Modelling and simulation of the biomass fired dual fluidized bed gasifier at Guessing/Austria.

Priyanka Kaushal, Tobias Pröll and Hermann Hofbauer
Vienna University of Technology, Institute of Chemical Engineering,
Getreidemarkt 9/166, A-1060 Vienna/Austria.

Abstract
A one-dimensional steady state model of the gasification reactor of a dual fluidized bed biomass steam gasification system has been developed. The gasification reactor is operated in bubbling regime. The model distinguishes two zones: dense zone and freeboard zone. The dense zone is the bubbling bed and is modelled with modified two phase theory while freeboard is modelled as a plug flow reactor. The main fuel is biomass (wood) and is introduced into the dense zone. Biomass is modelled as a homogeneous matrix of C, H, and O. The solids within the dense zone are considered to be well mixed while the gases are in plug flow regime. Energy balance is solved globally in each zone. Results show that the wood is only partly converted in the gasifier. The gas composition profile and temperature profile predicted by the model is in good agreement with the values measured at 8 MW (fuel power) plant in Guessing/Austria.

Keywords
Biomass, steam gasification, fluidized bed, model.

1. Introduction
The prime objective of biomass gasification is energy refinement i.e. to convert the chemical energy in biomass into the chemical energy of the producer gas. There is a large potential for biomass utilization as a renewable energy source. Efficient conversion of solid biomass (i.e. wood chips) to a medium calorific product gas by means of steam gasification allows the combined production of heat and power (CHP) [1]. In Austria, a dual fluidized bed steam gasification technology has been developed and is successfully demonstrated at the 8 MW (fuel power) CHP plant in Güssing/Austria. The gasification unit consists of two fluidized bed reactors (gasification and combustion reactor) coupled via a circulating bed material loop. The energy needed for the endothermic steam gasification reactions in the gasification reactor is generated by combustion of residual char in the combustion reactor. The gasification reactor is operated in bubbling regime while the combustion reactor is operated as a fast fluidized bed (riser). The process has recently been described [2].

This paper focuses on the mathematical modelling of the gasification reactor as shown in Fig. 1. The boundaries of the investigated system are marked by the broken line in Fig. 1. The bed material leaves the gasifier together with the residual biomass char via the chute at the bottom towards the riser. After separation of the solids from the flue gas in the cyclone at the top of the riser the solid cycles back into the gasifier via a steam-fluidized loop seal. A number of circulating fluidized bed (CFB) models have focussed on coal combustion [3,4] but biomass processing in CFBs has received less attention so far [5]. This model is capable of predicting the average temperatures in the zones, the concentration and distribution of each species in the vertical direction of the bed in both the bubble and emulsion phase, the composition of the producer gas, the heating value and production rate of the producer gas. Directly measured validation data from the Güssing plant is limited to several temperatures along the height of the reactor and the final producer gas composition. Mass and energy balances for the entire plant yield most of the input parameters to the riser simulation: net biomass combustion rate, bed material circulation rate, char composition.

2. Mathematical modelling
a. Model structure
This is a one dimensional steady state model for a bubbling fluidized bed biomass gasifier. The model assumes gases as ideal and in plug flow regime, the solids are assumed to be attrition free and uniform in size. The inorganic is classified as Geldart’s type B. Biomass is modelled as a homogeneous matrix of carbon, hydrogen and oxygen whose composition changes post devolatilization. The gasifier is divided into two zones with different hydrodynamic characteristics: dense zone and freeboard. Superheated steam is introduced at the lower boundary of dense zone. Each zone is further divided into cells and each cell calculates its local hydrodynamic and thermodynamic state based on the theoretical principles. The cells are solved sequentially from bottom to top with the output of each cell considered as input for the next cell. The
conservation equations for biomass, bed material and energy are not evaluated in each cell but across the entire zone. Therefore each zone shows a homogeneous biomass concentration in the bed material and a uniform temperature. Further input parameters to the model are geometric data, material properties, gas flow rates and inlet temperatures.

Table 1
Input parameters to the model (typical operating condition from Guessing plant)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Diameter (maximum) of gasifier</td>
<td>0.67 m</td>
</tr>
<tr>
<td>Height of column</td>
<td>6 m</td>
</tr>
<tr>
<td>Diameter of particle</td>
<td>500E-6 m</td>
</tr>
<tr>
<td>Density of bed material</td>
<td>2960 kg/m³</td>
</tr>
<tr>
<td>Density of coke</td>
<td>200 kg/m³</td>
</tr>
<tr>
<td>Bed circulation</td>
<td>37 kg/s</td>
</tr>
<tr>
<td>Steam feed rate</td>
<td>700 Nm³/hr</td>
</tr>
</tbody>
</table>

Flue gas
Solid
Solid
Air
Producer gas

Figure 1: Modelling boundary of the DFB boundary.

b. Bed hydrodynamics
The dense zone (bubbling bed) is modelled according to the modified two phase theory [6] as shown in equation (1). Y is always below unity, the reported values of Y scatter in a wide range [7]. In present model, Y is calculated as a function of the height. The bubble size is one of the most critical parameter since it affects the bubble rising velocity, the bubble fraction and the mass transfer between the phases.

\[ Q_B = Y(U_0 - U_{mf}) \] 

The bubble size is calculated (Equation 2) as a function of bed height and it is assumed that all bubbles at any cross section are of uniform size [8].
As the bed height increases, bubbles coalesce and the increased bubble size leads to an increase in the bubble rising velocity formulated according to Davidson & Harrison [9] as shown in equation (3).

The interphase mass-transfer between bubble and emulsion, essential for the gas-solid reactions, is modelled by a semi-empirical approach [10] using the specific bubble surface as the exchange area, the concentration gradient and mass-transfer coefficient, as shown below in equation (4):

\[ K_{bl} = \frac{U_{mf}}{4} + \frac{4\varepsilon_{mf}D_{U_b}}{\pi d_b} \]

\[ d_b = 0.54(U_b - U_{mf})^{0.4} \left( z + 4 \sqrt{\frac{A}{N_{mf}}} \right)^{0.8} g^{-0.2} \]

(c. Reaction system)
Gasification is in general a very complex process due to combination of different mechanisms as mass transfer, chemical reaction and heat transfer. Several attempts have been made to understand and describe the reaction mechanism [11]. In present work, gasification process is divided in three steps: Drying is the first step that the biomass undergoes. The moisture content within the biomass is an input parameter to the model. Drying is followed by devolatilization (devolatilization is the thermal decomposition of biomass in the absence of oxygen, to produce char and medium-heating-value gas).

\[ \dot{m}_v = \dot{m}_{vc} + \dot{m}_{vr} + \dot{m}_{vo} \]

From the extensive research work done [12] it can be concluded that the kinetics of the devolatilization process are dependent on temperature, particle size, solid residence time, composition of the feedstock and heating rate etc. Still, the devolatilization step of the biomass is a source of high uncertainty. The proposed model assumes instantaneous drying and devolatilization. The products of devolatilization are CO₂, CO, H₂O, H₂ and CH₄. The simplification of considering the primary gaseous products to consist of these five compounds has some literature and some experimental support [13,14].

The steam and gas released from drying and devolatilization are not added instantaneously to the upflow gas stream. They are added in each cell of the dense bed according to some predefined profile (Fig.2).

Figure 2: Some of the defined profiles for gas addition in main gas stream
a: increasing;b: decreasing;c: first increases than decreases;d: equally.

The final step that the biomass encounters in a gasifier is the gasification process. This step completes the thermal conversion of biomass. Here, the residual solid, the char, which is a product of the
preliminary drying and devolatilization step undergoes conversion. The freeboard of the gasifier is modelled as a plug flow reactor where only homogeneous reaction takes place.

\[
\begin{align*}
\text{Heterogeneous Reactions} \\
C + H_2O &\rightarrow H_2 + CO \quad A \\
C + CO_2 &\rightarrow 2CO \quad B \\
C + 2H_2 &\rightarrow CH_4 \quad C \\
\text{Homogeneous Reactions} \\
CO + H_2O &\leftrightarrow CO_2 + H_2 \quad D \\
CH_4 + H_2O &\leftrightarrow CO + 3H_2 \quad E
\end{align*}
\]

\textit{d. Conservation of mass and energy}

While the elementary mass balances inside every single cell are covered by the stoichiometry of the reaction formulations, the mass balance for solid carbon and the energy balance is applied globally across the dense zones. The general carbon balance is

\[
m_{C,\text{solid, out}} + m_{C,\text{gas, out}} = m_{C,\text{solid, in}} + m_{C,\text{gas, in}} \tag{6}
\]

All feed rates on the right hand side of Eq. 6 are input parameters to the model. Since a uniform solid concentration is assumed, the solid carbon exit rate and the carbon hold-up in the zone are directly linked to each other. The carbon conversion rate is correlated by the reaction model to several parameters and depends strongly on the carbon hold up within each cell. The energy balance is formulated globally across the entire zone using total enthalpies including the standard enthalpy of formation with the assumption that the total amount of energy entering the system is actually leaving the system.

\[
\sum H_{\text{out}} = \sum H_{\text{in}} \tag{7}
\]

The enthalpy of ideal gas mixtures is calculated using the NASA polynomials with coefficients reported by Burcat and McBride [15]. The enthalpy of the inert bed material is calculated by interpolation of data reported by Barin [16]. The sensible heat of char is calculated using the correlations reported by Merrick [17]. The enthalpy of formation of char is calculated from the heating value, estimated from ultimate analysis using the Boie formula [18].

\section{3. Results and discussions}

The model presented here provides an insight of the gasifier, predicts the performance, gas phase composition and temperature profile along the height of reactor. Table 1 lists the input parameters for a typical plant operation. Figure 3 shows the average gas composition of the producer gas over the height of the gasifier. It shows that with the increase of height the steam fraction decreases while those of hydrogen, carbon monoxide, carbon dioxide and hydrocarbon increase. Most of the conversion takes place in the dense bed at the bottom of the gasifier. In the freeboard the changes in gas composition are insignificant. Figure 4 shows the gaseous composition in the dense zone (bottom bed).

A two-dimensional Newton-Raphson algorithm is applied where the components of the Jacobian matrix are calculated analytically. The iteration is performed for the dense zones where the order is again from bottom towards top of the gasifier. After convergence, the model yields the gas phase concentration profiles, the average temperature in each zone, the solid char flow rate leaving the reactor.
Figure 3: Average gas phase composition along the height of the riser.

Table 2
Comparing the measured and predicted gas composition (at the exit) and temperature of gasifier.
(Gas composition reported in volume percent; Temperature in degree celsius)

<table>
<thead>
<tr>
<th></th>
<th>Predicted</th>
<th>Measured</th>
</tr>
</thead>
<tbody>
<tr>
<td>CO</td>
<td>12.77</td>
<td>13.23</td>
</tr>
<tr>
<td>CO₂</td>
<td>11.29</td>
<td>12.75</td>
</tr>
<tr>
<td>CH₄</td>
<td>10.80</td>
<td>6.21</td>
</tr>
<tr>
<td>H₂</td>
<td>22.12</td>
<td>21.38</td>
</tr>
<tr>
<td>H₂O</td>
<td>41.06</td>
<td>42.79</td>
</tr>
<tr>
<td>Temperature (dense zone)</td>
<td>857</td>
<td>860</td>
</tr>
<tr>
<td>Temperature (Freeboard)</td>
<td>855</td>
<td>857</td>
</tr>
</tbody>
</table>

Figure 4: Gas profile in dense zone (in bubble and in emulsion phase).
4. Conclusions

A one dimensional steady state model of a gasifier has been developed to analyze the gasification of biomass in a bubbling fluidized bed. The model is based on mass and energy balances. The model includes different sub-models that are linked together to describe the overall gasification process. The hydrodynamic sub-model highlights the physical characteristics of the bed material while the reaction sub-model deals with the chemical reactions in the different phases of the gasifier. Global reaction rates are used for the description of chemical kinetics. Model validations have been performed with measured results obtained at the 8 MWth dual fluidized bed gasification plant at Guessing. The model is in its first stage of development and is yet to overcome some of its shortcomings. The major challenge is to prepare a robust model for the pyrolysis process. Nevertheless the model predictions are in good agreement with the measured data.

Acknowledgements

The authors gratefully acknowledge the financial support from RENET Austria (Knet/Kind public funds program, Austria).

Nomenclature

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>Area (cross-sectional area)</td>
<td>[m²]</td>
</tr>
<tr>
<td>D</td>
<td>Molecular diffusivity</td>
<td>[m²/s]</td>
</tr>
<tr>
<td>d_b</td>
<td>Bubble diameter (equivalent diameter of a sphere)</td>
<td>[m]</td>
</tr>
<tr>
<td>g</td>
<td>Gravity</td>
<td>[m/s²]</td>
</tr>
<tr>
<td>H</td>
<td>Enthalpy</td>
<td>[J/mol s]</td>
</tr>
<tr>
<td>K_{b,e}</td>
<td>Mass transfer coefficient between bubble and emulsion (Eq.6.14)</td>
<td>[S⁻¹]</td>
</tr>
<tr>
<td>\dot{m}</td>
<td>Mass flow rate</td>
<td>[kg/s]</td>
</tr>
<tr>
<td>N_o</td>
<td>Number of orifice</td>
<td>[-]</td>
</tr>
<tr>
<td>Q_b</td>
<td>Volumetric flow rate in bubble</td>
<td>[m³/s]</td>
</tr>
<tr>
<td>U_o</td>
<td>Superficial velocity</td>
<td>[m/s]</td>
</tr>
<tr>
<td>U_b</td>
<td>Bubble velocity</td>
<td>[m/s]</td>
</tr>
<tr>
<td>U_{b,c}</td>
<td>Velocity of a single isolated bubble</td>
<td>[m/s]</td>
</tr>
<tr>
<td>U_{inf}</td>
<td>Minimum fluidization velocity</td>
<td>[m/s]</td>
</tr>
<tr>
<td>Y</td>
<td>Correction factor for modified two phase theory</td>
<td>[-]</td>
</tr>
<tr>
<td>z</td>
<td>Height</td>
<td>[m]</td>
</tr>
</tbody>
</table>

References

