

## Modelling and Optimisation of Dual Fluidisation Bed Gasifiers for production of chemicals

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Biomass gasification is used in a variety of processes that range from heating application to the production of chemicals. Dual Fluidised Bed Gasifiers (DBFG), with their efficient operation and clean output syngas, are being proposed for many such applications. However, each application has a specific input syngas quality requirement. The quality of the syngas is a function of the biomass feedstock used, the gasifier technology employed, and the gasification conditions. A gasifier model can serve as an effective tool in the understanding of the effect of different parameters on the quality and quantity of syngas. Furthermore, these parameters could also be optimised to systematically meet the requirement of syngas. This study presents a kinetic-based compartment model for DBFGs that are developed in ASPEN Plus®. The model takes into account devolatilisation, catalytic and homogenous gasification reactions for syngas and tars (using a lumped species approach); it also considers combustion of char and heat transfer through bed circulation. The model results were found to be in good agreement when compared with the operational data of an 8 MW CHP gasifier in Gussing, Austria. Furthermore, Multi-Objective Optimisation using the NSGA-II algorithm was also performed for the DBFG model. The optimisation aim was to derive a set of process conditions that are most favourable for the production of ammonia from syngas.

### 1. Introduction

Biomass gasification is seen as one of the front runners for sustainable utilisation of bio-energy. Many technologies for biomass gasification have been proposed; the prominent ones are the updraft gasifier, the downdraft gasifier, the bubbling fluidised bed gasifier, the circulating fluidised bed gasifier and entrained flow gasification. Apart from these, many other technologies have been proposed, based on the combination of the prominent ones. The relative advantages of each technology are related to the biomass that has been gasified, the scale of gasification and the syngas quality required. This study focusses on understanding the working of the Dual Fluidised Bed Gasification (DFBG) technology. As its name suggests, two fluidised beds are used to carry out gasification and combustion separately. The gasification is carried out with steam, and air is used to sustain the combustion reactions. The heat transfer takes place through the circulation of hot bed material between the two beds. Since the gasification is carried out with steam, the nitrogen and tar content in the output syngas is quite low. A wide range of feedstocks can be gasified due to the compact design and easy feeding—requiring little pre-treatment of the biomass. Additionally, the gasifiers are known for their low investment costs. The use of bed material as a catalyst, in the application of chemical loop combustion, and in absorption-enhanced reforming has also been proposed (Göransson et al., 2011).

The presence of a large number of gasification configurations makes it difficult to choose the best one for fulfilling the aims of a particular process. The construction of different lab-scale models would not only consume time and energy but might also not be economically feasible. To overcome these problems, researchers in the past have relied on simulation models to predict the syngas output for particular process configurations. The simulation models for biomass gasification can be grouped under four major methodologies, namely, the equilibrium model, the kinetic model, the Computational Fluid Dynamic (CFD)

model, and the Artificial Neural Network (ANN) model. Equilibrium models are based on the assumption that the reacting system reaches its most stable composition. In other words, Gibbs energy is minimised or the entropy is maximised. The equilibrium models largely act as useful tools for initial estimation, but they are unable to predict precise results for different process configurations. Kinetic models are more detailed when compared to equilibrium models. The reactions are modelled according to their kinetics, which takes into consideration the gasifier design and other physical conditions. Kinetic-based compartment models that focus mainly on reaction kinetics and neglect the hydrodynamics aspect have also been proposed. Kinetic models are frequently used in fluidised bed reactor modelling because the process is kinetically limited. A CFD-based model involves the solving of mass, momentum, elemental and energy balance equations over a defined space. The simulations are usually computationally expensive. Lastly, an ANN model provides an alternate approach to replicate complex systems such as biomass gasification. A unique aspect of this approach is that the model needs to be trained with real time data. The data is used to adjust the parameters inside the ANN, giving it the ability to predict the output of any given input. This modelling approach is useful to predict the output of a real-time gasification process rather than to understand or optimise the process.

Process modelling and simulation is followed by process optimisation. Often it is found that the optimisation objectives conflict, that is, improvement in one objective leads to a decline in others. The traditional approach has been to place different weights on objectives. and to optimise a single objective. Multi-Objective Optimisation (MOO) provides an alternative to this approach by giving a range of optimal solutions that are called Pareto-optimal solutions. This means that any available solution, if optimum for one objective, will be sub-optimal for another objective. No solution on a Pareto curve will be better than any other point with respect to all objectives. It contains a collection of equally good points, and offers a variety of optimal points for the user to choose from. The modelling and optimisation for DFBG is presented below.

## 2. The Gasifier Model

The gasifier selected for the model is the 8MW CHP gasifier at Gussing, Austria. It is based on the dual fluidised bed technology. A kinetic-based compartment model offers a trade-off between accuracy of results and the complexity involved. The present study uses this model to simulate a DFBG in ASPEN Plus® simulation software. The software uses a sequential modular approach to calculate the mass and energy balance. The thermodynamic property method used for simulation was Redlich Kwong Soave Boston Mathias (RKS-BM). The model incorporates both conventional and non-conventional solids without Particle Size Distribution (PSD). Biomass, char and ash were modelled as non-conventional species (François et al., 2012). The simulation model is shown in Figure 1.

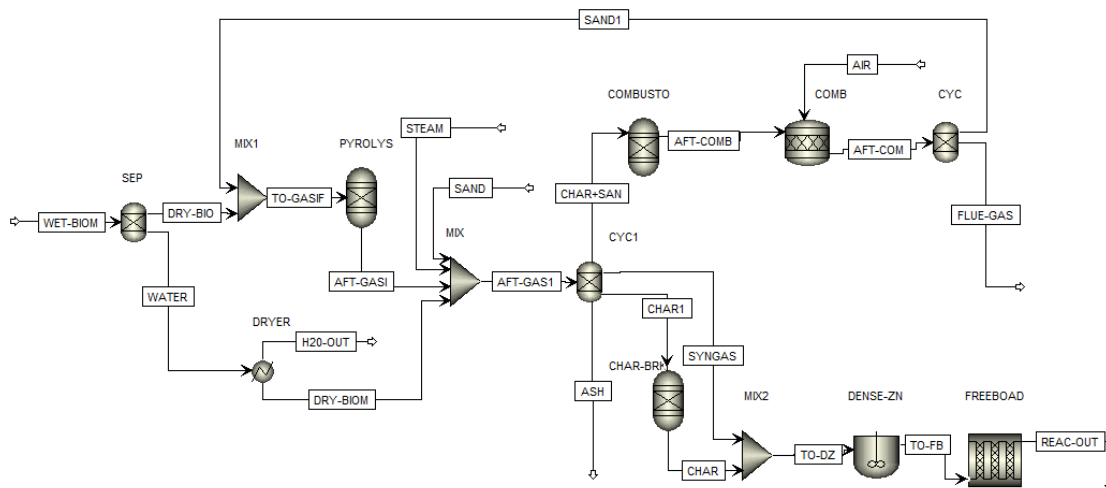


Figure 1: Gasifier flowsheet

The input is modelled as wet biomass. A dryer is used to remove excess moisture. The biomass is mixed with the recycled bed material (modelled as sand) and is introduced into the pyrolysis reactor. The pyrolysis is assumed to be instantaneous and is modelled with the help of the experimental data reported by Dufour et al.(2009a). The data reports the gas, tar and char yields for biomass pyrolysis in the

temperature range of 700 °C to 1,000 °C, and for particle heating rates varying from 20 °C/s to 40 °C/s. The heating rates are in agreement with experimental values for fluidised bed gasifiers (Abdelouahed et al. 2012). For gas yield, data was reported for six major gaseous components, namely, carbon monoxide (CO), hydrogen (H<sub>2</sub>), carbon dioxide (CO<sub>2</sub>), methane (CH<sub>4</sub>), ethene (C<sub>2</sub>H<sub>4</sub>), and ethane (C<sub>2</sub>H<sub>6</sub>). The tars were represented by four model compounds, namely, benzene (C<sub>6</sub>H<sub>6</sub>), phenol (C<sub>7</sub>H<sub>8</sub>), toluene (C<sub>6</sub>H<sub>6</sub>O), and naphthalene (C<sub>10</sub>H<sub>8</sub>). In reality, tars are a mixture of more than 200 compounds, but to simplify the simulations, they are lumped into a few major compounds. Building on the data reported, correlations were formulated by Abdelouahed et al. (2012) to give the mass yields of various compounds, based on the bed material temperature in the pyrolysis reactor. The same correlations are used in this study.

After the pyrolysis reactor, the pyrolysis products are mixed with steam, which is used as fluidisation medium in the gasifier. Make-up bed material is also added here. The combined stream is then sent to a splitter to split the char and the bed material for the combustor. The combustor is modelled as a combination of a yield and stoichiometric reactor. The combustion reactions considered are listed in Table 1.

The combustion reactions heat up the bed material. The heated bed material is then sent to a cyclone, modelled as a splitter. Here the flue gases are separated from the hot bed material. It is assumed that along with the flue gases, 15 % of the bed material that enters is lost. This percentage is higher than that is experienced in practice. However, it accounts for heat losses and maintains the temperature difference between the gasifier and the combustor. The heated bed material is recycled to be mixed with the anhydrous biomass.

The syngas that contains a small percentage of char is sent to the gasification reactor. It is assumed that 5 % of the char produced in the pyrolysis products is gasified and the rest is sent to the combustor to heat up the bed material. The char is broken down into its elemental constituents before it enters the dense zone of the fluidised bed, which is modelled as a continuous flow stirred-tank reactor (CSTR). Here the heterogeneous tar-cracking reactions take place. The gases then enter the freeboard of the gasifier, which is modelled as a plug flow reactor (PFR). Here homogenous gasification reactions take place. The water gas shift reaction is the most important homogenous reaction that dictates the composition of the syngas; it is the only reaction that reaches equilibrium. Other important reactions are the water gas reaction, the methanation reaction and the steam methane reforming reaction. It is reported that hydrogen and steam play an inhibiting role in the steam methane reforming reaction, in a reducing atmosphere (Dufour et al. 2009b). Thus, care must be taken while choosing the appropriate kinetics. Tar reforming reactions also take place in the freeboard but to a very limited extent. The homogenous and the heterogeneous reactions involved, along with their associated kinetics are listed in Table 1.

For optimisation of the process, the Non-dominated Sorting Genetic Algorithm-II (NSGA-II) proposed by Deb et al. (2002) has been used. The algorithm was coded in Visual Basic (VB)/MS Excel® and linked to ASPEN Plus® by Rangaiah et al. (2008). The algorithm has been modified for the optimisation of the gasifier. The MOO framework is depicted in Figure 2. The output syngas composition is optimised for ammonia production. According to a biomass-to-ammonia flowsheet proposed by Arora et al. (2014) the output syngas should have high hydrogen content and a low carbon dioxide and methane content. Thus, the optimisation is aimed at maximising the hydrogen content and minimising the combined carbon dioxide and methane content in the syngas. The optimisation problem is a multi-variable, non-linear, multi-objective optimisation problem solved by using the genetic algorithm NSGA-II.

The gas compositions were found to be within the range that was predicted by the literature. The tar output is higher than the experimental results. This study relies on three model reactions for tar decomposition, whereas, many more reactions are reported in the literature. A sensitivity analysis was also performed in order to study the change in syngas composition when the steam-to-biomass ratio changes. The steam-to-biomass ratio was varied from 0.3 to 1.2 to understand its effect on the quality of the syngas produced—shown in Figure 3. It was seen that an increase in the steam-to-biomass ratio led to an increase in the concentration of H<sub>2</sub> and CO<sub>2</sub> and a decrease in the concentration of CO in the product gas. An increase in steam shifts the equilibrium in favour of H<sub>2</sub> and CO<sub>2</sub>. However, an increase in steam also leads to a lowering of the combustor temperature. This further results in lowering the pyrolysis temperature and a smaller amount of H<sub>2</sub> is produced, as governed by the correlations presented earlier. Thus, the increase in H<sub>2</sub> concentration is much lesser than the increase in CO<sub>2</sub> concentration. A similar trend has been reported by experimental results (Hofbauer and Rauch, 2000).

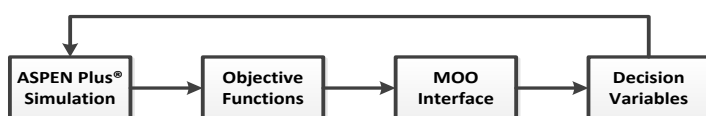


Figure 2: MOO methodology

Table 1: Reaction kinetics

Reaction	Kinetics	Reference
<b>Heterogeneous tar reaction</b>		
$C_{10}H_8 \rightarrow 9C + 1/6 C_6H_6 + 7/2 H_2$	$r = 21.11 \exp\left(-\frac{61,000}{RT}\right) C_{C_{10}H_8}$	(Abdelouahed et al., 2012)
$C_6H_6 + H_2O \rightarrow 3C + 2CH_4 + CO$	$r = 21.11 \exp\left(-\frac{61,000}{RT}\right) C_{C_6H_6}$	(Abdelouahed et al., 2012)
$C_7H_8 + H_2 \rightarrow C_6H_6 + CH_4$	$r = 21.11 \exp\left(-\frac{61,000}{RT}\right) C_{C_7H_8}$	(Abdelouahed et al., 2012)
$CH_4 \rightarrow C + 2H_2$	$r = 10^{-2} \exp\left(-\frac{263,000}{RT}\right) p_{C_{10}H_8}$	(Abdelouahed et al., 2012)
<b>Homogenous reactions</b>		
$CO_2 + H_2 \rightarrow CO + H_2O$	$r = 1.26 * 10^5 \exp\left(-\frac{47,290}{RT}\right) C_{CO_2} C_{H_2}$	(Abdelouahed et al., 2012)
$CO + H_2O \rightarrow CO_2 + H_2$	$r = 2780 \exp\left(-\frac{12,560}{RT}\right) C_{CO} C_{H_2O}$	(Abdelouahed et al., 2012)
$CH_4 + H_2O \rightarrow CO + 3H_2$	$r = 4.7 * 10^4 \exp\left(-\frac{211,000}{RT}\right) p_{CH_4}^{1.48} p_{H_2O}^{-0.11} p_{H_2}^{-0.91}$	(Dufour et al., 2009b)
$C + H_2O \rightarrow CO + H_2$	$r = 2 * 10^8 \exp\left(-\frac{49,884}{RT}\right) C_{H_2O} C_C$	(Inayat et al., 2010)
$C + 2H_2 \rightarrow CH_4$	$r = 120 \exp\left(-\frac{148,995}{RT}\right) C_{H_2} C_C$	(Inayat et al., 2010)
$C_{10}H_8 \rightarrow 9C + 1/6 C_6H_6 + 7/2 H_2$	$r = 3.4 * 10^{14} \exp\left(-\frac{350,000}{RT}\right) C_{C_{10}H_8}^{1.6} C_{H_2}^{-0.5}$	(Abdelouahed et al., 2012)
$C_6H_6 + H_2O \rightarrow 3C + 2CH_4 + CO$	$r = 4 * 10^{16} \exp\left(-\frac{443,000}{RT}\right) C_{C_6H_6}^{1.3} C_{H_2}^{-0.4} C_{H_2O}^{0.2}$	(Abdelouahed et al., 2012)
$C_7H_8 + H_2 \rightarrow C_6H_6 + CH_4$	$r = 1.04 * 10^{12} \exp\left(-\frac{247,000}{RT}\right) C_{C_7H_8} C_{H_2}^{0.5}$	(Abdelouahed et al., 2012)
<b>Combustion Reactions</b>		
$C + O_2 \rightarrow CO_2$	95 % conversion	
$H_2 + 0.5 O_2 \rightarrow H_2O$	100 % conversion	

### 3. Results

Both qualitative and quantitative results are presented. The simulation results compare well with the experimental results reported for the CHP gasifier at Gussing (E4tech, 2009), as shown in Table 2.

Table 2: Gasifier model validation

Variable	Literature	This Model
Biomass input	2.3 t/h	2.3 t/h
Moisture	27 %	27 %
Output Gas (Dry basis)		
H <sub>2</sub>	38 - 45 %	41.1 %
CO	20 - 25 %	19.9 %
CO <sub>2</sub>	20 - 23 %	19.3 %
CH <sub>4</sub>	9 - 12 %	8.8 %
C <sub>6</sub> H <sub>6</sub>	8 g/Nm <sup>3</sup>	15.1 g/Nm <sup>3</sup>
C <sub>7</sub> H <sub>8</sub>	0.5 g/Nm <sup>3</sup>	7.5 g/Nm <sup>3</sup>
C <sub>10</sub> H <sub>8</sub>	2g/Nm <sup>3</sup>	1.1 g/Nm <sup>3</sup>
Steam to Fuel Ratio	.2 - .8 kg/kg dry biomass	0.4
Gas yield	0.9 - 1.1 kg/kg dry biomass	0.9 kg/kg
Gasifier Temperature	850 - 900 °C	866 °C
Combustor Temperature	950 - 1,000 °C	965 °C

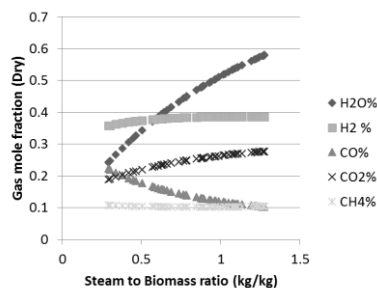


Figure 3: Variation in syngas concentration (dry basis) with respect to steam-to-biomass ratio

The MOO results are now presented. For production of ammonia, the syngas needs to be cleansed of all the gases but hydrogen. A typical gas conditioning plant section would begin with reforming of methane, followed by water gas shift reactors, and finally, the removal of  $\text{CO}_2$ . The aim of the MOO is to maximise the molar flowrate of  $\text{H}_2$  and at the same time to minimise the molar flowrate of  $\text{CO}_2$  and  $\text{CH}_4$ . For the ammonia synthesis process, a rise in  $\text{H}_2$  is linearly linked to the final amount of ammonia produced. A high  $\text{CH}_4$  content increases the load on the reformer downstream of the gasifier.  $\text{CO}_2$  is a waste gas, and any reduction in the amount of  $\text{CO}_2$  increases the production of  $\text{CO}$  (which is converted into equal moles of  $\text{H}_2$  after the shift reactor). Not much variation is expected in the amount of the total  $\text{CO}_2$  released from gas conditioning, since most of the carbon contained in the syngas would eventually be converted to  $\text{CO}_2$ . The manipulated variables include the steam-to-biomass ratio, the bed circulation rate and the percentage division of char between the gasifier and the combustor. The impact of a changing steam-to-biomass ratio has already been illustrated in Figure 3; it is varied between 0.2 and 1.

The percentage of char going to the gasifier was varied from 5 % to 20 %. An increase in the percentage of char going to the gasifier from 5 % to 15 % leads to a decrease in the temperature of the combustion reactor (as char going to the combustor is decreased); and hence, a decrease in the temperature of bed material. This further decreases the pyrolysis temperature. It leads to a decrease in the  $\text{H}_2$  and  $\text{CO}$  concentration and an increase in the concentration of  $\text{CO}_2$  and  $\text{CH}_4$  in the final gas composition. However, the percentage of char going to gasifier when increased beyond 15 %, enhances char gasification reaction in the gasifier and leads to an increase in concentration of  $\text{H}_2$ ,  $\text{CO}$ ,  $\text{CO}_2$  and  $\text{CH}_4$  (nullifying the effect of combustor temperature).

An increase in bed circulation rate leads to a decrease in the concentration of  $\text{H}_2$  and  $\text{CO}$  and an increase in the concentration of  $\text{CO}_2$  and  $\text{CH}_4$  in the final gas composition. It is observed that a decrease in the bed circulation rate leads to an increase in the combustor temperature because the same amount of heat is now absorbed by a smaller mass of bed material. This leads to a small increase in the pyrolysis as well as in the gasification temperature. A higher bed material temperature enhances the production of gaseous products as per the pyrolysis correlations used. However, this effect is noticed when the percentage of char going to the gasifier is less than 15 %. If this percentage is more than 15 %, an increase in combustor temperature results in lowering of pyrolysis temperature and the result effect on gas composition is reversed. The bed circulation rate was varied between 17 to 50 kg/kg biomass. The results obtained after running the NSGA-II based MOO for a population size of 50 and 100 generations are shown in Figure 4(a) and 4(b) and explained below.

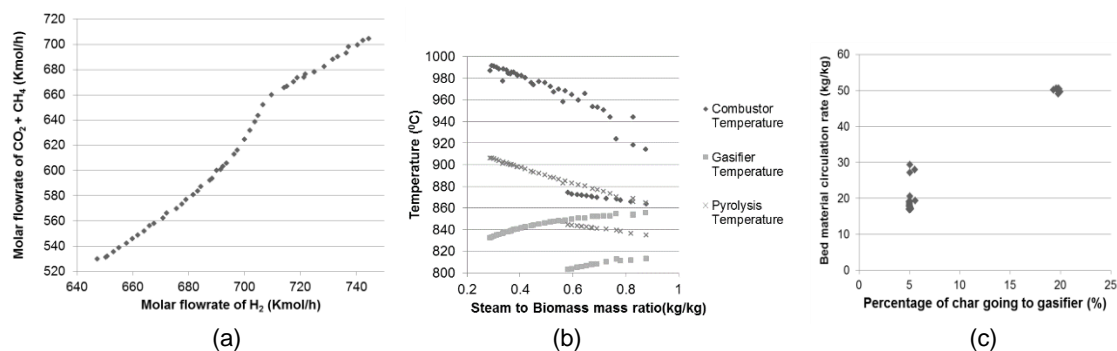


Figure 4: (a) MOO results for optimisation of syngas output, (b) Temperature variations and (c) Distribution of decision variables.

The Pareto plot in Figure 4(a) predicts two kind of relationship between the two objectives, namely, the initial parabolic relationship and later linear relationship. The steam-to-biomass ratio was found to have the maximum influence on the results. Both the percentage of char going to gasifier and bed material circulation rate converged either to the lowest value or the highest value in the range provided, as shown in Figure 4(c). For lower values of percentage char distribution and bed circulation rate, the CO<sub>2</sub> flowrate increased much faster than the H<sub>2</sub> flowrate, with increasing steam-to-biomass ratios. An increase in the steam-to-biomass ratio beyond 0.9 led to a steep rise in the production of CO<sub>2</sub>. At this point, the relationship between the two objectives changes to a linear relationship, which is experienced at higher bed circulation rates and percentage char distribution. Figure 4(b) shows the variation in combustor and gasifier temperatures with changing steam-to-biomass ratios. The temperatures predict a viable energy integration between the combustor and gasifier. The results from the Pareto plot need to be validated by experimental results. The results mentioned, however, show that the MOO methodology can be effectively used to optimise gasifier operations. For an effective ammonia production optimisation, downstream processes need to be modelled and included in the MOO.

#### 4. Conclusions

A kinetic-based compartment-based model for dual fluidised bed gasifier in ASPEN Plus® has been proposed. The model results are found to be in good agreement with reported industrial data. The flowsheet has been connected to an Excel-based MOO framework. A multi-objective optimisation to enhance the output syngas composition, which leads to ammonia production, has been carried out. The results of this modelling methodology predict:

- The effect of changing the steam-to-biomass ratio, percentage of char going to gasifier and bed circulation rate on pyrolysis, gasification and combustor temperatures.
- The effect of process temperatures on pyrolysis and kinetics of gasification reactions.
- A range of optimum syngas compositions that result from different process configurations.

Thus, this study highlights the potential advantages of modelling and optimisation of gasifier systems.

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