Simulation of air-biomass gasification in a bubbling fluidized bed using CPFD model

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Abstract

Biomass is a renewable energy source. Biomass gasification process produces producer gas, which can be further used for power generation or as raw materials for the production of secondary fuels. Experiment on the air gasification of biomass in a bubbling fluidized bed reactor was performed in a pilot-scale reactor located at the University of South-Eastern Norway (USN). A kinetics-based simulation model was developed based on MultiPhase Particle-In-Cell MP-PIC approach, using commercial software Barracuda®, and the results were compared with the experimental data. The average volume percentage of carbon monoxide, hydrogen, methane and nitrogen were found to be around 20%, 10%, 7% and 38% respectively in the experiment. The simulation results agree well for carbon monoxide, hydrogen and methane, but there is a difference in nitrogen volume percentage compared to the experimental results. The oxygen concentration during the experiment was around 1% suggesting a good performance of the gasifier. The char partial oxidation is less significant compared to the homogenous phase reactions. This shows that devolatilization reaction and the homogenous phase reactions dominate the char gasification reaction.

Keywords: air-biomass gasification, bubbling fluidized bed, CPFD

1 Introduction

Due to the rapid increase in the consumption of conventional fossil fuels, the global temperature is rising quite fast. One of the alternatives to counteract the increase in temperature is the use of renewable energy sources. Biomass gasification is one of the renewable energy production technologies and includes thermochemical conversion of carbonaceous fuels mainly into syngas (a mixture of CO and H_2) with the application of gasifying medium such as air, steam, and oxygen. Among the different biomass gasification technologies, fluidized bed reactors are commonly used. The fluidized bed technology uses bed material such as sand, or olivine to heat up the biomass particles at a temperature range of 700-900°C (Franco *et al.*, 2003). The gasification temperature is comparatively low, and

this inhibits the agglomeration and sintering of the ash, which prevents causing serious problems during the operation of the gasifier. In addition, even distribution of heat and mass transfer, and excellent solid mixing make the fluidized bed reactor one of the attractive technologies for biomass gasification.

The product of gasification can be used for power generation in a gas engine, methanol synthesis or as the raw materials for production of secondary fuels, such as biodiesel, bio-ethanol and methanol (Bandara *et al.*, 2018). The operation of the fluidized bed gasification involves multiphase flow, various chemical reactions and heat transfer. It is a big challenge to investigate the effects of different parameters from the experimental study only, because of the requirements to build different setup configurations and procedures. Instead, modeling and simulations give better ideas for a wide range of design and operational parameters.

Modelling and simulation of such complex systems are needed for a good understanding of the process, designing and optimization. Computational fluid dynamics (CFD) are used to model the systems handling the fluid flow. Conventional CFD is a well-accepted technique for single-phase systems. Multiphase CFD models use either a Eulerian-Eulerian, or Eulerian-Lagrangian approach. The Eulerian-Eulerian approach models the solid and gas phase separately with the Navier-Stokes equation. The discrete particle phase is not considered in Eulerian modelling and is solved with the kinetic theory of granular flow. In the Eulerian-Lagrangian approach, fluid is treated as a continuous phase and the particles as a discrete phase. The solid particles are approximated with Newton's law of motion. This gives high loading to CPU during simulations and is often limited to 2D or quasi-3D and in the order of 10^4 number of particles (Ku *et al.*, 2015). The MP PIC modelling is based on the Eulerian approach for fluid particles and Lagrangian approach for the solid particles. Barracuda® is a software package based on the MP PIC modelling, which is known as the Computational Particle Fluid Dynamics (CPFD) approach.

Air is commonly used as the gasifying agent, which gives product gases with a Higher Heating Value (HHV) of 4-7 MJ/Nm³. The low HHV is due to the dilution of

the produced gas by nitrogen. Oxygen/steam blown biomass gasification produces gas with HHV of 10-18 MJ/Nm^3 (Schuster *et al.*, 2001; Li *et al.*, 2004). However, there will be an additional cost to produce oxygen/steam. There are many CFD models reported in the literature on steam gasification of biomass. CPFD modelling was chosen in this study because of its reliability and shorter simulation time. However, no previous work was found for the modelling of air gasification of biomass in a bubbling fluidized reactor using CPFD approach.

1.1 Previous works

Schuster et al. and Li et al. have studied the gasification of biomass based on the thermodynamic equilibrium model. Such models deviate significantly from the experimental results compared to the kinetics-based models (Schuster *et al.*, 2001, Li *et al.*, 2004).

Xie et al. have developed a model based on the MP-PIC approach for coal gasification in a fluidized bed reactor. Flow patterns, particle species profile, gas compositions, distributions of reaction rates were studied during their study (Xie *et al.*, 2013). The obtained results from the simulation model agree well with the experimental data.

Most of the biomass gasification simulations based on the MP-PIC approach have been applied with steam as the gasifying agent. Loha et al. have studied the flow pattern, gas composition and pressure distribution for different temperature and steam to biomass ratio in a laboratory scale bubbling fluidized bed gasifier. The gasification of rice husk during the experiment agreed well with the simulation based on the reaction kinetics of the gasification process (Loha *et al.*, 2014).

Further, the MP-PIC modelling has been applied to simulate the dual circulating bubbling fluidized bed (DCBFG) gasifier. Liu et al. studied the gasification of almond prunings in a dual fluidized bed gasifier. The model showed that the H$_2$ production, as well as CO production, was increased with increase in gasifier temperature and steam to biomass ratio (Liu *et al.*, 2016). Thapa et al. have developed a model for biomass gasification in DCBFG based on the MP-PIC approach. The published result agrees well with the experimental data obtained from the biomass gasification plant in Güssing, Austria (Thapa *et al.*, 2014).

In the present works, a simulation model for a bubbling fluidized bed gasifier has been developed in barracuda, and the results have been compared with the experimental data. The objective of this paper is to develop a model for air-gasification of biomass and validate the model against the experimental results.

2 Methods

2.1 Experimental Setup

The gasification rig installed at the University of South-Eastern Norway (USN) is a bubbling fluidized bed reactor with a fuel capacity of 20kW. Figure 1 and Figure 2 show the block diagram and the picture of the gasification rig at USN.
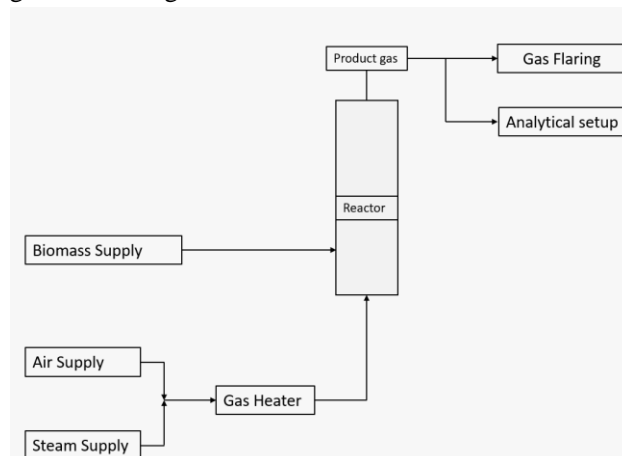

Figure 1. Block diagram of biomass gasification reactor at USN

The gasifier consists of a preheater (A), which heats up the fluidizing agents (air or steam) to about 450°C. The screw conveyors (B1 and B2), transfer the biomass from the fuel silo (C) to the reactor (D). Biomass is added into the silo before starting the experiments. The system is purged with nitrogen during the idle conditions of the reactor. The reactor is installed with pressure and temperature sensors at different locations to monitor the pressure and the temperature of the reactor. The product gas leaves from the top of the reactor for the gas analysis (F) and the flaring (E). The different parameters were controlled/changed/monitored during the experiment with the help of a computer program available at the experimental facility.
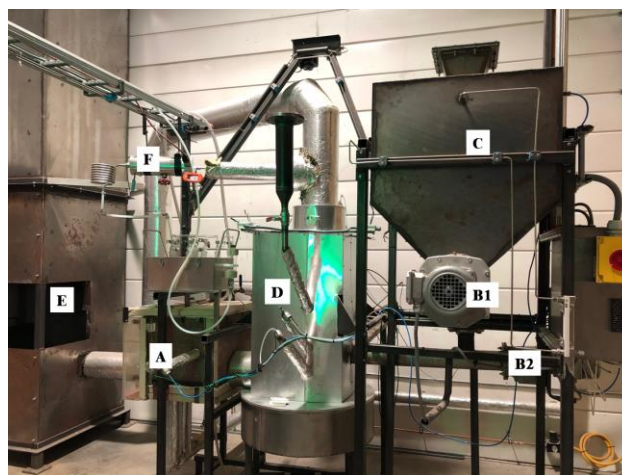

Figure 2. Picture of the bubbling bed reactor at USN

There are two screw conveyors as shown in Figure 3. The cold screw conveyor supplies the biomass from fuel silo to hot conveyor and the hot conveyor introduces the biomass into the reactor bed. The conveyors are perpendicular to each other.
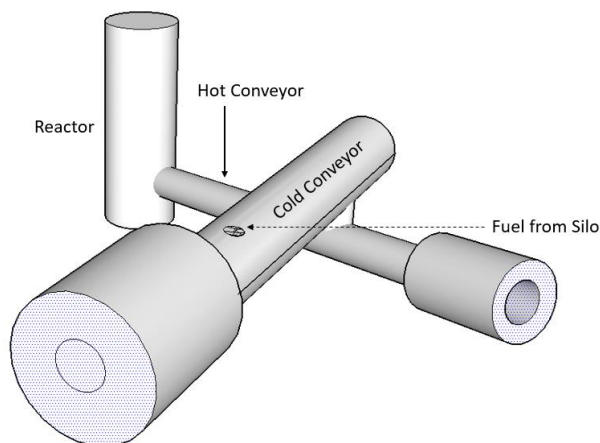

Figure 3. Cold and hot conveyor

The reason for separating the two-screw conveyer is to avoid the combustion of wood chips during the transportation process. The reactor is insulated to reduce heat loss during the experiments. The reactor is 100 mm in diameter and 1000 mm in height.

Sand with an average particle diameter of 285µm was used as bed materials during the experiments. Wood chips with approximately 0.5 cm average diameter was used for the experiments. The reactor was heated initially to about 700°C before the introduction of the biomass into the reactor for gasification experiments. Gas collected on syringe were analyzed on SRI 8610C gas chromatograph.

2.2 CPFD Simulation setup

A simulation model was developed by using Barracuda VR17 software. Wen-Yu drag model was used with 60% momentum loss after the particle collision. The reactor was designed as an open cylinder with a diameter of 100 mm and a height of 1000mm.
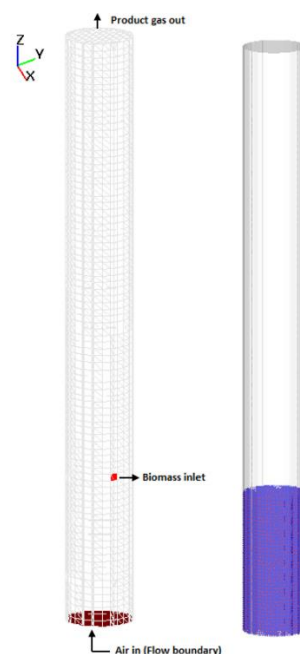

Figure 4. (a) Boundary conditions (b) Initial bed material

Figure 4 shows the boundary conditions and the initial height of bed material used for the simulation. The developed geometry was divided into 7128 computational cells.

Table 3 shows the properties of the bed material, and the gasifying agent used for the simulation process. The exit of particles from the reactor was set to zero by default, and the pressure boundary at the top of the reactor ensures the out flow of the product gas from the

Table 1. Reaction kinetics for air gasification

Reaction	Rate Kinetics
Char partial combustion (Xie *et al.*, 2013) $2C + O_2 \leftrightarrow 2CO$	$r = 4.34 \times 10^7 \, m_s \theta_f \exp\left(\frac{-13590}{T}\right)[O_2]$
CO oxidation (Xie *et al.*, 2013) $CO + 0.5O_2 \leftrightarrow CO_2$	$r = 5.62 \times 10^{12} \exp\left(\frac{-16000}{T}\right)[CO][O_2]^{0.5}$
H$_2$ oxidation (Bates *et al.*, 2017) $H_2 + 0.5O_2 \leftrightarrow H_2O$	$r = 5.69 \times 10^{11} \exp\left(\frac{-17610}{T}\right)[H_2][O_2]^{0.5}$
CH$_4$ oxidation (Xie *et al.*, 2013) $CH_4 + 2O_2 \leftrightarrow CO_2 + 2H_2O$	$r = 3.552 \times 10^{11} \, T^{-1} \exp\left(\frac{-15700}{T}\right)[CH_4][O_2]$
Water gas shift reaction (Xie *et al.*, 2013) $CO + H_2O \leftrightarrow CO_2 + H_2$	$r = 7.68 \times 10^{10} \, T \exp\left(\frac{-36640}{T}\right)[CO]^{0.5}[H_2O]$
Methane reforming (Solli *et al.*, 2018) $CH_4 + H_2O \leftrightarrow CO + 3H_2$	$r = 3.00 \times 10^5 \exp\left(\frac{-15042}{T}\right)[CH_4][H_2O]$

reactor. The air supply into the bed was kept constant during the experiments and the simulation process. Air at 1000K was supplied during the simulation to reduce the simulation time. During the experiments, preheating of air was done before introducing into the reactor bed. The reaction rate kinetics are presented in Table 1 based on the Arrhenius reaction rate model. The properties of the wood chips used in the simulation model are presented in Table 2 (Doherty *et al.*, 2013)

Table 2. Properties of wood chips

Proximate analysis (dry basis, wt. %)	
Volatile matter	80
Fixed carbon	18.84
Ash	1.16
Moisture	*20*

Table 3. Initial conditions

Items	Parameters
Bed material	285 µm average diameter, 0.54 volume fraction, density 2650 kg/m^3, 200 mm initial bed height
Gasifying fluid	Air, 0.2 m/s, 1000K, 101325Pa

3 Results and discussions

Experiments were done with wood chips and air in the bubbling fluidized reactor. The gas composition from the simulation is presented in Figure 5. The gas composition is irregular because of different physical and chemical transformation occurring inside the reactor, whereas the average gas compositions seems to be stable throughout the simulation.
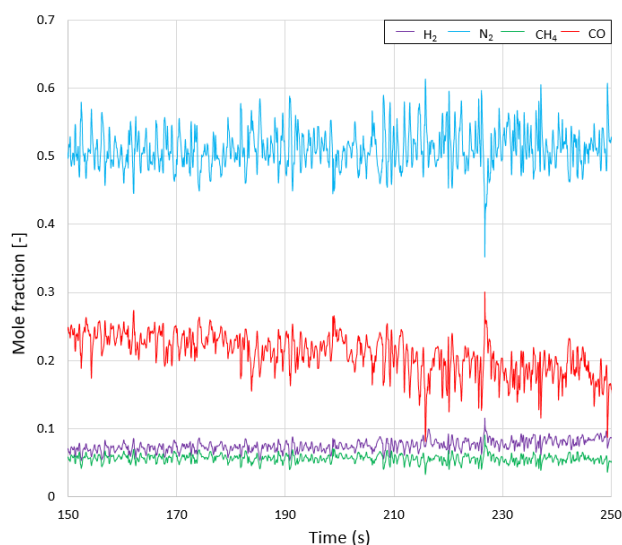
Figure 5. Gas composition for the simulation model

In the beginning, the hydrogen concentration in the product gas is due to the devolatilization of the biomass in the hot bed. Water vapor that is produced during methane oxidation favors the water gas shift reaction which slightly increases the hydrogen production with time. Further, the average gas composition from the simulation results are compared with the experimental results and is presented in Figure 6.

The simulation model predicts well the fraction of the different gas components and there is a good agreement between experimental and computational results regarding the hydrogen, carbon monoxide and methane concentration.
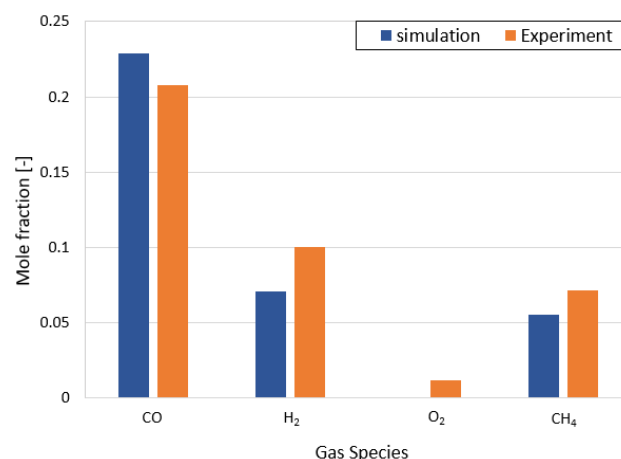
Figure 6. Comparison of average gas species

There are several reactions occurring during the gasification process. The major chemical reactions are modelled using the six major reactions presented in Table 1. The other minor chemical reactions are not included in the barracuda simulations, as they require a lot of computer capacity and time. The average oxygen concentration during the simulation was found to be zero whereas oxygen concentration during the experiment was around 1% of the total volume composition. This may be due to the sampling procedure, as the samples were taken in a syringe for the gas analysis. This shows that the CPFD model gives a comprehensive result.

The product gas compositions during the simulation were monitored at the different heights along the reactor. Figure 7 shows the mole fractions of carbon monoxide, hydrogen and the methane along the height of the reactor. There are not any distinct variations up to the biomass feeding position. The char partial oxidation is less significant compared to the homogenous phase reactions. Devolatilization as well as chemical transformations of biomass inside the bed give different gas compositions. The increasing hydrogen concentration along the reactor indicates the dominance of the water gas shift reaction and the methane reforming reaction.
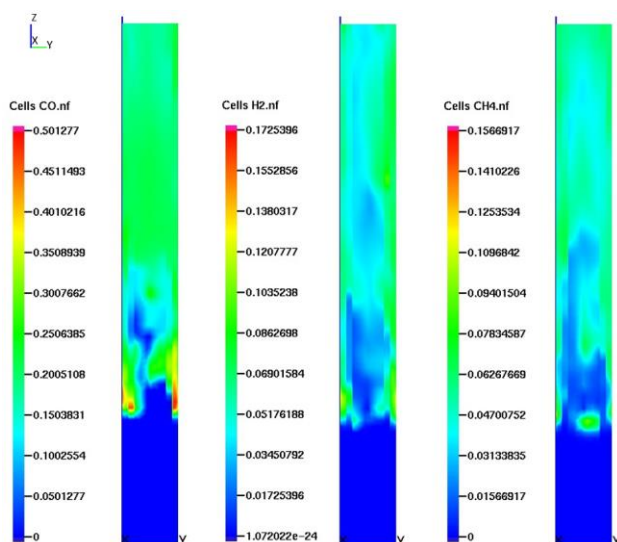
Figure 7. Gas composition along the reactor (Mole fraction)

This shows that the chemical transformations as well as the bed hydrodynamics is quite complex in a bubbling fluidized bed reactor. The operation of the optimized reactor would give uniform particle distribution and ensure operation in the bubbling fluidization regime. Figure 8 shows the particle volume fraction and the particle temperature distribution along the reactor height.
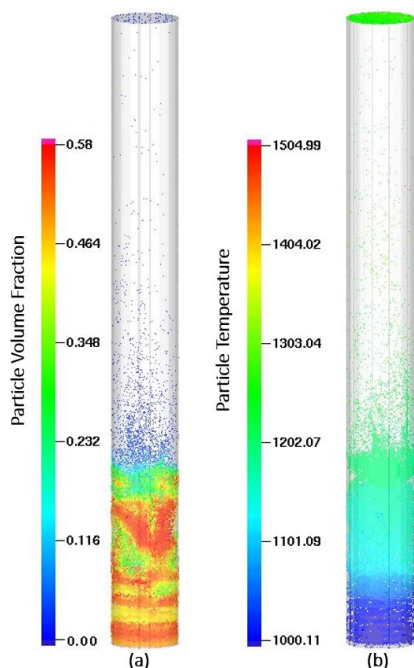

Figure 8. Simulation bed hydrodynamics at 200 s (a). Particle volume fraction (b). Particle temperature

Figure 8 (a) shows that the reactor operates at the bubbling fluidization regime with entrainment of few particles in the freeboard region. The solid volume fraction after the onset of the bubbling regime in the bed is reduced from the solid volume fraction of the static bed. Although the system was set to a temperature of 1000K, due to the exothermic nature of the reactions, the temperature rises up to around 1200K inside the reactor.

4 Conclusions

Air gasification of biomass in bubbling fluidized bed reactor was performed in a pilot-scale reactor at USN. A kinetic-based CPFD simulation model was used to simulate the gasification of biomass using Barracuda. The experimental setup as well as the simulation model were operated in the bubbling fluidizing regime. The results from the simulation were compared with the experimental data. The average volume percentage of carbon monoxide, hydrogen and methane were found to be around 20%, 10%, and 7% respectively during the experiment. There is a good agreement between experimental and computational results regarding the hydrogen, carbon monoxide and methane concentration. Oxygen concentration during the experiment was around 1%. The small amount of oxygen during the experiment may be due to manual sampling process used for gas sampling. The char partial oxidation is less significant compared to the homogenous phase reactions during the gasification process.

References

J. C. Bandara, B. ME. Moldestad and M. S. Eikeland. Analysing the effect of temperature for steam fluidized-bed gasification of biomass with MP-PIC simulation. *International Journal of Energy and Environment,* 9(6): 529-542, 2018.

R. B. Bates et al., Steam-air blown bubbling fluidized bed biomass gasification (BFBBG): Multi-scale models and experimental validation. *AIChE Journal,* 63(5): 1543-1565, 2017. doi:10.1002/aic.15666.

W. Doherty, A. Reynolds and D. Kennedy. Aspen plus simulation of biomass gasification in a steam blown dual fluidized bed. 2013.

C. Franco, F. Pinto, I. Gulyurtlu and I. Cabrita. The study of reactions influencing the biomass steam gasification process. *Fuel* 82(7): 835-842, 2003. doi:10.1016/S0016-2361(02)00313-7.

X. Ku, T. Li and T. Løvås. CFD–DEM simulation of biomass gasification with steam in a fluidized bed reactor. *Chemical Engineering Science,* 122: 270-283, 2015. doi:10.1016/j.ces.2014.08.045.

X. Li et al., "Biomass gasification in a circulating fluidized bed. *Biomass and Bioenergy,* 26(2): 171-193, 2004. doi:10.1016/S0961-9534(03)00084-9

H. Liu, R. J. Cattolica and R. Seiser. CFD studies on biomass gasification in a pilot-scale dual fluidized-bed system. *International Journal of Hydrogen Energy,* 41(28): 11974-11989, 2016. doi:10.1016/j.ijhydene.2016.04.205

C. Loha, H. Chattopadhyay and P. K. Chatterjee. Three dimensional kinetic modeling of fluidized bed biomass gasification. *Chemical Engineering Science,* 109: 53-64, 2014. doi:10.1016/j.ces.2014.01.017

G. Schuster, G. Löffler, K. Weigl and H. Hofbauer. Biomass steam gasification–an extensive parametric modeling study. *Bioresource technology,* 77(1): 71-79, 2001. doi:10.1016/S0960-8524(00)00115-2

K.-A. Solli, R. K. Thapa and B. ME. Moldestad. Screening of kinetic rate equations for gasification simulation models. Proceedings of The 9th EUROSIM Congress on Modelling and Simulation, EUROSIM 2016.

R. Thapa, C. Pfeifer and B. M. Halvorsen. Modeling of reaction kinetics in bubbling fluidized bed biomass gasification reactor. *Int. J. Energy Environment,* 5: 35-44, 2014.

J. Xie, W. Zhong, B. Jin, Y. Shao and Y. Huang. Eulerian–Lagrangian method for three-dimensional simulation of fluidized bed coal gasification. *Advanced Powder Technology,* 24(1): 382-392, 2013. doi:10.1016/j.apt.2012.09.001