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Modeling of reaction kinetics in bubbling fluidized bed biomass gasification reactor

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Abstract
Bubbling fluidized beds are widely used as biomass gasification reactors as at the biomass gasification plant in Güssing, Austria. The reactor in the plant is a dual circulating bubbling fluidized bed gasification reactor. The plant produces 2MW electricity and 4.5MW heat from the gasification of biomass. Wood chips as biomass and olivine particles as hot bed materials are fluidized with high temperature steam in the reactor. As a result, biomass undergoes endothermic chemical reaction to produce a mixture of combustible gases in addition to some carbon-dioxide (CO_2). The combustible gases are mainly hydrogen (H_2), carbon monoxide (CO) and methane (CH_4). The gas is used to produce electricity and heat via utilization in a gas engine. Alternatively, the gas is further processed for gaseous or liquid fuels, but still on the process of development level. Composition and quality of the gas determine the efficiency of the reactor.
A computational model has been developed for the study of reaction kinetics in the gasification rector. The simulation is performed using commercial software Barracuda virtual reactor, VR15. Eulerian-Lagrangian approach in coupling of gas-solid flow has been implemented. Fluid phase is treated with an Eulerian formulation. Discrete phase is treated with a Lagrangian formulation. Particle-particle and particle-wall interactions and inter-phase heat and mass transfer have been taken into account.
Series of simulations have been performed to study model prediction of the gas composition. The composition is compared with data from the gasifier at the CHP plant in Güssing, Austria. The model prediction of the composition of gases has good agreements with the result of the operating plant.

Keywords: Biomass gasification; Fluidized bed; Computational Particle Fluid Dynamic CPFD; Eulerian-Lagrangian approach; Reaction kinetics; Dual fluidized bed; FICFB-gasification.

1. Introduction

Biomass is a source of renewable energy neutral to CO_2 emission. It is the oldest source of energy known to mankind. At present time it is the fourth largest source of energy after oil, coal and gas. Today, biomass contributes 14% world's energy consumption [1, 2]. Biomass is used in power plants to produce heat and power. In conventional power plants, biomass is combusted to produce steam. The steam is then used in steam cycles for power production. The overall efficiencies of those power plants are relatively low.
During the past two decades many researches are focused on the gasification of biomass. The technology allows producing a mixture of combustible gases in addition to some gases like CO_2 and water vapor.

The gas can further be utilized for heat and power production. One of those areas is dual fluidized bed gasification, formerly called Fast Internally Circulating Fluidized Bed (FICFB) gasification system. The technology was developed jointly by Vienna University of Technology and AE Energietechnik in Austria [3, 4]. The fundamental principal of the gasification process is shown in Figure 1. The basic concept behind the technology is to separate the gasification reactor from the combustion reactor. The gasification reactor is operated as a bubbling fluidized bed fluidized by high temperature steam. In the gasification reactor, biomass undergoes endothermic reaction to produce a mixture of combustible gases in addition to CO_2 and water vapor. The combustible gases are mainly hydrogen (H_2), methane (CH_4) and carbon-monoxide (CO). The mixture of gas is called producer gas. The combustion reactor is operated as a circulating fluidized bed reactor fluidized by air. The combustion reactor is used to heat the bed material. The heated bed material is then circulated to the gasification reactor in order to supply necessary heat for endothermic reactions in the gasification reactor.

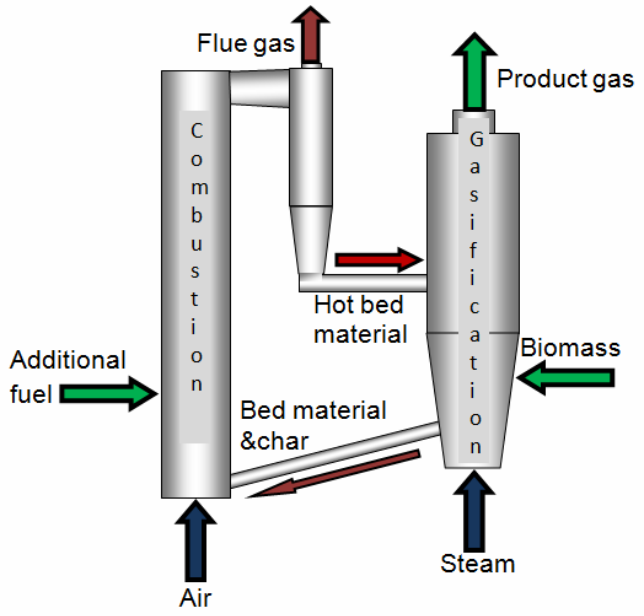


Figure 1. Principle of dual fluidized bed-gasification process

The producer gas can be used for several applications. It can be used in gas engines, gas turbines or fuel cells to produce electricity and heat. The gas can further processed through Fischer-Tropsch (FT) or dimethyl ether (DME) synthesis. The energy efficiency of the technology is higher than conventional technologies. The technology has less environmental impacts such as NO_x and particulate production [5]. The technology has been demonstrated as biomass gasification plant for combined heat and power (CHP) production. The $8MW_{fuel}$ plant is located in Güssing, Austria. The plant produces 2MW electricity and 4.5MW heat from the gasification of wood chips [6]. The technology produces almost nitrogen free, producer gas with high calorific value of about 12-14 MJ/Nm^3 [7].

Besides the novelty of the technology, the overall efficiency of the technology needs to be further increased. This makes the technology more competitive with other sources of energy in the world energy market. Gasification reactor is the heart of the technology and it is believed that the efficiency of the technology mainly depends on the thermo-chemical and fluid dynamic behavior in the reactor. Study of those parameters in an operating plant is almost impossible due to its high operating temperature. Down-scaled lab-models allow the study of fluid-dynamic behaviors [8, 9]. Nevertheless a detailed study of thermo-chemical behavior is still a major challenge. A validated computational model with CFD simulation could be the solution. The model prediction is helpful for improving efficiency of the technology. In addition, it can predict the optimized parameters in design for improvements and scaling of such plant.

2. The gasification reactor

The modeling in the present work is focused only on the gasification reactor excluding the combustion reactor. The gasification reactor is a bubbling fluidized bed. In the reactor, hot bed material, olivine

particles are fluidized by high temperature steam. The geometry of the model reactor is shown in Figure 2. Biomass in the form of wood chips is fed to the reactor. The heated bed material of temperature about 900^0C is also fed to the gasification reactor from the combustion reactor. Biomass undergoes endothermic gasification reaction taking necessary heat from the hot bed material. The bed material with some amount of unreacted char particles leaves the gasification reactor to the combustion reactor. The producer gas leaves the reactor at the top.

Inside the reactor, biomass first undergoes a drying process and the moisture content of the biomass is removed in the form of water vapor. The second process is devolatilization. This is the process of thermal decomposition of biomass in the absence of oxygen where the biomass is decomposed to char particles and gases. The process can be shown as in Equation 1 [10]. The composition of the gases depends on the operating condition of the reactor.

$$wood \rightarrow H_2, CO, CO_2, CH_4, HC, H_2O, tars, char(s) \quad (1)$$

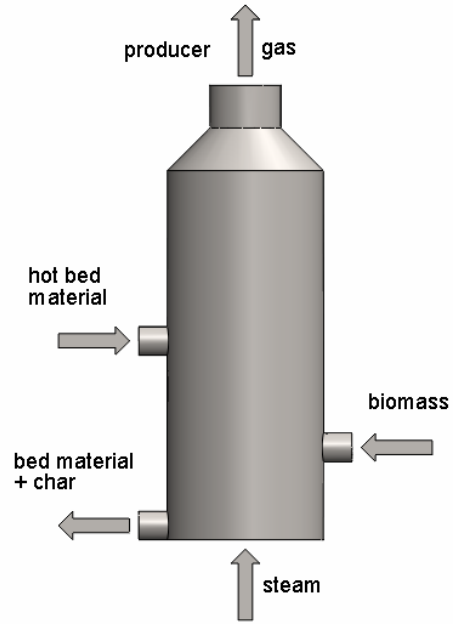


Figure 2. fModel of gasification reactor

The third step include sheterogeneous and homogeneous reactions. The reactions with the corresponding reaction kinetics are presented in Table 1 [11-14].

The process should be optimized in order to get the maximum fraction of H_2 and CO with reduced amounts of condensable water and organic vapor in the product gas. The reactions are depending on the heat and mass transfer as well as fluid dynamic behavior in the gasification reactor. Modeling and simulation of the reactor using Computational Particle Fluid Dynamics (CPFD) allows study of the reactor with varying parameters.

3. Computational model

There are mainly two approaches in modeling of gas-solid flow in fluidized bed reactors: Eulerian-Eulerian and Eulerian-Lagrangian. Eulerian-Eulerian approach assumes both the gas and solid phase as continuum and the two phase flow as interpenetrating continua. The major disadvantage encountered in this approach is that the model does not have the possibility to account for the particle size distribution in the bed. This is because separate momentum and continuity equation have to be solved for each size of particle [15]. However, the particle size distribution has significant influence on the performance of fluidized bed [16-18]. Eulerian-Lagrangian approach treats solid phase as discrete elements. The motions of individual particles are tracked using Newton's law. The particle-particle, particle-wall and fluid-particle interaction forces are taken into account [19]. This approach simulates the gas solid flow with wide range of particle size distribution [20, 21].

Eulerian-Lagrangian approach is implemented for the modeling of gas-solid flow and chemical reactions in the biomass gasification reactor. Governing equations of the fluid phase are solved using continuum model. The particle phase is solved using Lagrangian model. The computational methods applied in this work is developed by D.M. Snider et al. and the details of the approach can be found in [22-24]. 3D simulations of gas-solid reacting flow are performed using commercial computational particle fluid dynamics (CPFD) software Barracuda VR 15.

One of the important advantages of CPFD software is that it allows simulating particles with different size and distribution. Figure 3 shows the particle size distribution of biomass and bed material feed to the reactor. It should be noted that the particle size are measured in their corresponding radius in Barracuda VR 15 instead of diameter.

Table 1. Reactions in the gasification reactor and their reaction kinetics

Reaction	Reaction kinetics
Steam gasification $C + H_2O \underset{r_{1r}}{\overset{r_{1f}}{\Leftrightarrow}} H_2 + CO$	$r_{1f} = 1.272\, m_s\, T \exp\left(\frac{-22645}{T}\right)[H_2O]$ $r_{1r} = 1.044\times10^{-4} m_s T^2 \exp\left(\frac{-6319}{T} - 17.29\right)[H_2][CO]$
Carbon-dioxide gasification $C + CO_2 \underset{r_{2r}}{\overset{r_{2f}}{\Leftrightarrow}} 2CO$	$r_{2f} = 1.272 m_s T \exp\left(\frac{-22645}{T}\right)[CO_2]$ $r_{2r} = 1.044\times10^{-4} m_s T^2 \exp\left(\frac{-2363}{T} - 20.92\right)[CO]^2$
Methanation $0.5C + H_2 \underset{r_{3r}}{\overset{r_{3f}}{\Leftrightarrow}} 0.5CH_4$	$r_{3f} = 1.368\times10^{-3} m_s T \exp\left(\frac{-8078}{T} - 7.087\right)[H_2]$ $r_{3r} = 0.151 m_s T^{0.5} \exp\left(\frac{-13578}{T} - 0.372\right)[CH_4]^{0.5}$
Water- gas shiftreaction $CO + H_2O \underset{r_{4r}}{\overset{r_{4f}}{\Leftrightarrow}} CO_2 + H_2$	$r_{4f} = 7.68\times10^{10} m_s T \exp\left(\frac{-36640}{T}\right)[CO]^{0.5}[H_2O]$ $r_{4r} = 6.4\times10^{9} m_s T \exp\left(\frac{-39260}{T}\right)[H_2]^{0.5}[CO_2]$
Methane reforming $CH_4 + H_2O \underset{r_{5r}}{\overset{r_{5f}}{\Leftrightarrow}} CO + 3H_2$	$r_{5f} = 3.0\times10^{5} T \exp\left(\frac{-15042}{T}\right)[CH_4][H_2O]$ $r_{5r} = 0.0265\ T \exp\left(\frac{-32900}{T}\right)[CO][H_2]^2$

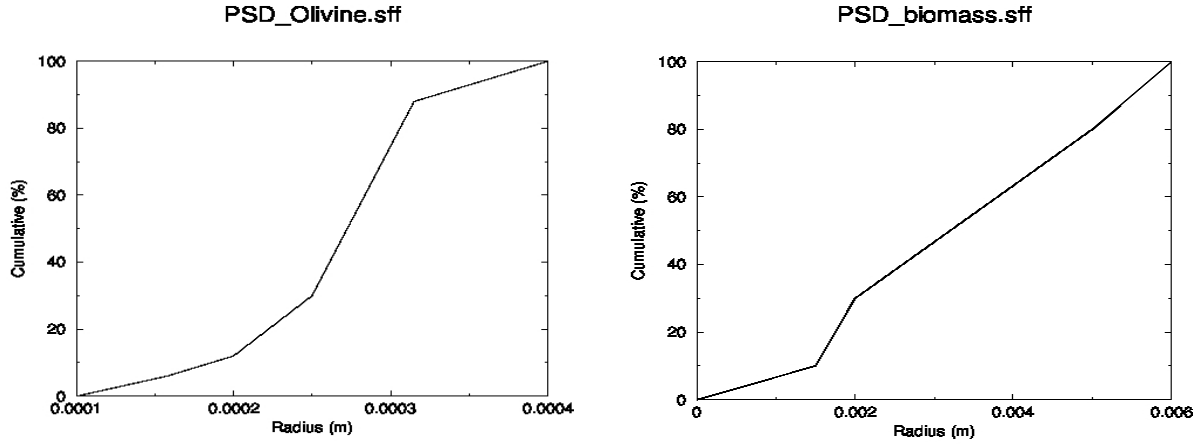


Figure 3. Particle size distribution of the bed material and biomass

Wood chips are fed to the hot bed material in the operating plant. The model assumes that the drying and devolatilization takes place immediately at the inlet of the reactor. The assumption makes sense because

the temperature of the reactor is very high. The reaction temperature is about 1123 K. Feed of the reactor at biomass inlet is divided into char and volatile matters instead of wood chips [25]. The main products of wood pyrolysis are volatile matter, char, moisture, tar, higher hydrocarbons and some other components. As a simplification of the model, the tar, hydrocarbons and other compounds of the pyrolysis are neglected and the volatile matter is divided to91% of gases (CH_4,CO,CO_2 and H_2) and 9% of char particles on dry basis [26]. The wt% of the composition of gases is given in Table 2. The inlet of biomass is modeled as inlet of char particles and volatile matter.

Some of the physical properties of biomass and bed materials are presented in Table 3. Biomass feed rate as volatile matter and char is 28 kg/h. Bed material circulation is 40 times higher than biomass feed. The steam-fuel ratio is 0.6.

Initially the reactor is filled with hot bed material, char particles and superheated steam. The pressure and flow boundary conditions of the reactor are shown in Figure 4. The product gas outlet is pressure boundary. Biomass, bed materials and char particles inlet and outlets are flow boundaries as shown in the figure. The particles and gases passing through these boundaries are monitored by corresponding flux-planes. In addition to this, flow of the product gas is monitored by the flux planes located at 1.4m, 1.9m, 2.4m and 3m along the height of the reactor.

Table 2. Composition of volatile matters in wood

Components	Wt%
CH_4	0.1213
CO	0.6856
CO_2	0.1764
H_2	0.0167

Table 3. Properties of biomass and bed material

Material	Density [kg/m^3]	Flow rate [kg/h]
Olivine	2960	1120
Char	200	25.7
Volatile matter	1.200	2.3
Steam	0.204	16.8

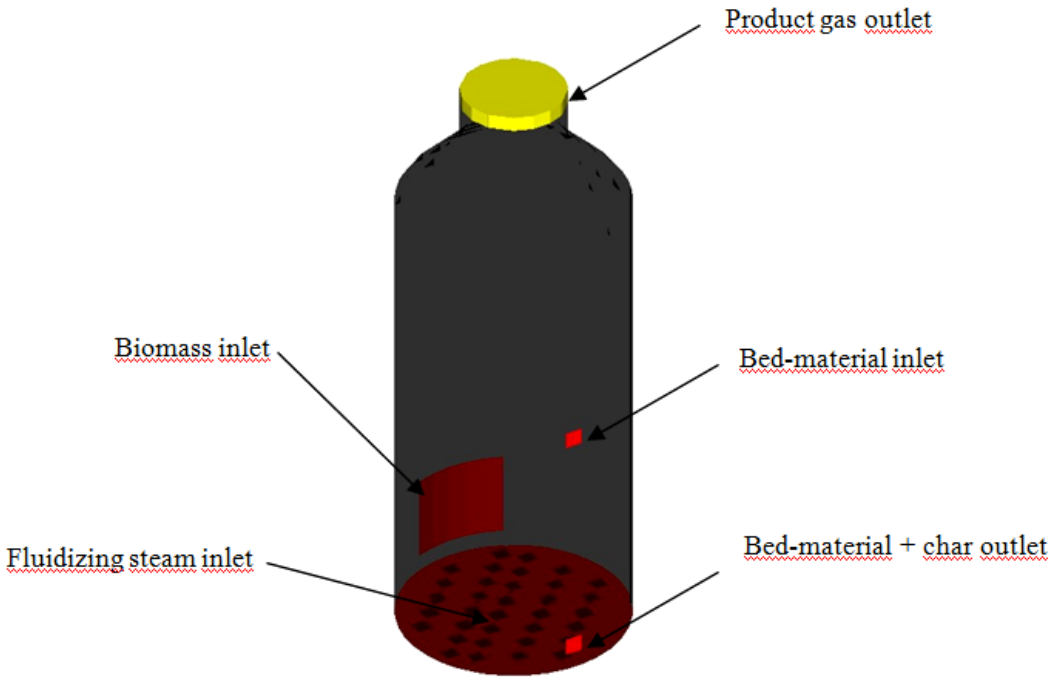
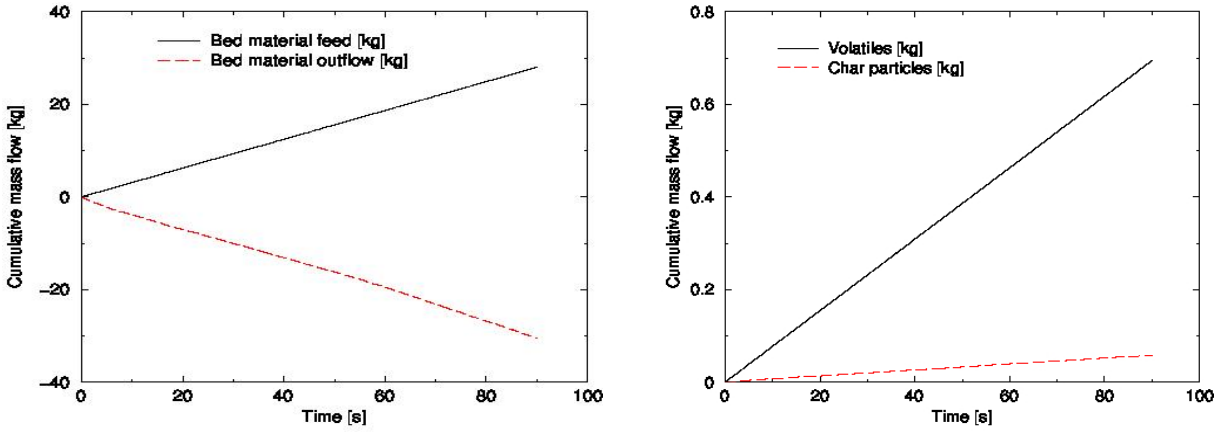


Figure 4. Pressure and flow boundary condition of the model

4. Results and discussion

The simulation was performed to gain 90 seconds of fluidizationas well as gasification reactions in the reactor. Average data was recorded after 10seconds of simulation in order to avoid the fluctuation of different parameter in starting of the reactor. The average data and transient data for different simulation parameters are assigned in different flux planes and transient data points respectively.

Analysis of the results is started from the flow parameters. During simulation, it is important that the flow of bed materialand biomass are consistent with the given feed rate. The in-flux and out-flux rates of bed material and biomass through corresponding flux planes are stored influx-data files. The cumulative rate of inflow and outflow of bed material is shown in Figure 5(a). The figure shows that circulation of bed material is maintained properly during the simulation period. Figure 5(b) shows cumulative mass flow rate of biomass feed. Biomass is divided to 91% volatiles and 9% of char. The figure shows consistent flow of biomass during the simulation period.



(a) (b)

Figure 5. (a) Cumulative flow of bed material; (b) Cumulative flow of biomass

Another significant parameter to be examined is temperature. Different transient points along the height of the reactor are assigned to record temperatures during the simulation. The contours of particle temperature and fluid temperature at 90s of simulation are shown in Figure 6.

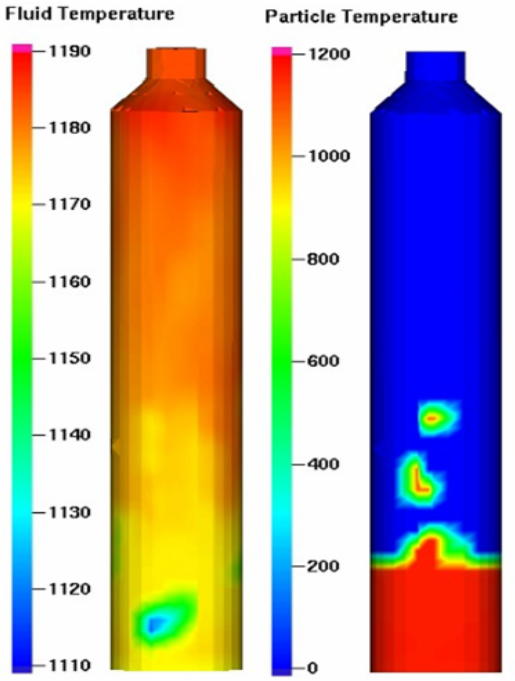


Figure 6. Variation of fluid temperature and particle temperature along the height of reactor

The particle feed temperature is 1173 K. The steam feed temperature is 1073 K. The average gasification temperature is 1073K-1123K. The figure shows both the particle temperature and fluid temperature is above 1073K. This means gasification reaction in the reactor is maintained constantly. The figure indicates that the average temperature of the fluid in freeboard is about 1110 K. The temperature distribution in the dense region as well as the freeboard region of the reactor is consistent with required reaction temperature.

Mass flow rate of the components of the product gas is recorded in different flux planes along the height of reactor. The flow rate through the flux plane located at the top of the reactor is presented in Figure7. Initially, the mass flow rate of CO and CH_4 is higher. This is the result of steam gasification and methanation. After some time, there is decrease in CO, CH_4 and water vapor with increase in H_2 and CO_2 indicating homogeneous water gas shift and methane reforming reactions. After few seconds of reaction the flow rate of gas does not vary significantly.

The mole flow rate of gas components are shown in Figure 8. The flow rate is transient data recorded in a point at the top of the reactor. The mole flow rate from transient data is similar to that of mass flow rate from the flux plane as shown in Figure 7. The more fluctuation of mole flow is due to transient nature of the data. Moreover it is the mole passing through a point monitor in the plane.

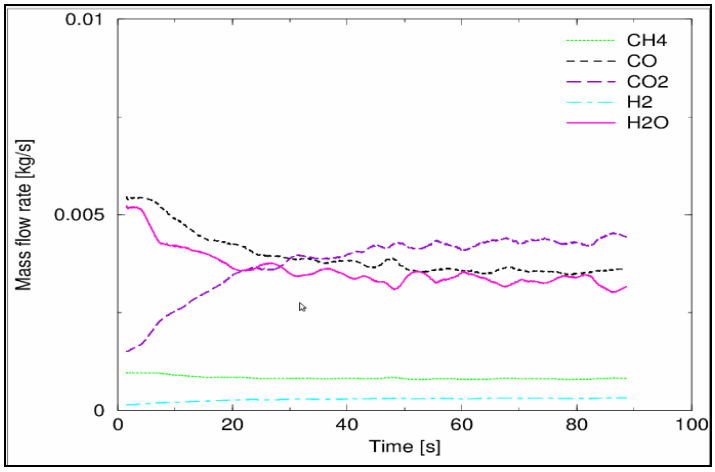


Figure 7. Mass flow rate of gas components through the top of reactor

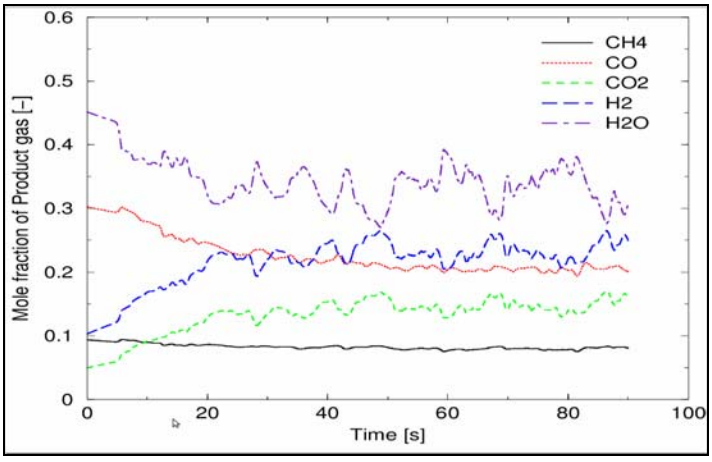


Figure 8. Mole fraction of product gas passing through a point on the top of the reactor

Figure 9 shows that the mass fraction of CO and H_2O is highest at the bottom of the reactor in the dense region of the bed. Steam gasification, CO_2 gasification and methanation reactions are responsible for the higher mass fraction of those components. Moreover, the pyrolysis of wood produces large mass fraction of CO.

The mass fraction of CO_2 and $H_2$is highest at the top of reactor. The fraction of CH_4 is decreasing slightly and continuously from the dense region to the freeboard. This indicates methane reforming reaction starts

immediately at the freeboard region near to the dense region of the bed and continues along the height of the bed.

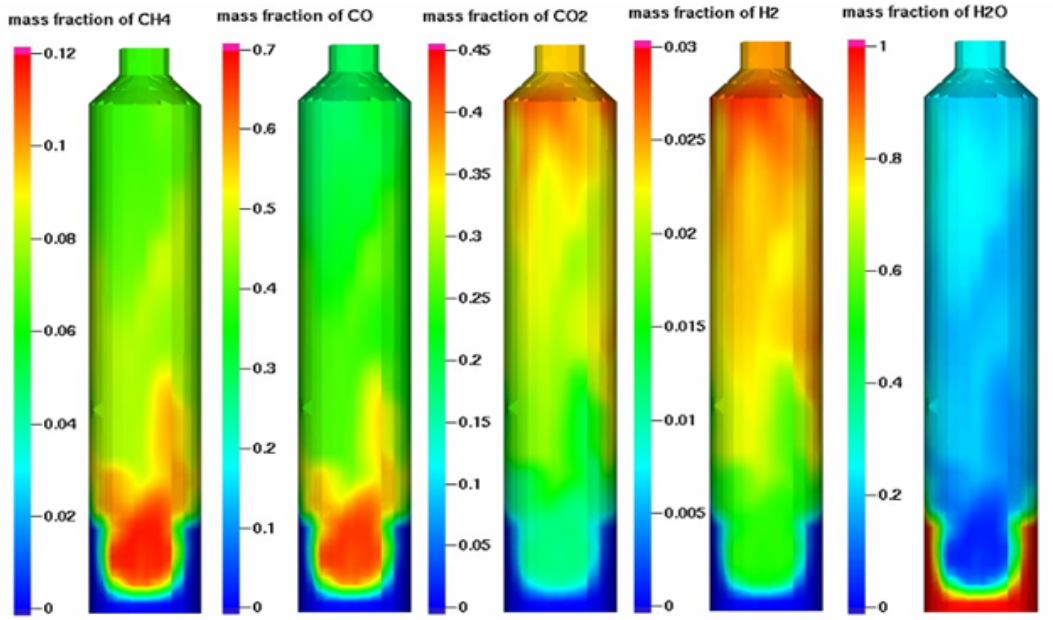


Figure 9. Mass fraction of the product gas components at simulation time of 90s

At the dense region of the reactor, chemical reactions occur to produce CH_4 and CO. At the freeboard region the mass fraction of CO and CH_4 is decreased forming more H_2 and CO_2. The fraction of steam is also decreased significantly at the freeboard region indicating the fact that more steam is consumed during homogeneous reactions in the freeboard.

The product gas compositions are recorded at the four different heights of the freeboard region of the reactor. The mass fractions are converted to volume fractions and presented in Figure 10. The product gas composition varies significantly at the dense region of the bed and its nearest freeboard region. As the product gas flows higher and higher along freeboard, the gas composition becomes more constant. This indicates less and less reactions as the gas moves along the height of the reactor.

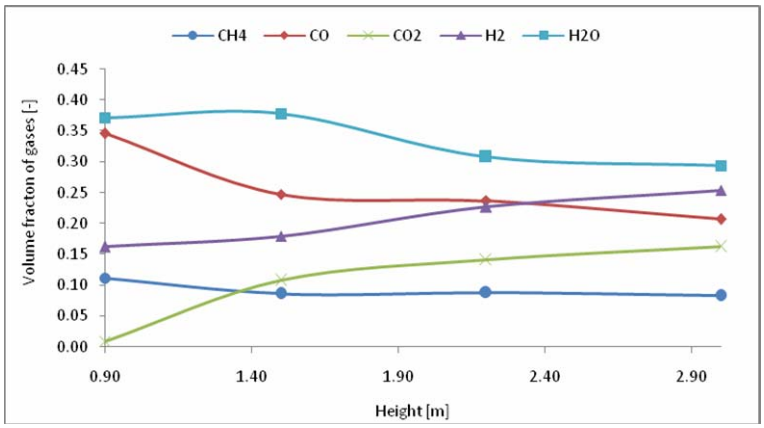


Figure 10. Gas volume fraction along the height of the reactor

The composition of producer gas in the Güssing plant can be found in many published literatures [3, 4, 27]. Simulated producer gas composition is compared with the measured composition of the CHP plant in Güssing. The data is presented in Table 4. The gasification temperature is about 800-850^{0}C at atmospheric pressure. The measured values are in dry basis. It should be noted that 9vol% of gases are assumed as tar and other hydrocarbons which are not included in the predicted results as well as in measured data from the CHP plant in Güssing.

Table 4. Comparison of simulated and measured product gas composition

Components	Predicted vol%	Measured vol%
Hydrogen (H_2)	34	32
Carbon monoxide (CO)	25	25
Carbon dioxide(CO_2)	22	22
Methane (CH_4)	10	12

5. Conclusion

A 3D gas solid reacting flow in the bubbling fluidized bed part of the dual fluidized bed biomass gasification reactor has been modeled. The model is simulated using computational particle fluid dynamic (CPFD) software Barracuda VR 15. Biomass is modeled as a 91wt% of volatile gases and 9wt% of char particles. The heterogeneous reactions considered are the steam gasification, CO_2 gasification, and methanation. Homogeneous reactions occurring in the gasification reactor are water-gas shift and methane reforming.

The results of the simulation shows most of the reactions occur at the dense region of the bed and the vicinity of the dense region in the freeboard. As the gases passes through the freeboard region, the composition of the gas becomes consistent. The predicted composition of the product gas is compared with measured data from the gasifier at the combined heat and power plant in Güssing, Austria. The compositions agree well.

A computational model of a wood gasification reactor has been established. The model can be used to study various parameters of the reactor such as influence of temperature, residence time and steam-fuel ratio as well as other parameters.

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