CPFD SIMULATION OF A FIXED BED GASIFICATION REACTOR

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ABSTRACT

Biomass gasification is regarded as one of the most promising energy recovery technologies. The gases produced from the biomass gasification can be used for heat and power production. Alternatively, they can be used for the production of liquid biofuel. Fixed bed downdraft gasification reactors are easier to use in small scale gasification processes. A three-dimensional Computational Particle Fluid Dynamic (CPFD) model has been developed to gain a better understanding of the gasification process in a fixed bed downdraft gasification reactor. The processes considered in the model are volatilization, partial combustion and gasification. Using the model, the product gas composition is calculated. The computational results are compared with published results from experimental measurements in a fixed bed gasification reactor. There are reasonable agreements between computational and experimental results confirming that the model can be used for further investigation of the fixed bed biomass gasification reactor. The model is used to investigate the effect of the air–fuel ratio on the product gas composition.
Keywords: biomass, fixed bed gasification, downdraft gasifier, CPFD model, air–fuel ratio.

1 INTRODUCTION

Biomass gasification is one of the most promising energy recovery technologies. The gases produced from the biomass gasification can be used for heat and power production. They can also be used for liquid biofuel production.

Gasification is an endothermic process, which requires continuous heat supply for the reactions. There are mainly two types of gasification processes with respect to heat supply methods: autothermal and allothermal. Fixed bed downdraft gasification is an autothermal gasification process, which supplies the heat required for the gasification by partial combustion of biomass in the reactor. These types of reactors are usually air blown. The reactor can be operated for small scale gasification systems. The simple construction makes it easy to operate and to use fuels with various sizes, shapes, types and moisture contents.

Fixed bed reactors are widely used in gasification. There are two main reasons for that. The first one is that the gasifier can be used to gasify small amounts of biomass. Another is that the gasifier has flexibility for a wide range of biomass feedstock. Therefore, it is essential to investigate the gasification process in the reactor to make it more efficient and economically competitive in energy markets and at the same time to overcome various challenges that exist.

Biomass is fed at the top of the gasifier. Usually, biomass feeding is a batch process. The reactor is virtually divided into drying, pyrolysis, oxidation and reduction zones. Air is supplied continuously through air nozzles in an oxidation zone. Biomass that comes in contact with air in this part of the reactor gets air–fuel ratio sufficient for combustion. A part of the biomass in this zone is combusted and heat released by the combustion is supplied partly for the drying and pyrolysis of the biomass in corresponding zones. Another part of the heat is used for gasification of char. This process continues in the reactor as long as the reactor receives a sufficient supply of biomass.

In fixed bed downdraft gasifiers, the oxidant and product gas move in a countercurrent direction. The product gas flows downward through a high-temperature zone. Therefore, the

tar is cracked thermally forming producer gas with lower content of tar [1]. If the temperature of the oxidizing zone is not high enough, a part of the tar can pass through the zone without being converted into smaller molecules [2]. Therefore, maintaining a high temperature in the reactor is crucial in order to produce clean product gas. Maintaining a high temperature requires sufficient combustion of biomass in the oxidation zone. This leads to an increase in air–fuel ratio. At the same time, it is vital not to have over combustion so that the product gas becomes more diluted with CO_2. Optimal air–fuel ratio is important to produce a high-quality product gas.

Low cost, simple design and a relatively higher product gas quality are the advantages of the reactor. However, a large part of the fuel is oxidized increasing the content of CO_2 [1]. The product gas is mixed with the nitrogen from the air, which makes it more dilute. Moreover, the product gas passing through the combustion zone collects small ash particles. These are the disadvantages or challenges in the fixed bed gasifiers. In order to overcome these challenges, a threshold between air–fuel ratio, gasification temperature and product gas composition should be determined.

One of the most used investigation processes is modelling and simulation. The modelling and simulation of a fixed bed gasification is limited mostly to coal gasification or one-dimensional modelling [3], [4]. Literature on 3D modelling and simulation of fixed bed gasification reactors using Computational Particle Fluid Dynamic (CPFD) modelling and simulation approach are rare. 3D modelling gives an overview of the whole process that occurs inside the reactor, including the gas–solid flow and chemical reactions. The results from simulations of the models, provide the means to analyse the behaviour of gas–solid flow and chemical reactions separately. This work attempts to model the particle–gas flow and chemical reactions in a fixed bed gasification reactor. The model is implemented and the results are compared to experimental measurements published in the literature. The CPFD approach is adopted for modelling, and commercial software Barracuda has been used for simulations.

2 COMPUTATIONAL MODEL

There are mainly two approaches for modelling of the gasification process in the literature: thermodynamic equilibrium models [5], [6] and kinetics based models. Kinetics based models are widely used with Computational Fluid Dynamics (CFD) and CPFD. In this study, a 3D kinetic based model for the fixed bed gasification reactor is developed using the CPFD method. The CPFD numerical methodology incorporates the multi-phase-particle-in-cell (MP-PIC) method [7]. The gas phase is solved using the Eulerian approach, and the particles are modelled as Lagrangian computational particles. Gas and particle momentum equations are solved in three dimensions. The fluid is described by the Navier–Stokes equation with strong coupling to the discrete particles. The particle momentum follows the MP-PIC description, which is a Lagrangian description of particle motions described by ordinary differential equations with coupling to the fluid [8]. In the CPFD numerical method, actual particles are grouped into computational particles, each containing a number of particles with identical densities, volume, and velocities located at a particular position. The computational particle is a numerical approximation similar to the numerical control volume where a spatial region has a single property for the fluid. With these computational particles, large commercial systems containing billions of particles can be simulated using millions of computational particles. The governing equations and numerical procedures for the CPFD models can be found in the literature [9], [10].

2.1 Modelling of fixed bed gasifier

A model geometry is developed for the fixed bed gasification reactor using software SolidWorks. The geometry is divided into 7436 uniform grids, as shown in Fig. 1. The figure also shows the model boundaries. Biomass is fed at the top of the reactor and is defined as a flow boundary. There are injection boundaries at the oxidation zone. Air is supplied from six uniformly distributed nozzles. There is a grate under the oxidation zone. After the partial combustion, the ash and char particles pass via this grate. This grate is modelled here as a baffle plate. The baffle plate is defined as a two-dimensional sub-grid structure with zero thickness in CPFD that affects the particle and fluid flow. Mainly, baffle plates are used to model thin walls that would be challenging to capture with the coarse grid, as in the case of this modelling. The baffles act as solid walls for the particles, while they can be used as a transparent medium for the fluid flow when the k factor appearing in eqn (1) is set to zero:

$$\Delta P = (1/2)\rho k v^2, \tag{1}$$

where, ΔP is the pressure drop across the baffle, ρ is the fluid density and v is the velocity of the fluid. The product gas (syngas) leaves the reactor at the bottom and is defined as a pressure boundary.

Wood chips are used as biomass feed and air as a gasifying agent. Table 1 shows the elemental analysis of wood chips, whereas the fractions of char, ash and volatiles in the wood chips, are presented in Table 2. The results are obtained from the proximate and ultimate analysis of the wood chips [9].
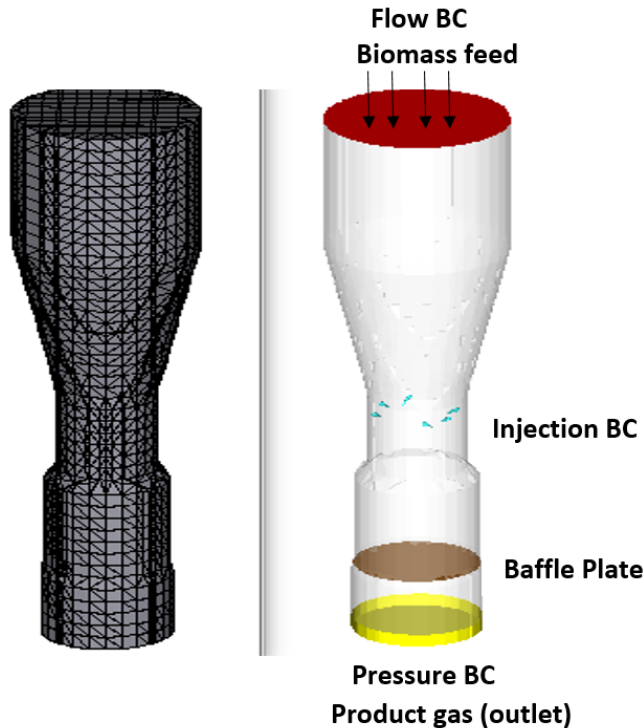

Figure 1: Grid of geometry and boundaries.

Table 1: Elemental analysis of wood.

Elements	Wt.%
Carbon, C	48.6
Hydrogen, H	5.6
Oxygen, O	45.6
Nitrogen, N	0.2

Table 2: Basic components of wood in the model.

Components	Fraction (%)
Char	15.2
Ash	0.3
Volatiles:	84.5
Methane (CH_4)	0.112
Carbon monoxide (CO)	0.635
Carbon dioxide (CO_2)	0.163
Hydrogen (H_2)	0.015
Moisture (H_2O)	0.073

The ash content (composition of elements such as potassium, calcium, sodium, silicon, phosphorous and magnesium) in wood is less than 1% [10]. The nitrogen content of wood is 0.2%. For simplicity of modelling, all these minor components are neglected. Finally, the process of devolatilization of wood can be modelled, as shown in eqn (2):

$$C_x H_y O_z = aCH_4 + bCO + dCO_2 + eH_2 + fC_x H_y + gC + gH_2O. \tag{2}$$
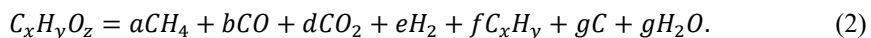
The kinetics of de-volatilization is given by eqn (3):

$$k = 0.05 T e^{(-5500T)}. \tag{3}$$

The thermochemical process in the gasifier comprises several reactions. Identification of all the reactions and their kinetics, in addition to simulating them, is nearly impossible. However, the processes can be virtually divided into a group of separate sub-processes that constitute the major global processes. The major chemical reactions in the reactor are shown in Table 3.

The chemistry described in Table 3, is specified as mass action kinetics. The reactions are described by stoichiometric equations and their rates. The effect of particle concentration on the reaction rate, will be included within the reaction coefficient k. During the overall process of gasification, the biomass particles are heated from the ambient temperature up to the gasification reaction temperature.

Table 3: Reactions and rate kinetics used in the CPFD model.

Chemical reactions	Kinetics
Biomass partial combustion [13] $2C + O_2 \leftrightarrow 2CO$	$r = 4.34 \times 10^{10} \, m_s \theta_f \exp\left(\frac{-13590}{T}\right)[O_2]$
CO oxidation [13] $CO + 0.5O_2 \leftrightarrow CO_2$	$r = 5.62 \times 10^{12} \exp\left(\frac{-16000}{T}\right)[CO][O_2]^{0.5}$
H_2 oxidation [15] $H_2 + 0.5O_2 \leftrightarrow H_2O$	$r = 5.69 \times 10^{11} \exp\left(\frac{-17610}{T}\right)[H_2][O_2]^{0.5}$
CH_4 oxidation [13] $CH_4 + 2O_2 \leftrightarrow CO_2 + 2H_2O$	$r = 5.0118 \times 10^{11} \, T^{-1} \exp\left(\frac{-24357}{T}\right)[CH_4][O_2]$
Water–gas shift reaction [13] $CO + H_2O \leftrightarrow CO_2 + H_2$	$r = 7.68 \times 10^{10} \, T \exp\left(\frac{-36640}{T}\right)[CO]^{0.5}[H_2O]$
Methane reforming [14] $CH_4 + H_2O \leftrightarrow CO + 3H_2$	$r = 3.00 \times 10^5 \exp\left(\frac{-15042}{T}\right)[CH_4][H_2O]$

The simulation is started for the air–fuel ratio 0.7. Part of the air is used for the partial combustion of the woodchips, and the rest is used for volatilization of biomass and gasification of char particles. A series of simulations are run at different air–fuel ratios.

3 RESULTS AND DISCUSSION

The result of the simulation with an air–fuel ratio of 0.7, is presented in Fig. 2. The product gas composition is monitored at the outlet. The gases monitored are N_2, CH_4, H_2, CO and CO_2. The simulation is run for 550 s. The quantity and quality of volatiles produced in the pyrolysis process affect the overall gas composition of the final product gas significantly. This is because about 84% of the product gas is released during pyrolysis of the biomass. Part of the gas is combusted in the oxidation zone, adding more N_2 and CO_2. This contributes further dilution of the product gas. In the beginning of the process, it is mostly nitrogen from the air that leaves the reactor. The fraction of nitrogen in the product gas decreases when partial combustion and pyrolysis of the biomass begin to add flue gas as well as the product gas from pyrolysis and char gasification as shown in the figure.

Simulations were run with different air–fuel ratios. The fractions of different components in the product gases are calculated, excluding nitrogen. Nitrogen is excluded, because it is an inert gas and does not take part in the process. This means that the amount of nitrogen entering the reactor is equal to the amount of nitrogen leaving the reactor. The nitrogen content in the product gas only affects the Lower Heating Value (LHV) of product gas per volume. However, it is not desirable to have excess nitrogen gas in the product gas. This makes extra handling of the gas without calorific value. Therefore, it is important to control the air–fuel ratio in the reactor. Excess air makes the product gas more diluted reducing its calorific value. On the other hand, insufficient air can reduce the production of gases such as CO, H_2 and CH_4 with calorific value.

The results show the fluctuation of product gas composition with time. Many factors contribute to the fluctuation. There is a lack of uniform heat distribution in the fixed bed gasifier. Non-uniform heat distribution affects the reaction kinetics of pyrolysis and gasification process, making the product gas rate to fluctuate. It is not possible to accurately control the amount of biomass used for partial combustion in the oxidation zone. More investigation should be carried out to overcome such challenges.
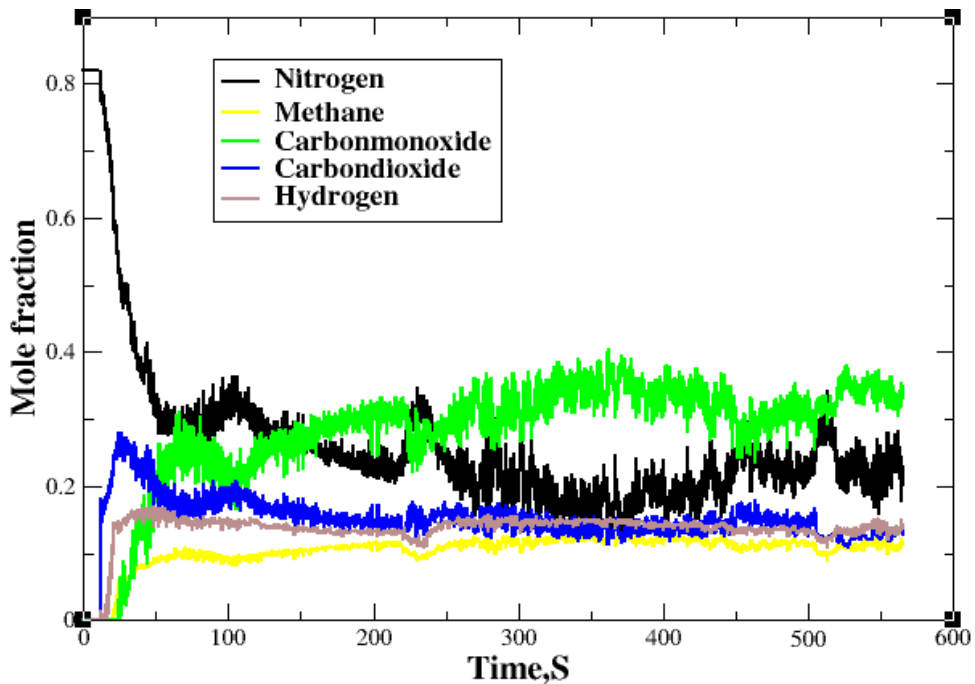
Figure 2: Mole fraction of product gases at an air–fuel ratio of 0.7.

The product gas composition for different air–fuel ratios is compared with the experimental data published in the literature and is presented in Fig. 3. The experimental results are from the gasification of birch wood chips in a fixed bed downdraft gasification reactor [16]. The product gas composition is presented excluding the nitrogen content. The simulation results for air–fuel ratio of 0.45 is nearest to the experimental measurements. The computational results show good agreement with experimental measurements in the case of carbon monoxide. Computational results for carbon dioxide and methane are higher than the experimental. The simulation result for hydrogen is lower in comparison to experimental. There can be various reasons for the deviations. The gas compositions in experimental measurements fluctuate a lot. Prediction of the product gas composition by Barracuda is more consistent.

The woodchip sizes (averaging 11.5 mm) in experiments are larger than in the simulation (4–11 mm). Modelling in Barracuda does not allow having a particle size larger than the grid size. On the other hand, very large grid sizes do not give accurate results. There should be a balance between grid size and accuracy. This is the reason for having smaller particles in simulations. This could contribute to the deviations between numerical and experimental gas compositions. Moreover, the gasification temperature in the experiments fluctuates significantly making the average reactor temperature lower than that in simulations.

The figure also shows the product gas composition at increasing air–fuel ratio. The results indicate that the fraction of methane increases whereas the fraction of hydrogen decreases with increasing air–fuel ratio. The air–fuel ratio does not show a significant effect on the fraction of carbon monoxide. The fraction of carbon dioxide shows decreasing trend with increasing air–fuel ratio.
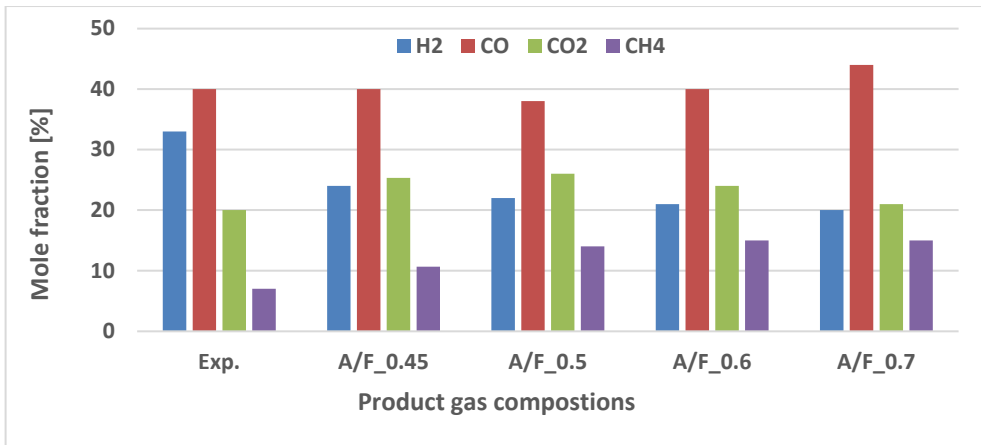
Figure 3: Comparison of experimental and computational product gas compositions.

The composition of the product gas is changed with air–fuel ratios. All these gases have different calorific values. Therefore, the gases are not equally valuable in terms of energy contents. In order to get an idea about the efficiency of the reactor, it is important to have an overview of the total calorific value of the product gas. The product gas calorific value in the experiments and the simulations with various air–fuel ratios are presented in Fig. 4. The calorific values are presented in terms of LHV.

The figure shows that the experimental and computational results of product gas LHV are nearly similar for an air–fuel ratio of 0.45. The deviation is 3%. Although there are some deviations in the fraction of product gas composition, the experimental and computational product gas LHV shows very close results.

The product gas LHV increases with increasing air–fuel ratio. This fact indicates that there is still a possibility for increasing product gas LHV in the downdraft gasification reactor. According to the simulation results, the air–fuel ratio can be increased further to increase the LHV of product gas.
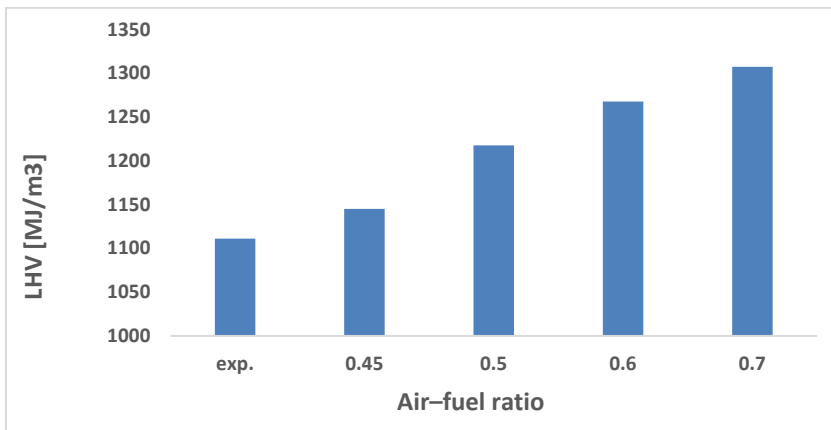

Figure 4: LHV of product gas at different air–fuel ratio compared with experimental.

4 CONCLUSIONS

The conclusions of this work are summarized as follows:

- A three-dimensional Computational Particle Fluid Dynamic (CPFD) model has been developed to obtain a better understanding of the gasification process in a fixed bed downdraft gasification reactor.
- The processes considered in the model are pyrolysis, partial combustion and gasification.
- Using the model, the product gas composition is calculated. The computational results are compared with published results from experimental measurements in a fixed bed downdraft gasification reactor.
- The computational results show good agreement with experimental measurements in the case of carbon monoxide. Results for carbon dioxide and methane are higher than that of experimental. The simulation result for hydrogen is lower in comparison to experimental.
- There is a good agreement between experiment and simulation results in terms of the product gas LHV.
- A series of simulations are run to calculate the product gas composition with increasing air–fuel ratios. The fraction of methane increases whereas the fraction of hydrogen decreases with increasing air–fuel ratio. The air–fuel ratio does not show significant effect on the fraction of carbon monoxide. The fraction of carbon dioxide shows decreasing trend with increasing air–fuel ratio. The LHV of product gas increases with increasing air–fuel ratio.

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