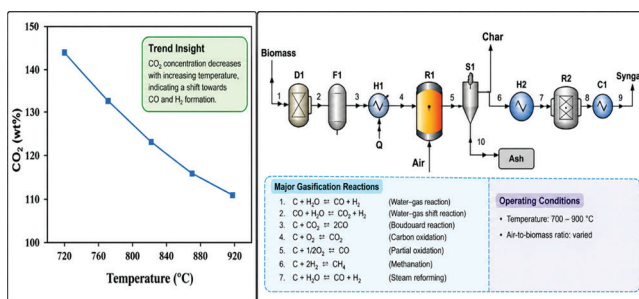




Process Modelling and Parametric Analysis of *Casuarina equisetifolia* Biomass Gasification

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Graphical Abstract



Restricted-equilibrium Aspen Plus model of biomass gasification of air-blown *Casuarina equisetifolia*, showing the process flowsheet and the impact of gasification temperature on CO₂ production.

Abstract

The paper depicts the process of simulation and application to biomass such as *Casuarina equisetifolia* to gasify by Aspen Plus with air-blown gasification under reactor temperatures ranging from 700°C to 900°C. The process model included drying, separation, and reaction processes. In this case, the biomass feed rate and air-to-biomass (A/B) ratio were constant, and when the reactor temperature increased, initially, a rise in the hydrogen mass flow rate occurred and then remained constant when the reactor temperature was above 800°C. Concurrently, the carbon dioxide (CO₂) became less, which can be inferred that the essence of the run of the chemical reactions was switched to carbon monoxide (CO) and hydrogen (H₂) being formed, such that the conventional chemical reactions were producing CO₂. As the A/B ratio increased for a fixed temperature of 750°C, the

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CO₂ concentration increased, though CO and methane (CH₄) decreased, and then the H₂ concentration was approximately steady. Such behavior caused the syngas mass-flow rate to fall when A/B is considerably high; then, syngas constituents would cross over into more complete combustion to produce more CO₂ at the expense of CO and CH₄, as demonstrated in this paper, to indicate significant understanding of the gasification process. This paper provides novel, valuable, nuanced guidance for work on *Casuarina equisetifolia*, a less-understood and infrequently studied but locally relevant biomass material, while simultaneously addressing the disconnect between equilibrium behaviors and the behavior of reactors found in industrial applications. The unified use of these components is a value-added step that, in their use together, advances the field in the future by providing another accurate, flexible, and practical simulation tool for biomass gasification.

Keywords: Biomass gasification, Operating parameters, Temperature Sensing, Modelling.

1. Introduction

Gasification is a thermochemical process in which the feedstock is reacted with a controlled amount of oxidizing agent, e.g. air, oxygen, steam or CO₂ at a high temperature to produce a combustible (Abuelgasim et al., 2021) gaseous product. Gasification involves partial oxidation of the carbonaceous material to yield a product gas (syngas) containing mainly CO, H₂, CO₂, CH₄ and other light hydrocarbons and heat. The composition and energy content of the product gas are highly sensitive to the characteristics of the feedstock, gasifying agent, operating conditions and temperature and pressure. Biomass is a key sustainable energy source, encompassing all organic materials from plants and animals. It also comprises liquids and gases that are produced when the decomposition of organic materials occurs, which are biodegradable and not fossilised. In India, abundant biomass resources are available (Abuelgasim et al., 2021). In reality, a large portion of it is disposed of by burning in open fields, which causes air pollution. It is essential to convert biomass to energy to make the most of these resources. On the other hand, there are several thermochemical processes like Pyrolysis, partial oxidation, combustion, gasification, etc. Gasification generates useful gaseous fuels or chemical feedstock from carbonaceous materials (Dhrioua et al., 2022). The conversion of carbonaceous materials into product gases is also called combustion. There are some distinctions between gasification and combustion. Unlike the gasification product gas, the combustion product gas does not have a high heating value. Gasification, which requires a certain amount of energy or temperature, occurs in an oxygen-deficient environment, whereas combustion occurs in an oxygen-rich environment,

releasing heat. Once the biomass is introduced into the gasifier, final drying occurs, utilizing heat from the downstream hot zone (HajiHashemi et al., 2023; Shabbar et al., 2013; Loweski Feliz M et al., 2024). When the temperature surpasses 100°C, the loosely bound water in the biomass is permanently removed. As the temperature increases, low molecular weight compounds begin to volatilize; this process continues up to around 200°C (Roddy & Manson-Whitton, 2012; Aboelela et al., 2023). Efficient moisture removal is crucial for optimising gasification efficiency and reducing the energy required for the process. Preheating is vital in enhancing the gasifier's efficiency and ensuring a more consistent and controlled gasification process (Tavares et al., 2020).

Thermochemical conversion of biomass to valuable gaseous products is a promising path to sustainable energy and resource recovery, especially as it makes renewable carbonaceous feedstocks into fuel-rich product gases like syngas. The performance of biomass conversion process however depends heavily on feedstock composition, operating temperature, pressure, gasifying reagent ratio and reactor conditions, etc. (Zaccariello, A., et al. (2023) which often requires time consuming and resource intensive experiments to optimize the process. Different modelling tools have been developed to forecast biomass conversion and product-gas characteristics, but it is still difficult to simultaneously obtain good results of the relationships between the operating conditions, the properties of the feedstock and the characteristics of the product-gas while keeping the computation time low. Hence, a flexible and reliable modelling framework is needed which can predict the process behaviour, provide information on the dominant operating parameters and enable process optimization without a large number of experimental trials. This study aims to fill this void by developing a predictive model of biomass conversion and testing the capability of this model to describe the formation and composition of product gas for different operating conditions.

Biomass gasification is an effective and economically viable method for producing thermal energy through the thermochemical conversion of biomass into a gaseous mixture using steam, air, or a combination of both (Halder et al., 2025; De et al., 2023). The efficiency of a gasifier depends on factors like temperature, pressure, gasifying agent, feedstock type, and biomass moisture content. Several developments have been studied in the experimental and computational aspects of biomass gasification. Mathematical models must be developed to account for several intricate processes, such as rapid pyrolysis, gasification of the char produced, and the conversion of tar and the water-gas shift reaction. In addition to predicting the impact of key input factors, including moisture amount, air/biomass ratio, component and their amount, and energy value of the product gas, these models can analyze the thermochemical processes involved in gasifying biomass. Several gasification models based on Thermodynamic equilibrium,

Aspen Plus, ASPEN, and ASPEN have been presented and analyzed in this work. The developed mathematical models enable designers to optimize gasifier operations by utilizing experimental data from pilot or existing plants. Operating under extreme conditions to enhance gasifier performance can be hazardous without prior analysis. Modeling provides a cost-effective way to assess the benefits and risks of operating modern gasifiers under extreme conditions, such as high temperatures and pressures (Shi et al., 2025).

Aspen Plus makes examining a range of chemical, biological, and physical processes easier. Model building and updating become simpler using Aspen Plus because small pieces of intricate and combined structures may be adopted and validated through this method. A sizable property data bank with a variety of stream properties is included in Aspen Plus. These are necessary to represent the material streams in a gasification plant (Li et al., 2004). There is a provision for including internal property data (Shi et al., 2025; Mandal et al., 2025). Nikoo & Mahinpey have studied the gasification process using ASPEN software and modified an atmospheric fluidized bed gasifier accordingly (Nikoo & Mahinpey, 2008). This model takes into account both response kinetic modeling and hydrodynamic factors. Four types of reactor schemes and nested exterior FORTRAN codes are used in Aspen to predict the gasification process. In Aspen Plus, an external Fortran code refers to custom Fortran subroutines that can be integrated into Aspen simulations to perform specialized calculations that the standard built-in models do not cover. Carbon is converted more effectively as the temperature rises, and H_2 is produced. The equivalent ratio is directly proportional to the generation of CO_2 and the effectiveness of the carbon sequestration (Naderi et al., 2025). Increasing the air-to-biomass ratio makes it possible to produce more H_2 and CO while reducing carbon dioxide and conversion efficiency. The average size of the particles has no bearing on the composition of the resultant gas. Aspen Plus was used to develop the model, and it was based on Gibbs Free Energy Minimization (Wayne Doherty, Reynolds, & Kennedy, 2008). Restrictive equilibrium was used to calibrate the model results against the experimental data. A Restrictive Equilibrium, also known as a Limited or Conditional Equilibrium, is a state where a chemical system reaches equilibrium under specific constraints or restrictions rather than complete thermodynamic equilibrium. The model anticipated the composition of Syngas, conversion efficiency, and heating parameters (Puig-Arnavat et al., 2013). The model's findings and the data from the experiment agreed. The variables that affect the composition of syngas include temperature, equivalence ratio (ER), preheating of gasifier medium, the moisture of feedstock on its heating value, and its conversion efficiency. An ER denoted the temperature range where hydrogen and carbon monoxide were produced in the highest amounts (Dhrioua et al., 2022).

Thus, a cold gas economy (CGE) and high heating value were ensured. The value of gas heating decreased as ER decreased. With air preheating, more hydrogen and carbon monoxide are produced. As a result, CGE and gas heating values increased. Air preheating was found to work better at lower ERs. With more moisture present, performance was shown to suffer. It was discovered that pre-drying the input gasoline was necessary to prevent this. Steam injection was being used to obtain hydrogen-rich syngas. Using Aspen Plus, the thermochemical processes in wood biomass gasifiers were modelled. For the thermochemical models, the reactants are presumed to reach chemical equilibrium. The model predicted both the ultimate component of the producer gas and pyrolysis gas (Paviet, Chazarenc, & Tazerout, 2009). Parametric research based on air/fuel ratio modification was carried out. The model was modified to account for the operational parameters of a staged gasifier created by the Technical University of Denmark (DTU). The impact of humidity with a modest air injection was found using parametric analyses. The same model could simulate the Downdraft Gasifier (DDG) and DTU. Data on the composition of the exit gas and flaring pyrolysis were acquired. Combining Aspen Plus and specific Fortran files, the biomass gasification process was modeled in Dual Fluidized Bed (DFB) reactors (Abdelouahed et al., 2012; W. Doherty et al., 2013). Biomass pyrolysis, secondary reactions, and char combustion are the three main chemical processes that separate the DFB into three modules. Mass yields of char, water, tar species, and permanent gases were modelled based on the reactor temperature using a correlation of pyrolysis. The secondary processes were represented by a brief kinetic approach that controls the gas ambience and catalytic conversions over lumped tar components and CH₄ char, gas phase water-gas shift reaction (WGSR), and char conversion. The WGSR kinetics were discovered to be sensitive to the syngas composition and flow rate. An improved kinetic law for WGSR was provided after a review of the rate laws for WGSR. Different gasification stages, i.e., devolatilization, mild oxidation, and reforming, are represented by a mix of modules in the Aspen Plus simulator.

For this simulation to produce scientifically acceptable results, reactor temperature and air-to-biomass ratio had to be systematically varied while keeping the other parameter constant in each set of experiments. This study design allows a clear assessment of the impact of each parameter by minimizing confounding effects, following the studies published on equilibrium modeling of biomass gasification. The choice of fixed values came from maximizing the yield of syngas and following experimental norms cited for air-blown gasification of biomass in the literature to enhance comparability and rigor.

The restricted equilibrium approach is utilized to remedy the divergence brought on by the gasification systems in complete equilibrium

(Bhattacharjee et al., 2024; Bhakta et al., 2024). The effects of operating factors, including the steam/MSW ratio (S/M), oxygen percentage in the enriched air (OP), the temperature of gasification, equivalence ratio (ER), and MSW moisture content, are analysed concerning the syngas composition and gasifier efficiency. When the temperature increases, more H_2 and CO are produced, resulting in higher gasification efficiency. By raising ER, MSW's CO production and carbon conversion are enhanced. The product gas's energy value and reactor efficiency may be boosted, and the concentration of combustible components also increases with increasing air concentration. The syngas quality and cold gas efficiency deteriorate at a larger moisture level. Due to air injection, the H_2 /CO ratio and gasification efficiency increase. The Aspen model was used to predict syngas composition, energy value, and cold gas efficiency (CGE) by Reynolds and Kennedy (2013). The experimental facility for the gasifier was designed with the necessary cooling and filtration systems in place (Keche, Gaddale, & Tated, 2015). The obtained experimental data for babul wood, neem wood, mango wood, and bagasse were used to confirm the model's findings. The model accurately anticipated H_2 , CO, and CO_2 compositions but significantly underpredicted the composition of CH_4 . Babul wood was shown to have a greater gasifier conversion efficiency than other types of biomass. Its high quantities of carbon, hydrogen, and less ash could cause this. An Aspen Plus simulation model of biomass gasification for the generation of syngas and subsequent syngas adjustment was done as the gasifying agent employed was steam, and the model developed was based on the minimization of Gibbs' free energy (Pala, Wang, Kolb, & Hessel, 2017). The calibration procedure made use of the constrained equilibrium approach. The impact of significant variables such as temperature required in gasification, steam to biomass ratio, and the temperature needed for the shift reaction was examined on the concentration of H_2 , concentration of carbon monoxide (CO), conversion of CO and CO_2 , and H_2 /CO ratio in the product gas. For several types of biomass feedstock, the composition of syngas was anticipated. The syngas composition was changed to get the H_2 /CO molar ratio near the 2.15 value needed for the shift reaction to produce FT (Valderrama et al., 2018).

This research presents a dynamic process model for gasification of *Casuarina equisetifolia* biomass (CEB) in Aspen Plus for air-blown gasification temperatures from 700°C-900°C, contributing to the knowledge base on biofuels. The unique contribution of this research is worth noting. This research examines the differences between theory and experiments using a restricted equilibrium approach. It will aid in evaluating and predicting the syngas produced by gasification, primarily hydrogen and carbon monoxide. The study is based on combining chemical reactions and not the traditional Gibbs free energy minimization models. The model used in this study considers a more complete chemical dissociation approach to

gasification, including Boudouard reaction, water-gas shift, methanation, and species such as tar-free biomass, which other researchers may have overlooked. A systematic analysis of temperatures and air-to-biomass ratios (A/B) revealed the highlight findings of understanding the importance of the Boudouard reaction at high temperatures, the competition of CO_2 and combustible gases at A/B ratios that may further be refined for industrial grant applications. Applying the Peng-Robinson (PR) equation and Boston-Mathias (BM) modification for thermodynamic property calculation, which is capable of better representing light gases and polar mixtures, is novel. The concentrations of CO and hydrogen were changed to accomplish this. Research scale fluidized bed gasifier experiments using experimental data from steam biomass gasification literature were used to validate the model's predictions. Food wastes were steam gasified to yield a product gas composition with an H_2/CO molar ratio that was almost 2.15. Direct feeding of a Fischer-Tropsch synthesis facility is possible with this. To get the H_2/CO molar ratio around 2.15, the rest of the feedstocks needed the adjustment of syngas, either via WGS or RWGS processes. The experimental data were contrasted with the model results. It was observed that characterizing tar and its dynamics improved the model's believability and performance. As a result of enhanced H_2 production and decreased tar content, the gasification process was improved at higher temperatures (A.M. Sharma et al., 2012).

2. Methodology

In a fluidized bed reactor, biomass is gasified using air as the gasifying agent. The principal constituents of the gasification product gas include hydrogen, carbon monoxide, etc., and contaminants such as tars, ammonia, Hydrogen sulphide, etc. After that, within the separator, solids like tar, ash, and char are eliminated from the product (M. Martín, I.E. Grossmann, 2011; Bhattacharjee et al., 2025). The steps required to produce diesel from biomass are depicted in Figure 1.

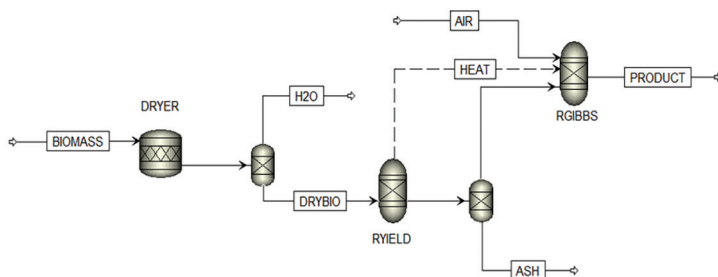


Figure 1: Process Flow for Gasification of Biomass with Air in Aspen Plus.

Aspen Plus syngas product composition is computed by minimizing the total Gibbs free energy at a specified temperature and pressure, by applying

restricted equilibrium conditions to mimic closer experimental observations. The revised methodology, by referencing the work of others and explaining why the calibration was necessary, articulates the strength and reliability of the process model for *Casuarina equisetifolia* biomass under air-blown conditions.

2.1. Flowsheet

Figure 1 depicts the flow sheet utilized for biomass gasification. The process requires the following steps in the model development process:

The detailed process of biomass gasification of *Casuarina* is depicted in Figure 1. The feed enters into the dryer block, where it undergoes drying and devolatilization to produce steam (H_2O), ash, carbon (C), H_2 , O_2 , N_2 , and S. The distribution of yield represents the amounts of the individual components produced at the time of the pyrolysis process. During the ultimate and proximate analysis, 100% of the ash was set aside under this component. The separator column (SEP1) receives the dryer block's outlet stream (M.K. et al., 2013). This separator column (SEP1) separates the remaining components and moisture. Some elements like C, H_2 , O_2 , N_2 , S, and Ash are present in the stream drybio, which enters the reactor's gasifier block through ryield. DRYBIOM is the primary fuel stream that travels to the gasification reactor, ryield, where the gasification process is carried out. The RGIBBS reactor block was operated over the specified gasification temperature range. The "RGIBBS" reactor block's gasification temperature is adjusted between 7000 °C and 7000 °C, and the mass flow rate of the "AIR" stream can be changed based on the air to biomass (A/B) ratio, which can range from 0.2 to 1. Equations (1) to (8) describe the gasification reactions specific to the RGIBBS block. Ash, CO, CO_2 , N_2 , CH_4 , H_2O , and H_2 are found in the block RGIBBS reactor's output stream, gasifier, which travels to the separator column, sep2.

A detailed Aspen Plus model of the air-blown gasification of *Casuarina equisetifolia* is shown in Figure 1. In the first step the biomass feed is dried and decomposed, and in the second step, the non-conventional biomass components are converted to conventional components in accordance with the desired yield ratio. The resulting stream includes the components which are needed as input to the gasification section. The gasification reactions in the RGIBBS reactor are represented in the restricted-equilibrium approach with the introduction of air as the gasifying agent. During the parametric simulation, the temperature of the RGIBBS reactor was changed from 750 °C to 900 °C, and the air flow rate was adjusted based on the air-to-biomass ratio chosen. The gaseous products and solid ash will be separated from the reactor outlet stream in the downstream separator.

Process simulation platforms like Aspen Plus can be very useful to model biomass thermochemical conversion in detail, by creating process

flowsheets, conducting thermodynamic calculations, modelling reactors and performing sensitivity analysis, but can be difficult to implement if thermodynamic data is extensive, reaction schemes are not adequately known and process specifications are not detailed. Whereas, data-driven and mathematical modelling can provide a more efficient alternative when the aim is to predict, estimate parameters, perform sensitivity analysis, or optimise a process rather than simulating the entire flowsheet, computation is avoided. These models can develop direct relationships between the important input variables and the characteristics of the product-gas, which allows the rapid evaluation of many operating conditions after the model is developed and validated. Thus, the selection of a process simulator like Aspen Plus or an independent predictive model will be dependent on the use the process is intended for: Aspen-based approach could be very useful for detailed process integration and mass-energy balances studies while predictive model could be useful for rapid screening, optimization and mass-energy balance prediction for general process. Ash and the remaining components, such as CO, H₂, CO₂, N₂, S, H₂O, and CH₄, are separated by this separator column as stream products. Table 3 explains the blocks that are utilized in the flow sheet.

The process flowsheet is defined by connecting the material and energy streams and utilizing unit operation blocks to specify the stream class, choose the property method, identify conventional and non-conventional components, and specify system components (from a database). Next, the unit operation blocks (chemical processes, thermodynamic conditions, flow rate, and composition) and feed streams (thermodynamic state) are specified.

In this study, the process is modelled based on the following assumptions:

- a) Biomass feed rate is 1000 kg/hr.
- b) The process is isothermal and steady state.
- c) Within the gasifier, the temperature and pressure are constant.
- d) Air was supplied at atmospheric pressure, and the temperature of the gasification reactor was varied according to the specified simulation conditions.
- e) There are no such occurrences of pressure or heat losses within the gasifier.
- f) All fuel bond sulfur (S) is transformed into H₂S, and tar production is not taken into account (Makwana et al., 2023).
- g) The product contains no such unconverted carbon.
- h) Ash and carbon are the only elements present in char (W. Doherty et al., 2009).

- i) Instantaneous pyrolysis and drying occur (W. Doherty, Reynolds, & Kennedy, 2013).
- j) Hydrogen, carbon monoxide, carbon dioxide, methane, nitrogen, and hydrogen sulphide are assumed to be present in gas components, and they all follow the ideal gas behaviour.
- k) The concerned gases follow the Boston-Mathematics (PR-BM) characteristic approach in the Peng-Robinson equation of state (W. Doherty, Reynolds, & Kennedy, 2013; T. Bridgwater et al., 2012).

Proximate analysis and Ultimate analysis of Casuarina biomass feedstock have been represented in Tables 1 and 2, respectively. It is commonly recognized that due to the short residence time in the gasifier, the real gasification process does not achieve chemical equilibrium. As a result of applying the Gibbs equilibrium model, significant differences have been discovered between the experimental and predicted values of the syngas composition. The restricted equilibrium approach with the Gibbs reactor model has improved agreement between the predicted and experimental syngas composition (C. Liao, M. Summers, 2014). The modified scheme is based on the restricted chemical equilibrium followed in the Gibbs reactor. Choosing the calculation option sets the restricted equilibrium to define an individual reaction; the temperature approach must be specified with zero degrees. This is known as the "Restrict chemical equilibrium" method. RGibbs determines the equilibrium gas composition for each reaction by evaluating the chemical equilibrium constant at reactor temperature and providing a zero temperature approach for each process. Several chemical reactions occur inside the gasifier during the complicated process of biomass gasification (Díaz González et al., 2023; Abdelouahed et al., 2012).

The key process variables that influence product-gas production should be the most sensitive factors for which an effective predictive model should demonstrate generalizability, accuracy, and computational efficiency. A large number of parameters should not be included in the model as these can either complicate the model or not enhance the prediction significantly, but should be focussed on those that have the most significant effect on gas yields and composition and how these relate to the desired outputs. A well-developed model should, therefore, be able to capture the nonlinear behaviour of the conversion process, give reliable prediction in the range of process conditions studied and be sufficiently flexible to analyze the effect of changes in conditions. These properties are especially relevant to the optimization process, as a model could be used to minimize the number of experiments needed to find the optimum operating conditions for the process, and could serve as a starting point for further analysis of other feedstocks and process configurations.

The challenges of biomass conversion is related to the heterogeneous nature of biomass and the simultaneous occurrence of several thermochemical reactions: drying, devolatilization, oxidation, reduction and gas phase reactions, which all influence the end result composition of the product gas. Variations in the temperature, pressure, equivalence ratio, moisture content and feedstock characteristic can then lead to variations in the relative concentrations of CO, H₂, CO₂, CH₄, and gaseous species in the process, which complicates establishing simple linear relationships between process inputs and outputs. The complexity of this scenario emphasizes the need to develop modelling tools that allow for modeling the interaction of different variables, but still be simple enough to be predictive and optimizable in a timely fashion. The model can be used to give more insight into the process behaviour without being a complicated or costly model since the most influential process parameters are incorporated in a predictive framework.

The primary goal of the present study is not to describe the behaviour of the particular biomass used, but rather to develop a modelling framework that can be readily applied to a wide variety of carbonaceous feedstocks. The proximate and ultimate composition, ash content, volatile matter, fixed carbon, moisture and elemental ratios are different in biomass resources, which is affecting the thermochemical conversion behaviour. Any good predictive model should, therefore, be able to incorporate these variations, not just one feedstock under specific operating conditions. The modelling methodology developed in this study is therefore expected to be transferable and applicable to the analysis of biomass gasification and product-gas formation in general renewable carbonaceous materials such as agricultural residues, forestry waste, energy crops, municipal biogenic waste and others, provided that they are calibrated and validated accordingly. The wider view point makes the model more useful for the practical application showing that the ability of the model to predict the behavior of the selected biomass is not only useful but it also offers a methodology that can be extended to other feedstocks and operating conditions.

The chemical processes that have been taken into consideration in this work for the gasification process are equations (1) to (8) in Table 3 (C.C. Sreejith, C. Muraleedharan, 2013; Bhattacharjee et al., 2023). However, the present model does not account for the fluid dynamics, limitations of the reactor heat transfer, and side reactions that result in tar production and deactivation of the catalyst. In this model, the thermodynamic properties of the conventional components have been calculated using the Peng-Robinson equation with the Boston-Mathias (PR-BM) characteristic approach. Light gases like CO₂, H₂S, and H₂ as well as nonpolar or slightly polar mixtures like hydrocarbons, are handled with this technique.

2.2. Biomass (Casuarina equisetifolia) and its Proximate and Ultimate Analysis

For the developed air-blown gasification model, the biomass of *Casuarina equisetifolia* was chosen. The biomass was modeled in Aspen Plus based on its proximate and ultimate analysis that were reported in the literature. The proximate analysis indicates the moisture content, volatile matter, ash content and fixed carbon fraction, while the ultimate analysis indicates the elemental composition of biomass, which includes carbon, hydrogen, nitrogen, sulphur, oxygen and ash. The proximate and ultimate analyses for defining the biomass feedstock are shown in Tables 1 and 2, respectively.

The biomass was considered as a non-conventional component in the Aspen Plus model. The conversion of the conventional chemical components were illustrated by the drying and decomposition processes before the gasification reactor. The information on the composition presented by proximate and ultimate analyses was utilized to define the distribution of conventional components produced during biomass decomposition stage. This section does not contain any performance interpretation or syngas-composition results, since this section is only limited to the definition of biomass feed and model inputs.

Table 1: Proximate analysis (wt.%, air dried basis)

Component	Percentage
Moisture	9.75
Volatile matter	81.28
Ash Content	0.34
Fixed carbon	8.63

Several chemical reactions have been considered: the Water gas reaction and Water gas shift reaction, Boudouard reaction, Carbon oxidation and partial oxidation, Methanation, Steam reforming of methane, Hydrogen partial combustion, and H₂S formation.

Table 2: Ultimate analysis (wt.%, air dried basis)

Component	Percentage
C	51.21
N	5.9
H	4.34
S	1.03
O	37.18 (by difference)
Ash	0.34

Table 3: Chemical reactions involved in the process (Molino, A., et al., 2016; Pala et al., 2017) ‘Steam gasification of biomass with subsequent syngas adjustment using shift reaction for syngas production: An Aspen Plus model’, Renewable Energy.):

Reaction number	Reaction scheme	Reaction name	Heat of reaction ΔH (KJ/mol)
1	$C + H_2O = CO + H_2$	Water gas reaction	+131
2	$CO + H_2O = CO_2 + H_2$	Water gas shift reaction	-41
3	$C + CO_2 = 2CO$	Boudouard reaction	+172
4	$C + O_2 = CO_2$	Carbon oxidation	-393.0
5	$C + \frac{1}{2}O_2 = CO$	Carbon partial oxidation	-112
6	$C + 2H_2 = CH_4$	Methanation of carbon	-74
7	$CH_4 + H_2O = CO + 3H_2$	Steam reforming of methane	+206
8	$H_2 + 0.5O_2 = H_2O$	Hydrogen partial combustion	-242
9	$H_2 + S = H_2S$	H_2S formation	-20.2

Table 4: Description of the reactor block utilized in the simulation (Zaccariello, A., et al. (2023):

Block ID	Aspen Plus name	Description
DRYER	RStoic	RStoic reactor - used in the conversion of biomass into conventional elements according to yield distribution data
SEP1	Sep	Separator - used in the separation of Moisture and DRY-BIOMASS
RGIBBS	RGibbs	Equilibrium reactor: minimization of Gibbs free energy. As temperature and pressure are defined.
RYIELD	RYIELD	Produces conventional elements from biomass based on yield distribution data.
SEP2	Sep	Separator - separates Ash and SYNGAS

The Peng–Robinson equation of state (PR–Boston–Mathias) was used for the calculation of the thermodynamic properties of the conventional gaseous components. The gaseous species involved in the gasification process has been chosen to be represented by this property method. This steady-state process model was run at atmospheric pressure. In the present simulation, heat losses and pressure losses in the gasification system were not considered. It was assumed that the biomass was dried and decomposed instantaneously to the components having the prescribed component yields. The formation of tar was not considered in the present model, and the chemical species and reactions used in the gasification reaction network were limited to the ones listed in Table 3. Downstream separator separated Ash from the gaseous

product stream. The various drying, separation, decomposition, gasification and product-separation stages are achieved using the Aspen Plus blocks shown in Table 4.

3. Results and discussion

The syngas composition was achieved by adjusting the A/B ratio between 0.5 and 1.0 and the gasification temperature between 750 °C and 900 °C.

The revision now accounts for the fact that biomass gasification processes may employ various gasifying agents, including air, steam, oxygen-enriched air, and, in rare cases, CO₂ mixtures. Each one of the agents works to bring about different hydrogen and carbon monoxide content in the syngas to varying degrees in tar formation and the energy balance of syngas. Giving the introduction a wider framework regarding agent selection would reveal a thorough understanding of the subject, familiarize it with experimental and simulation investigation, thus paving the way for future expansion into multi-agent gasification research.

3.1. Effect of temperature

The hydrogen mass flow rate increases as the reactor temperature increases, given a constant biomass feed rate and air/biomass ratio. Higher temperatures facilitate reactions that produce more hydrogen, enhancing the syngas’ overall hydrogen yield and mass flow rate. Optimal hydrogen production for the sample biomass typically occurs between 800°C and 900°C. Figure 2 and Figure 3 represent the effect of temperature on the mass flow rate of hydrogen at the A/B ratio of 0.5.

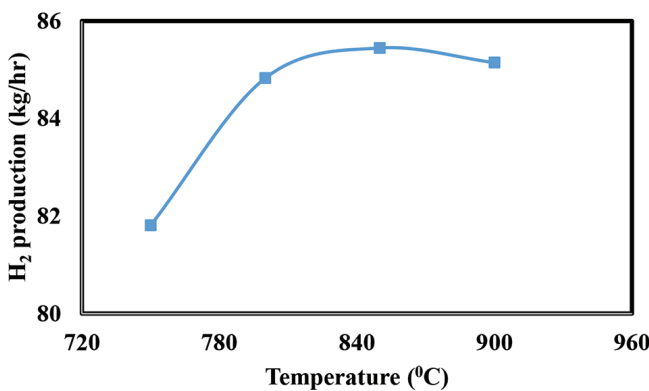


Figure 2: Effect of the gasification temperature on the Hydrogen mass flow rate at an A/B ratio of 0.5.

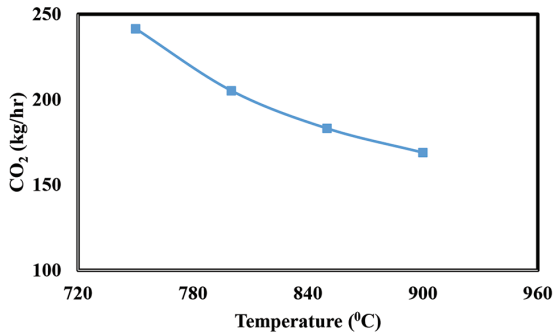


Figure 3: Effect of temperature on mass flow rate of CO₂ at 0.5 A/B ratio.

As the gasification temperature increases, the CO₂ mass flow rate tends to decrease due to the shift in chemical reactions favoring the production of carbon monoxide and hydrogen over carbon dioxide. Lower temperatures result in higher CO₂ production due to direct combustion, while higher temperatures promote endothermic reactions that convert CO₂ to CO, reducing the overall CO₂ yield in the syngas (Cecilio et al., 2023; HASPENula et al., 2012). Optimal gasification temperatures (typically above 800°C) result in a lower CO₂ mass flow rate.

3.2. Impact of the air-to-biomass (A/B) ratio

Figure 4 shows that increasing the A/B ratio in biomass gasification at 750°C tends to increase CO₂ concentration, while decreasing CO and CH₄ concentrations are seen. The H₂ concentration remains relatively constant. The mass flow rate of syngas can be reduced with a higher A/B ratio due to the shift towards more complete combustion reactions, producing CO₂ rather than CO and CH₄. This highlights the importance of optimizing the A/B ratio to balance the desired syngas composition and overall efficiency of the gasification process. Similar trends were reported in Refs (A. Inayat, M.M. Ahmad,2010) as shown in Figure 5.

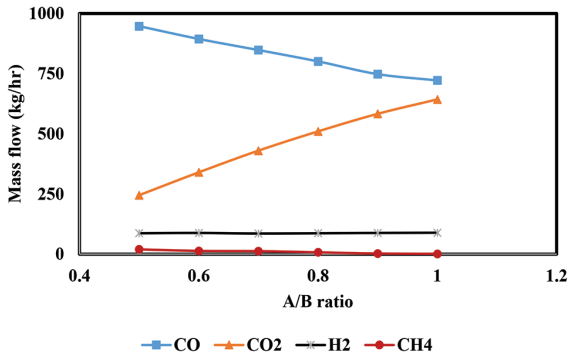


Figure 4: Impact of the air to biomass (A/B) ratio on the mass flow of different gaseous components at a reactor temperature of 750°C.

The model aims to move beyond the usual Gibbs free energy minimization, using a constrained equilibrium approach coupled with the Peng-Robinson equation, Boston-Mathias-modified, to predict the composition of syngas with greater precision, particularly for light gases. The simulation results are confronted with and tested against experimental results from fluidized-bed gasifier setups to keep the study relevant to actual industrial conversion scenarios. The workflow distinction is clarified; no external FORTRAN was intruded, though the model stands prepared for further expansion if advanced kinetic modeling is deemed necessary through the usage of custom subroutines. By including and studying in a systematic way within one united Aspen Plus simulation the key reactions – Boudouard, water-gas shift, methanation, and steam reforming – it becomes possible to pinpoint the important temperature and air-to-biomass ratio regimes favoring hydrogen and CO production for future process optimization and scale-up to industry.

3.3. Effect of temperature on H₂/CO Ratio

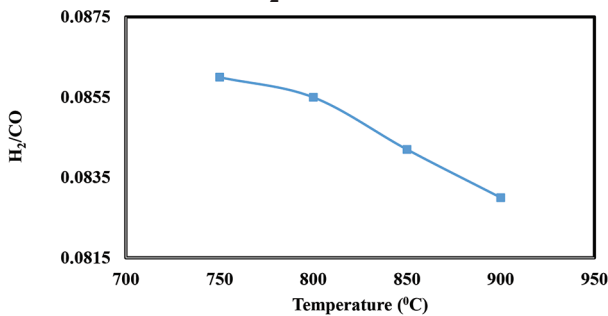


Figure 5: Effect of the gasification temperature on the H₂/CO mass flow rate ratio at an A/B ratio of 0.5

At the A/B ratio of 0.5, Figure 5 illustrates how the gasification temperature affects the mass flow ratio of H₂/CO in the final gas composition (S. Cheah et al., 2009; C.C. Sreejith et al., 2013). As the temperature of biomass gasification rises, it is noticed that the H₂/CO ratio decreases. The explanation is that while the H₂ mass flow was relatively constant, the CO mass flow increased due to the increasing gasification temperature. This suggests that the Boudouard reaction dominates the water gas reaction within the investigated gasification temperature range, as shown in Figure 5.

A model called Aspen Plus has been created specifically for the use of air gasification in biomass. The model is based on the constrained equilibrium method of Gibbs free energy minimization, with distinct temperature methods established for each gasification process reaction. The PR-BT equation of state has been selected as the base property technique. Studies

have examined the impact of various operational parameters, including gasification temperature and air-to-biomass ratio, on gas composition, CO, CO₂, and H₂ conversion. At an A/B ratio of 0.5, increasing the gasification temperature primarily increases the CO concentration due to the Boudouard reaction dominating the water-gas shift reaction, decreasing the product gas's H₂/CO molar ratio. Other parameters are to be validated in future studies using the model results. This model aims to provide a more accurate prediction of syngas composition under various operating conditions. Further research will focus on optimizing the model for industrial applications.

4. Future Scope and Research Directions

The results of this study lead to many potential avenues of research. Future efforts could include modeling tar dynamics and catalytic reforming reactions in addition to gasification reactions, because tars will significantly impact syngas composition and equipment performance, and validated experimental studies would help further strengthen the model performance. Adding computational fluid dynamics (ASPEN) software to Aspen Plus to model fluidized behaviors would help clarify heat transfers and gas-to-solids behaviors (Eikeland et al., 2015; Loweski Feliz M, et al., 2024).

Although there are some well-developed process-simulation and modelling methods for biomass conversion, there is still a need for efficient predictive models that can simultaneously: describe the effects of significant operating parameters, accurately predict product gases, and be flexible with the type of carbonaceous feedstocks. The novelty of the present work is the development of a modelling framework which is evaluated by its predictive ability, its parameter sensitivities and its transferability, but not only by its ability to simulate a specific biomass in detail. In this regard the study examines the relationship between the most important operating conditions and the product-gas properties, validates the model with available experimental or reference data (Loweski Feliz M, et al., 2024), elucidates the important parameters that affect the formation of gas, and evaluates the suitability of the developed approach to be applied for other biomass feedstocks. As a result, the framework can be used as an additional tool to conventional process simulators and experimental work as a fast analysis and optimization tool for biomass gasification systems.

5. Conclusions

The manuscript emphasizes the air-blown biomass gasification model in Aspen Plus, aimed specifically at the characterization of *Casuarina equisetifolia*, in addition to unique parametric studies that expand the application of this model. Expanding the model to include variability from additional biomass types (like agricultural residues or algae) and machine learning approaches to

generate carbon-specific feedstock predictions could increase stakeholders' interest in the work. The exploration of "coupled" systems like gasification to Fischer-Tropsch synthesis or fuel cells would allow end users to improve the efficiency of energy use and carbon utilization efficiency, possibly while conducting techno-economic analyses. Environmental lifecycle analyses should look into emissions and carbon footprints to set the process on track for circular economy goals. AI could then make operational changes in real time to maximize syngas yield and minimize energy penalties, thus turning this model into a full-fledged tool for sustainable biomass gasification and waste valorization.

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Declaration of Interest Statement

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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