Eulerian-Lagrangian simulation of air-steam biomass gasification in a bubbling fluidized bed gasifier

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Abstract

To numerically study biomass gasification in a three-dimensional bubbling fluidized bed, a CFD-DEM (computational fluid dynamics – discrete element method) model with heat transfer and homogeneous and heterogeneous chemical reactions is implemented. An ideal reactor model is used for the air-steam bubbling fluidized bed (BFB) gasification reactor assuming perfectly mixed solids and plug flow. A validated computational particle fluid dynamics (CPFD) model has been applied to investigate the sensitivity analysis of mesh grids as well as to find the optimum number of grids. The result shows that 7452 grid cells are the optimal number of cells for the existence BFB gasifier. The effects of key process operating parameters such as steam to biomass ratio (SB), as well as temperature shows that by enhancing the SB ratio or reactor temperature, gas yields increase. H_2 and CO_2 concentrations promote by increasing the steam to biomass ratio while CO and CH_4 production drop. The optimal value of SB for the gasification process can be found in the range of 0.3 to 1.

Keywords: bubbling fluidized bed gasifier, CPFD method, Steam-to-biomass ratio, mesh sensitivity analysis, Eulerian-Lagrangian simulation

1. Introduction

Gasification is the partial oxidation of the carbon in the biomass in the presence of a gasifying carrier such as air, oxygen, steam, or carbon dioxide. The biomass gasification process can convert a solid or liquid organic material into a multifunctional gaseous compound and a solid phase. The gas phase, called syngas, has a high heating value and can be applied to produce biofuel and generate power. Char consists of organic residue and inert material and comprises the solid phase (A. Samani et al., 2022).

The gasification of biomass consists of a sequence of successive, endothermic, and exothermic reactions that can be divided into the main subprocesses as can be seen in Fig. 1.

The gasification process consists of drying, pyrolysis, partial oxidation, reduction (char gasification), and cracking (Arena, 2012, Mahinpey and Gomez, 2016).

Heating and drying: The moisture content makes up 5-35% of the biomass feed. During the drying stage, the moisture is released from the feed, and it is decreased to 5%. The operating temperature of the drying stage depends on the pressure inside the reactor, for example, if the reactor is operating on a pressure of 1-60 bars, the boiling temperature of the water can be between 373 to 550 K. High moisture content can lead to some troubles in feeding or fluidization like agglomerate formation and jamming problems. Furthermore, it can decrease the lower heating value (LHV) of the production as well as the energy efficiency of the gasification. Therefore, the tar content in the syngas is more likely to increase due to the reduction of the reaction temperature (Arena, 2012, Mishra and Upadhyay, 2021).

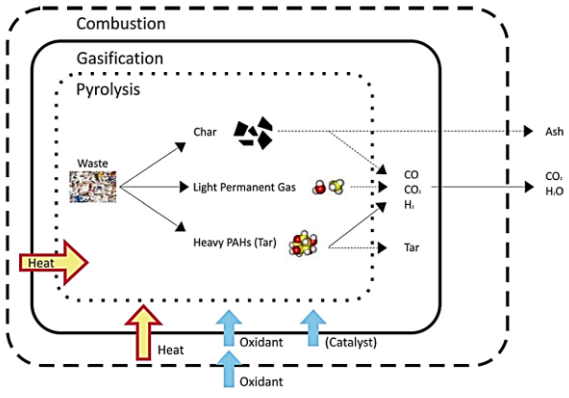

Figure 1: Schematic representation of pyrolysis, gasification, and combustion processes (Arena, 2012)

Devolatilization (pyrolysis): During the pyrolysis stage, the organic materials are decomposed into volatile and biochar (carbonaceous solid residue) in an oxygen-deprived atmosphere at higher temperatures (398‑773 K)(Mishra and Upadhyay,

2021). This process involves the breaking of the transitory bonds of the aromatic clusters in the feedstock. Thus, light gases (volatile matter) in the cooler part of biomass condense and produce high molecular weight hydrocarbons (tar). When dried biomass is heated to temperatures ranging from 200 to 500 °C during the pyrolysis step, it decomposes into solid char and volatiles (tar and gases), as shown in Fig. 2.

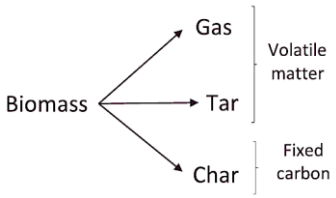

Figure 2: Pyrolysis output (Safarian et al., 2019)

Combustion(oxidation): Although the easiest and the most direct way of decomposition of biomass is the combustion, the overall heat released from the biomass in the combustion zone is lower than in the gasification process. Due to the exothermic chemical reactions, the temperature can be elevated to 1373 to 1773 K in the combustion zone. By controlling the gasifying agents, the temperature can be controlled in such a way that it does not approach the ash-slagging temperature and causes operational problems. The amount of pure oxygen or air is in the range of 25 to 40 percent. CO, CO_2, H_2, and H_2O are formed as the final products, and the heat released from the exothermic reactions can be applied to dry the particles in the pyrolysis process (Zhang et al., 2010).

Gasification/reduction: In this zone, some CO_2 and H_2O are reduced in the reaction of the remaining carbonized residue produced from pyrolysis. It can produce a gas with a high CO and H_2 content. The required energy for endothermic reduction reactions can be provided by the combustion of char and volatiles. Hydrogen, carbon monoxide, and methane can be generated through a sequence of reactions. Tar is one of the main problems in gasification of the biomass and can reduce the overall efficiency of the process and increase the cost of the plant (Mularski et al., 2020).

Consequently, gasifier reactors must be designed using either experimental data or numerical modeling and simulation. Modeling should be combined with experimental results as the most reliable option. Thus, at the R&D level, modeling, and simulation play an important role in the design and study of the gasification process. Modeling and simulations offer a low-cost method for optimizing existing gasifiers as well as scaling up and designing new gasifiers in terms of key operational parameters. Exploration of these operational parameters can provide insight into the relationship between the influences of the gasification variables and trends in process, cost, and implementation risks. (Baruah and Baruah, 2014, Safarian et al., 2019).

Some of the important operating parameters influencing the gasification process are feedstock flow rate, gasifying agent flow rate, equivalence ratio, reactor pressure, and reactor temperature. Any parameter change has a significant impact on the end-gas composition and, as a result, the gasifier's performance. Mathematical and computational fluid dynamics (CFD) models are created to provide a good representation of the chemical and physical phenomena that occur inside the gasification reactors (Basu, 2010). An Eulerian-Lagrangian model has been applied to study the influence of increasing the temperature, steam-biomass ratio, and equivalence ratio on the solid phase's gas voidage, fluid force, collision force, dispersion coefficient, as well as the various homogeneous reaction rates. The model offers important information about the hydrodynamics of the bubbling fluidized bed for biomass gasification, and they are expected to be useful for the operation, scale-up, and optimization of such systems for sustainable energy production (Yang et al., 2019). To simulate the gasification of pine sawdust in the presence of both air and steam, a comprehensive model was developed. The proposed model improved on the premise of an existing biomass gasification model based on ASPEN PLUS. The accuracy of the model's predictions was compared to actual experimental results to confirm validity. Furthermore, the comprehensive model's relative accuracy was compared to the original base model to see if there was any improvement. The model predicts the composition of H_2, CO, CO_2, and CH_4 with reasonable accuracy in varying temperature, steam-to-biomass, and equivalence ratio conditions (Pauls et al., 2016).

Since gasification is a thermodynamic conversion containing many solid-gas reactions, the gasification parameters such as temperature, pressure, feed composition, type of the gasification agents, and kinetics of the reaction are more likely to affect the syngas production. For this reason, the purpose of this paper is to apply CPFD simulation to evaluate the impacts of the steam to biomass ratio on the gasification process.

2. The CPFD method

CPFD is a numerical method based on the Eulerian-Lagrangian approach for the simulation of a large-scale multiphase (particle-fluid) flow system in three dimensions by adopting the multiphase particle-in-cell (MP-PIC) method and the particle parceling algorithm (Andrews and O'Rourke, 1996). The basis of the Eulerian-Lagrangian method is that a continuum model is considered for the fluid phase and a Lagrangian method is applied for the particle

phase. This can provide an appropriate numerical solution for a wide range of particle sizes, shapes, and velocities. For the fluid phase, the Navier-Stokes equation with coupling between the discrete particles is utilized (Samani et al.). However, in order to solve the particle phase, the direct element method (DEM) fits into the Lagrangian method (Jiang et al., 2014).
The method of solving is that the computational domain is divided into several computational parcels including particles with the same characteristics. Furthermore, conservation equations of momentum, mass, and energy are computed, including the coupling between the gas/solid phases. Therefore, the spatial distribution of key process parameters such as temperature, pressure, and velocities in the system can be calculated. Such information is necessary to find out the fluidization process, and that is why the CPFD scheme is widely used for the simulation of gas-particle fluidized reactors (Samani et al., 2020).

3. CPFD simulation set-up

Computational Particle Fluid Dynamics (CPFD) modeling is used to simulate the bubbling fluidized bed gasifier reactor at the University of South-Eastern Norway, with the goal of mesh sensitivity analysis to find the optimal number of grid cells to achieve accurate results. The CPFD hydrodynamic model has been validated against the results of Timsina's experiment for wood chips as biomass air gasification at 1000 K (Timsina et al., 2020) by A. Samani (A. Samani et al., 2022). In this paper, the model was used to investigate the effects of steam to biomass ratio as a key operating parameter on the steam gasification process.
The reactor was modelled as a cylinder with an inner diameter of 0.1 m and a height of 1 m. SolidWorks was used to create a computer-aided design (CAD) model of the reactor in stereolithography (STL) format, which was then imported into The CPFD Barracuda® VR software. Fig. 3 illustrates the initial bed conditions and boundary conditions.
The proximate and ultimate analysis of biomass species used in the experimental studies is shown in Tab.1. The rest of the physical and operational conditions used in the simulations are represented in Tab. 2 (Timsina et al., 2020).
In Barracuda, the Wen-Yu model takes into account the particle packing by including a dependence on the fluid volume fraction in addition to the single particle drag models upon which it is based. The Since Wen-Yu drag model is appropriate for more dilute systems, the Wen-Yu drag model has been applied with 60% momentum retention for the particle collision.

Table 1: Characterization of biomass (A. Samani et al., 2022)

Type of biomass	Wood chips
Proximate analysis (wt % basis)	
ash	1.16
volatiles	80
Fixed carbon	18.84
Moisture	11.1
Ultimate analysis (wt %)	
C	51.0
H	6.1
O	42.2
N	0.11
S	0.011
Cl	0.011
Ash	0.58

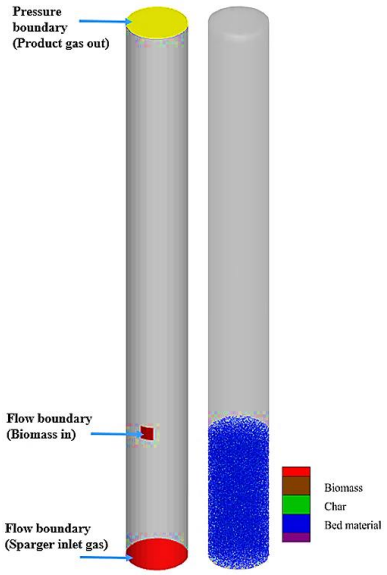

Figure 3: Boundary conditions and c) initial particle in bed (silica sand+char)

Table 2: Gasifier operating conditions (A. Samani et al., 2022)

Initial bed mass	Particle: **Silica** Particle size: 100-425µm 0.49 volume fraction Density: 2650 kg/m^3 Initial height: 250 mm
	Particle: **Char** Particle size: 500µm 0.05 volume fraction Density: 300 kg/m^3 Initial height: 250 mm
Solids close pack volume fraction	0.54
Initial gas in the reactor	Air (80% N_2, 20% O_2)
Initial solid and gas temperature	1000 K
Initial gasifier pressure	101325 Pa
Sparger inlet gas composition by mass	80% H_2O, 20% air (80% N_2, 20% O_2)
Sparger inlet gas temperature	1000 K
Sparger inlet gas superficial velocity	0.17 m/s
Biomass	Temperature: 500 K Mass flow rate: 2.08 kg/h

3.1 Main reactions of gasification:

The main global gasification reactions are divided into two groups, heterogeneous and homogenous.

3.1.1 Heterogeneous (solid-gas phase) reactions

The heterogeneous reactions are (Hejazi et al., 2017, Snider et al., 2011):
For all reactions, the kinetics rates [molm^{-3}s^{-1}] are represented. r_{f1} and r_{r1} are kinetics rates for the forward and reverse reactions. m_s is the mass of the solid, the solid volume fraction, and is the temperature of the reaction.

Boudouard:

$$C(s)+CO_2 \Leftrightarrow 2CO$$

$$\Delta H^{\circ}_{rnx} = +172kJ\ /\ mol$$

$$r_{f1} = 1.272 m_s T \exp(\frac{-22645}{T})[CO_2]$$

$$r_{r1} = 1.044\times10^{-4} m_s T^2 \exp(\frac{-2363}{T} - 20.92)[CO]^2$$

Water-gas:

$$C(s)+H_2O \Leftrightarrow CO+H_2$$

$$\Delta H^{\circ}_{rnx} = +131kJ\ /\ mol$$

$$r_{f1} = 1.272 m_s T \exp(\frac{-22645}{T})[H_2O]$$

$$r_{r1} = 1.044\times10^{-4} m_s T^2 \exp(\frac{-6319}{T} - 17.29)[H_2][CO]$$

Methanation:

$$0.5C(s)+H_2 \Leftrightarrow 0.5CH_4$$

$$\Delta H^{\circ}_{rnx} = -75kJ\ /\ mol$$

$$r_{f3} = 1.368\times10^{-3} m_s T \exp(\frac{-8078}{T} - 7.087)[H_2]$$

$$r_{r3} = 0.151 m_s T^{0.5} \exp(\frac{-13578}{T} - 0.372)[CH_4]^{0.5}$$

Combustion:

$$2C(s)+O_2 \rightarrow 2CO$$

$$\Delta H^{\circ}_{rnx} = -111kJ\ /\ mol$$

$$r_{f6} = 4.34\times10^{7} \varphi_p T \exp(\frac{-13590}{T})[O_2]$$

3.1.2 Homogeneous (gas-phase) reaction

Simple global homogeneous reactions are listed as (Snider et al., 2011):

Steam Methane reforming (SMR):

$$CH_4+H_2O \leftrightarrow CO+3H_2$$

$$\Delta H^{\circ}_{rnx} = +206kJ\ /\ mol$$

$$r_{f4} = 3\times10^{-5} \exp(\frac{-15042}{T})[H_2O][CH_4]$$

$$r_{r4} = 0.0265 \exp(\frac{-32900}{T})[CO][H_2]^2$$

Water-gas shift (WGS):

$$CO+H_2O \Leftrightarrow CO_2+H_2$$

$$\Delta H^{\circ}_{rnx} = -41kJ\ /\ mol$$

$$r_{f5} = 7.68\times10^{10} \exp(\frac{-36640}{T})[H_2O][CO]^{0.5}$$

$$r_{r5} = 6.4\times10^{9} \exp(\frac{-39260}{T})[H_2]^{0.5}[CO_2]$$

4. Results and discussion

4.1. Sensitivity mesh analysis

The CPFD method of solving is that the computational domain is divided into several computational cells including particles with the same velocity and properties. Furthermore, conservation equations of momentum, mass, and energy are computed, including the coupling between the gas/solid phases. The grid defines the spatial resolution for calculating the governing equations that result in gas-particle flow properties like pressure, velocity, and temperature. In order to achieve accurate results, it is necessary to define an optimum number of grid cells. As a result, the CPFD model for the BFB gasifier has been applied at the temperature of 1000 K, and the pressure of 101325 Pa for wood chips as biomass. The steam to biomass ratio of 0.8 and other gasification operating conditions are identical to Tab.2. The reason for choosing the SB ratio is that based on the results of the paper by Sharma (Sharma and Sheth, 2016), at this SB ratio, the hydrogen production could be maximum. The simulations have been carried out for 5 different mesh cells, 1450, 3577, 5376, 7452, and 10000 as shown in Fig.4. With 1450 grid cells, it was not possible to achieve results. This number of mesh is too coarse to achieve the results.

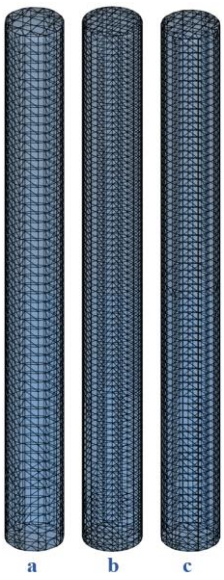

Figure 4: Computational grids, a: 1450, b: 7452, and c: 10000 grid cells

Fig. 5 and 6 investigate the effects of the grid sizes on the production of gas compositions and the concentration of CO production at the outlet cross-sectional area of the reactor. According to the results, since the error for 7452 and 10000 are very negligible (almost identical results), 7452 grid meshes are selected as an appropriate number of meshes for further analysis. By increasing the number of cells to more than 7452 grid cells, the results of gas production have not changed.

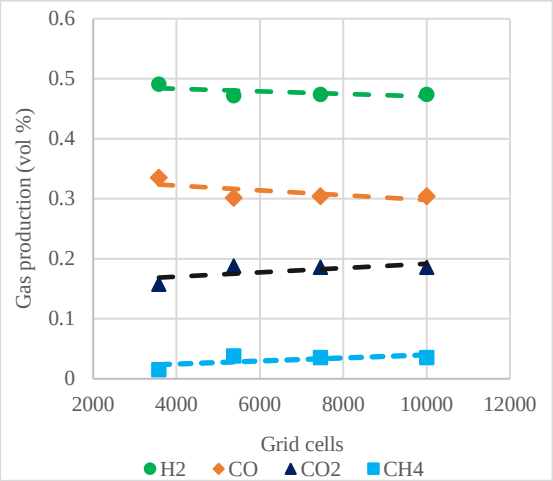

Figure 5: Effect of different grid cells on dry and N_2-free product gas composition for steam gasification of wood chips at a reactor temperature of 1000 K and S/B=0.8

4.2. The impacts of the gasification parameters

To investigate the impacts of SB on gas production as well as the temperature effects on the gas yield, the CPFD method has been applied to simulate the BFB gasifier for wood chips. The simulations have been conducted for 100 s to make sure that steady-state condition has been achieved.

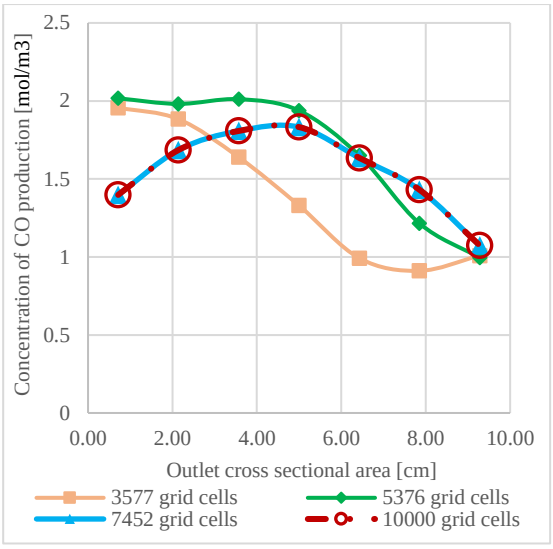

Figure 6: Concentration of CO production at the outlet cross-sectional of the cylinder for different mesh sizes

4.2.1. The effects of the steam to biomass ratio

This section discusses the variation of steady-state values of component production on the condition of dry and N_2 free, for air-steam gasification of wood chips at the temperature of 1000 K with steam to biomass ratio (SB) to identify the quantitative effects of steam addition on gasifier performance. Fig.7 presents particle volume fraction, particle temperature distribution, speed of the particle, and particle species distribution at the temperature at the simulation time of 100 s for SB equal to 0.8 and reactor temperature of 1000 K.

Owing to water gas shifts, which are aided by steam and are predominant at higher temperatures, increasing SB enhances H_2 and CO_2 concentrations and the heating value of syngas while decreasing CO and tar concentrations. Furthermore, because of the water gas and steam reforming reactions, the H_2 mole fraction in the product gas rises as the SB ratio is boosted. An excess of steam reduces temperature, favoring tar formation; additionally, the higher the SB, the more energy is required by the gasification process. The mole fractions of CO and CH_4 drop as the SB ratio promotes owing to increased WGS and SMR reactions as the results show in Fig.8. Higher H_2 and CO_2 concentrations were discovered for SB values ranging from 1.5 to 3. As can be seen in Fig.8, for the gasification process, the optimal value of SB can be found in the range of 0.3 to 1.

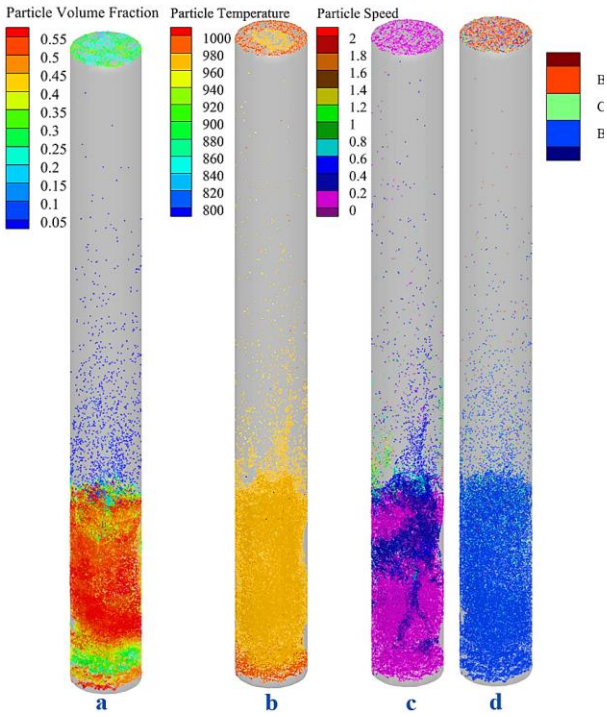

Figure 7: Bed hydrodynamics at 100 s simulation time, (a) Particle volume fractions, (b) Particle temperature distribution, (c) the speed of particle, and (d) Particle species distribution

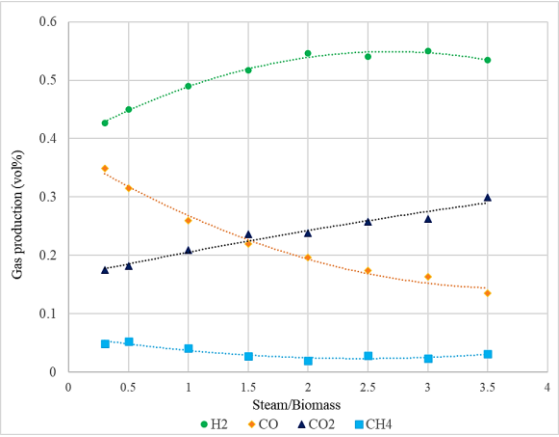

Figure 8: Effects of steam to biomass ratio on dry and N_2-free product gas composition for steam gasification of wood chips at a reactor temperature of 1000 K

4.2.2. The effects of the temperature on products yield

Gasification performance, syngas yield, and composition are all determined by the following operating parameters: partial pressure of Gasifying Agent (GA), heating rate and temperature, and gasification pressure. Fig.9 shows that by running the gasification process at high temperatures, it is possible to achieve high char conversion (the conversion of char into gases), low tar content, and high CO and H_2 contents owing to endothermic reactions of water-gas, Boudouard, and SMR. 750–850°C, 800–900°C, and 850–950°C are typical temperature ranges for gasification of agricultural waste, refused derived fuel (RFD), and woody biomass, respectively (Molino et al., 2018). Temperatures above 1000 °C have two major drawbacks: ash melting and strict reactor specification requirements. Thus, selecting a temperature range for operating the reactor is one of the most important parameters.

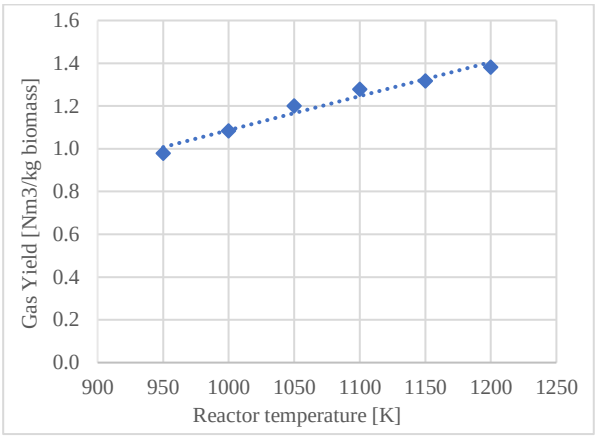

Figure 9: Predicted yield distribution of products from air-steam gasification of wood chips at different temperatures at SB=0.8

5. Conclusion

A validated three-dimensional numerical simulation was carried out to characterize the effects of the gasification parameters on the air-steam biomass gasification process in a BFB gasifier. In the first step, the mesh study has been carried out to find the optimum number of grid cells to have accurate results. It is illustrated that for the geometry of BFB in this paper, 7452 grid cells are chosen as the optimal number of meshes. By raising the steam-to-biomass (SB) ratio or reactor temperature, gas yields promote. Owing to the water gas, SMR, and WGS reactions, the H_2 mole fraction in the product gas rises by enhancing the SB ratio for steam gasification of wood chips in a BFB gasifier at a temperature of 1000 K. The CO_2 mole fraction rises as the SB ratio rises, most likely because the water-gas shift reaction becomes dominant at high gasifier temperatures. Due to increased WGS and SMR reactions, increasing the SB ratio brings the mole fractions of CO and CH_4 to drop. It is concluded that the optimal value of SB for the gasification process can be in the range of 0.3 and 1. By applying a more complex reaction for tar reforming and cracking, as well as using fuel-specific biomass gasification reaction kinetics to account for the catalytic influence of ash, the major factors affecting syngas production and composition such as gasification technologies (fixed bed reactors, fluidized bed reactors, entrained flow reactors), feedstock properties (biomass type, moisture content, particle

size, ash content), and operating gasification conditions (bed material, temperature, pressure, gas agent, equivalence ratio, SB) can be investigated.

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