} T_{OP}^{1.75} (1/M_i + 1/M_k)^{1/2}}{P(v_i^{1/3} + v_k^{1/3})^2}$ | (17) |
| $D_{ik,eff} = D_{ik}(\varepsilon/\exists)$ | (18) |
| $1/D_{i,eff} = 1/D_{ik,eff} + \frac{1}{D_{K,i,eff}}$ | (19) |
| $D_{A,eff} = D_{H_{2,eff}} \left(\frac{y_{H_2O}^0 P_{SOFC}}{P_{SOFC}} \right) + D_{H_2O,eff} \left(\frac{y_{H_2}^0 P_{SOFC}}{P_{SOFC}} \right)$ | (20) |
| $D_{C,eff} = D_{O_{2,eff}}$ | (21) |
| $\delta_{O_2} = \frac{{}^{D_{K,O_{2,eff}}}}{{}^{D_{K,O_{2,eff}} + D_{O_2} - N_{2,eff}}}$ | (22) |

To get the actual voltage (V_{real}) , the following equation was used:

$$V_{real} = V_{Nernst} - (V_{ohmic} + V_{conc} + V_{actual})$$
(23)

The following equations can be used to determine the current (I) and the current density (j), on the basis of the amount of H_2 used in electrochemical processes:

$$I = 2 * F * (H_{2,cons} * \frac{1000}{3600})$$
 (24)

$$j = \frac{I}{A} \tag{25}$$

F is Faraday constant and active area (A).

Using the information about the fuel (LHV_{fuel}) that is supplied into the SOFC and the information about the AC power (AC_{power}) that is fed into the SOFC, a Fortran codes in the D-5 design-spec was able to determine the electrical efficiency (E) of the SOFC. Using the following equation, we can get E after converting DC power (DC_{power}) to AC_{power} with an efficiency of 0.92:

$$E = \frac{{}^{DC_{power}*0.92}}{{}^{1000}}/LHV_{fuel} \times 100$$

3. Results

3.1. Bubbling Fluidized Bed Gasifier Model Validation

After BFBG model creation is complete, the model's correctness must be validated. Two independent experimental data sets from the published research were used to validate the developed process. The experimental conditions presented in Table 7 were used to input the system's operational parameters, fuel sample, and gasification agents' flow rates.

Table 8. Conditions in which the experiments were conducted

| | Experimental - 1 (Loha et al., 2013) | Experimental - 2 (Lv et al., 2003) |
|---------------------------|--------------------------------------|------------------------------------|
| Fuel Type | Rice Husk | Pine Sawdust |
| Gasifier Temperature (°C) | 850 | 800 |
| Fuel Feed Flow (kg/h) | 2.5 | 0.445 |
| Equivalence Ratio | 0.35 | 0.22 |
| Steam to Biomass Ratio | 0.5 | 1.35 |
| Gasification Agent | Steam, Air | Steam, Air |

The first set of experiments used rice husk as fuel, whereas the second set of experiments utilized pine sawdust. In both cases, researchers found that combining air and steam (in varying proportions) was used as gasifying agent. Molar fraction of syngas for CH₄, H₂, CO₂ and CO were evaluated after simulating under the same operating circumstances as experiments, and the results are presented in Table 9 and 10.

Table 9. Comparison of syngas composition from our model and first experimental study

| Component | Our Model | Experimental-1 (Loha et al., 2013) |
|-----------------|-----------|------------------------------------|
| CO | 14.50 | 14.80 |
| CO ₂ | 18.40 | 18.90 |
| H ₂ | 12.30 | 12.40 |
| CH ₄ | 3.00 | 1.90 |

Table 10. Comparison of syngas composition from our model and second experimental study

| Component | Our Model | Experimental-2 (Lv et al., 2003) |
|-----------------|-----------|----------------------------------|
| CO | 40.35 | 41.61 |
| CO ₂ | 16.85 | 17.53 |
| CH ₄ | 8.34 | 10.05 |
| H ₂ | 29.78 | 30.79 |

It was found via comparison that the model performs effectively even when mole fractions vary by a little amount. These variations in outcomes are consistent with those seen in earlier research investigations (Jarungthammachote & Dutta, 2008; Rupesh et al., 2016). The model demonstrated exceptional simulation performance in attempting to capture the understand of the gasification phenomenon.

3.2. SOFC Model Validation

This SOFC stack model was built using Aspen Plus simulation, and it is based on tubular SOFC technology. Validation of the constructed SOFC model against experimental or validated data sets is required. The model was validated using operational characteristics from Siemens Power Generation Inc.'s model of a 120 kW tubular SOFC stack. Results from both the simulation and the experiment were compared to one another as system outputs. You may find a summary of the SOFC's operational parameters in Table 11.

Table 11. Operating conditions of the model

| Parameters | Values |
|--------------------------------------|---|
| Fuel inlet composition (%, mole) | CH ₄ 81.3%, N ₂ 14.3%, CO 0.9%, C ₄ H ₁₀ 0.2%, C ₂ H ₆ 2.9%, C ₃ H ₈ 0.4%, |
| Active Area (m ²) | 96.1 |
| DC _{power} output (kW) | 120 |
| SOFC Operating Temperature (°C) | 910 |
| SOFC Operating Pressure (bar) | 1.08 |
| Inlet Fuel Temperature (°C) | 200 |
| Inlet Air Temperature (°C) | 630 |
| Cell Number | 1152 |
| Ua | 0.19 |
| Uf | 0.85 |
| DC to AC inverter efficiency (%) | 92 |
| P _{FUEL} /P _{SOFC} | 3 |

| Thermal Losses | 2% |
|-----------------------|-----|
| Steam to carbon ratio | 2.5 |

Similar to the experimental work, the system's working parameters were adjusted, and fuel was defined with specified composition in Table 11. Current density, cell voltage, gross AC efficiency, and other operatinfg parameters at the respective streams were used to evaluate the outputs. Table 12 displays the resulting comparisons.

Table 12. Comparison of SOFC results for our model and literature studies

| | Experimental | | |
|-----------------------------|-------------------------|-------------------------|-------------------------|
| | (Veyo & Lundberg, | Model | |
| Parameters | 1999) | (Doherty, 2014) | Our Model |
| Current Density | | | |
| (mA/cm ²) | 180 | 182.86 | 189 |
| | Not | | |
| Voltage (mV) | Available | 683 | 683 |
| Cathode Inlet | Not | | |
| Temperature (°C) | Available | 823 | 826 |
| Pre-reforming | | | |
| $Temperature \ (^{\circ}C)$ | 550 | 535 | 544 |
| Exhaust Temperature | | | |
| (°C) | 847 | 833 | 836 |
| | | 5.6% CO, | 5.6% CO, |
| | | 6.2% N ₂ , | 6.2% N ₂ , |
| | | 27.8% H ₂ O, | 27.8% H ₂ O, |
| | | 23.1% CO ₂ , | 23.1% CO ₂ , |
| Anode Inlet Gas | Not | 10.4% CH ₄ , | 10.4% CH ₄ , |
| Composition (%, mole) | Available | 26.9% H ₂ , | 26.9% H ₂ , |
| Anode Exhaust Gas | 5.0% N ₂ , | 5.1% N ₂ , | 5.1% N ₂ , |
| Composition (%, mole) | 48.0% H ₂ O, | 50.9% H ₂ O, | 50.8% H ₂ O, |

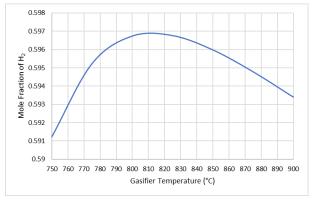
| Gross AC Efficiency (%, LHV) | 50.00 | 51.28 | 51.19 |
|------------------------------|-------------------------|-------------------------|-------------------------|
| | 5.0% CO | 7.4% CO | 7.4% CO |
| | 28.0% CO ₂ , | 24.9% CO ₂ , | 24.9% CO ₂ , |
| | 14.0% H ₂ , | 11.6% H ₂ , | 11.6% H ₂ , |

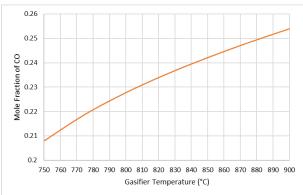
The model's predictions were quite consistent with the observed data. While there are some minor discrepancies in the model's composition and temperature readings, the model's performance was excellent based on current density, AC efficiency and voltage.

3.3. Evaluation of Operating Parameters on System Performance

3.3.1. Impact of Gasifier Temprature on Syngas Composition

The gasification part's operating temperature is a key factor in determining syngas composition and quality. Most of the equilibrium processes that take place during gasification are endothermic, therefore temperature has a huge impact on the whole process. Generally, fluidized bed reactors used in the biomass gasification process run at temperatures much below 1000 °C to preserve the integrity of the ash produced in the process. In this study, we analyze the effect of gasification temperature on syngas composition using the sensitivity analysis feature of the Aspen Plus simulator. Simulation findings for the concentration changes of H₂, CH₄, CO and CO₂ as a function of temperature are shown in Figure 2; this study was run with the steam to biomass ratio held constant at 0.8.





(a) (b)

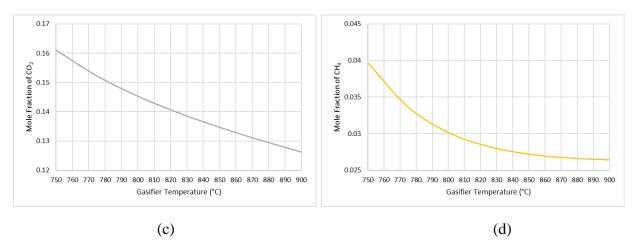


Figure 2. Impact of gasification step temperature on syngas composition: a) H₂, b) CO, c) CO₂ and d) CH₄

As can be seen in Figure 2, the gasification temperature has a direct impact on the state of chemical equilibrium of the reactions and the syngas composition due to the presence of endothermic and exothermic reactions. According to Le Chatelier's principle, as the temperature is increased, the chemical equilibrium shifts toward the reactant side for exothermic reactions and toward the product side for endothermic reactions (Shehzad et al., 2016).

The H₂ concentration in syngas showed a slight increase, which rose from 59.12% to 59.68%, at a temperature between 750 and 825 °C. The endothermic steam-methane reforming process raised the amount of H₂ gas in syngas while decreasing the amount of CO gas (Pang et al., 2020). Because of Le Chatelier's principle, when the mole fractions of H₂ and CO in syngas increase, the watergas shift, an exothermic process, moves to the reactant side. Furthermore, the Boudouard reaction, which generates CO and lowers CO₂ at quite high temperatures (>800 °C), is also favored by increasing temperatures. The data showed that when temperature increased, CO concentration rose from 20.80% to 25.30% while CO₂ concentration fell from 16.10% to 12.62%. According to the existing literature, these findings are consistent with expectations (Kartal & Özveren, 2020; Sezer & Özveren, 2021).

3.3.2. Impact of Gasification Step Temprature on SOFC

It is crucial to choose the right parameters to indicate overall system performance when assessing the system based on gasification step temperature. Since syngas composition fluctuated dramatically with gasification temperature, it was believed that this was the most important parameter in the integrated system. Directly or indirectly, the composition of the syngas and the molar flow are used to determine the SOFC's performance characteristics (electrical efficiency, voltage and current density). With the S/B and anode temperatures held constant at 0.8 and 910 °C, respectively, the impact of gasification step temperature on SOFC evaluation parameters was studied. The findings can be seen in Figure 3.

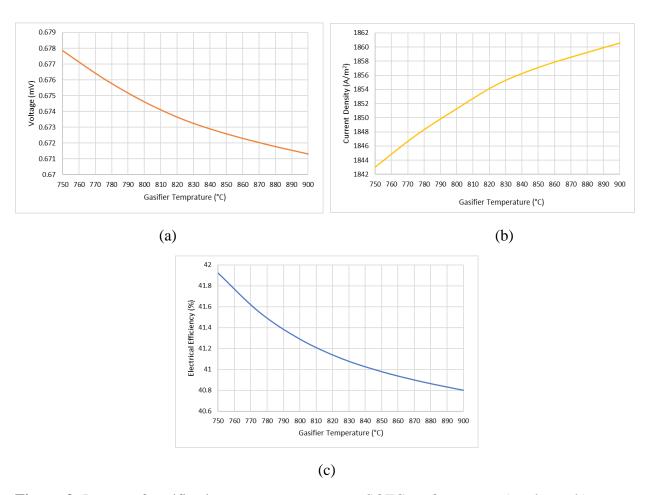


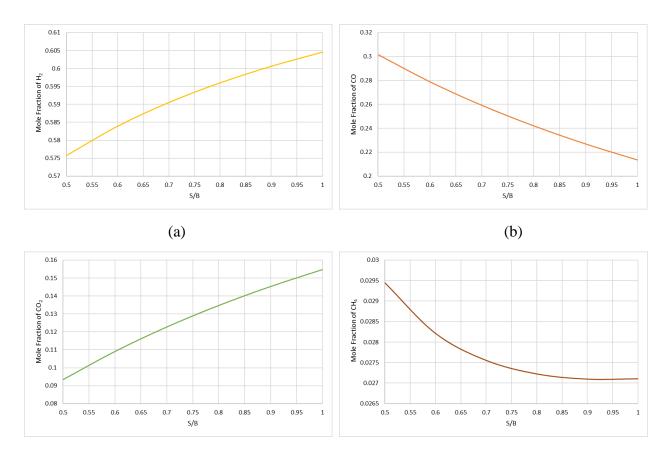
Figure 3. Impact of gasification step temperature on SOFC performance: a) voltage, b) current density, c) electrical efficiency

Figure 3.c shows how the temperature of the gasification step affects the electrical efficiency of the SOFC. As the temperature grew from 750 to 900 °C, the electrical efficiency steadily dropped from 42.92% to 40.80%. Syngas's CH₄ content changed drastically, which corresponded to a drastic decrease in electrical efficiency and voltage. Because it aids in conducting the anode reaction and yields 3 moles of H₂ every cycle, CH₄ reforming is attractive. Rising the operating temperature of the reformer facilitates the reverse water—gas shift reaction at higher temperatures

due to the previously noted decrease in CH₄ content in syngas with increasing temperatures. Since the anode inflow stream contains more and more H₂O due to the reverse water-gas shift reaction, this explains the declining trend in electrical efficiency. Tar in syngas may be generated at lower temperatures, therefore this should be considered even if increasing the temperature did not improve electrical efficiency. This resulted in a doubling of the current density to 120 kW DCP. Figure 3.a shows a decrease in voltage due to voltage losses calculated as a function of increasing current density. This is discussed in detail in subsection 2.2.2.1. Consistency with the findings found in the literature was shown (Abuadala, 2010; Bellomare & Rokni, 2013; Dey et al., 2014; Hosseinpour et al., 2018).

3.3.3. Impact of Steam to Biomass Ratio on Syngas Composition

In terms of syngas composition, the steam to biomass ratio (S/B) is a critical variable. The ratio of the mass flow rate of steam to the feed rate of biomass is named as S/B ratio. Figure 4 displays the findings on the influence of S/B on syngas gas concentrations. When the gasifier temperature was set at 850 °C, a measurement range of 0.5 to 1.0 was chosen for S/B.



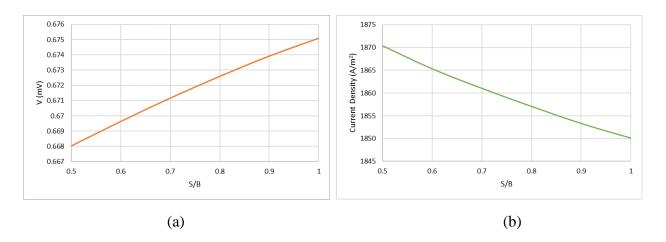
(c) (d)

Figure 4. Impact of S/B on syngas composition: a) H₂, b) CO, c) CO₂ and d) CH₄

When steam is introduced to a gasifier, the partial pressure of H₂O rises. Figure 4 illustrates how the forward processes of water-gas shift, water gas and steam methane reforming reactions are substantially accelerated by the larger partial pressure of H₂O. This action decreased CO₂ and CH₄ emissions while increasing H₂ and CO₂ output. The H₂ content dramatically rose from 57.57% to 60.46%. Unfortunately, adding steam raised CO₂ levels while lowering CO levels as consistent with the literature (Monteiro et al., 2017; Sezer et al., 2021). Therefore, it is crucial to choose the best possible value to produce syngas rich in H₂ and low in CO₂.

3.3.4. Impact of S/B on SOFC

While SOFCs can tolerate certain impurities in the fuel, the efficiency and output of electricity generated from them improves significantly when the H₂ percentage of the fuel is increased. As was discussed in the introduction, steam is a crucial factor in determining the precise composition of syngas. Parameters of SOFC performance were measured as a function of S/B as presented in Figure 5. As part of the parametric analysis, we held the temperatures of the gasification phase and the SOFC anode constant at 850 °C and 910 °C, respectively.



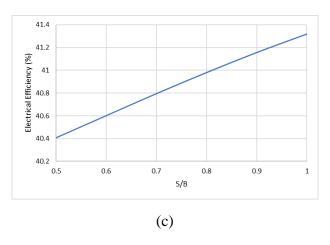


Figure 5. Impact of S/B on SOFC performance: a) voltage, b) current density, c) electrical efficiency

The influence of S/B on the concentration of syngas was demonstrated in the previous section, where it was established that the amount of CO₂ and H₂ rose in the produced gas with an enhancing ratio of steam. In addition, enhancing H₂ amount around 4.00% promoted the electrochemical reactions in anode. Figure 5.a shows that when the H₂ partial pressure at the anode inlet was raised, the voltage value also rose. The improved voltage results from a reduction in voltage losses made possible by the increase in current density. Thus, as shown in Figure 5.c, the electrical efficiency of SOFC rose from 40.41% to 41.32%. The results gained followed a trend that was seen in the existing literature (Sezer et al., 2022).

3.3.5. Impact of Anode Temperature on SOFC

Anode is the primary site of electrochemical processes. It is crucial to evaluate the influence of anode temperature on SOFC performance, since the pace of the reaction is highly affected by temperature. Anode working temperature was altered among 900 and 980 °C while S/B and gasification part temperature were kept stable at 0.8 and 850 °C, respectively. Voltage, electrical efficiency, and current density are used as evaluation parameters for SOFCs, and they are all shown to be affected by the anode temperature in Figure 6.

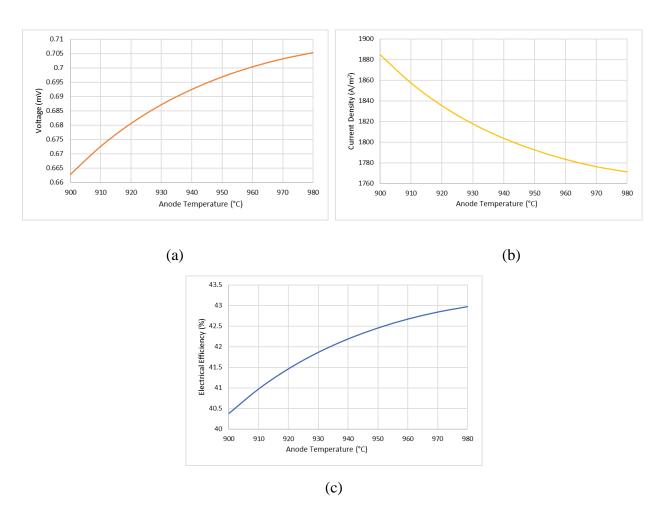


Figure 6. Impact of anode operating temperature on SOFC performance: a) voltage, b) current density, c) electrical efficiency

Increasing the SOFC's working temperature increases the rate of the electrochemical processes, which in turn improves the electrical efficiency, as shown in Figure 6.a. Significant progress was made in electricity efficiency, jumping from 40.38% to 42.98%. Because of this, more O₂ is being drawn into the anode region as the rate of electrochemical reactions rises. The increase in O₂ partial pressure improved voltage since it resulted in less current density and fewer voltage losses. High-temperature SOFCs need a more durable material than their low-temperature counterparts, despite the fact that their performance improved dramatically at higher temperatures. As a result, the cost of high-resistance materials and upkeep time should be minimized by optimizing the temperature of SOFCs.

Conclusion

In this study, the microalgae biomass sample was used as the fuel source for gasification with integrated SOFC system. Research in both theory and experiment has confirmed the accuracy of the Aspen Plus model of the bubbling bed gasifier with integrated SOFC. Sensitivity analysis study findings shown that operating temperatures and S/B had substantial effects on syngas composition. Produced gas from microalga gasification was reached high content of H₂ (60%) with steam addition. As the temperature climbed from 750 to 900 °C, a large fall in CH₄ concentration resulted in a gradual decline in electrical efficiency, from 42.92% to 40.80%. The influence of S/B on the composition of produced gas was demonstrated. The electrical efficiency of SOFC increased from 40.41% to 41.32% when the H₂ concentration was raised to roughly 4.00%, which aided the electrochemical processes in the anode. The another important parameter anode operatint temperature showed highly positive impact on SOFC. The electrical efficiency jumped from 40.38% to 42.98%.

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