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This is a submitted version of a paper published in *Biomass Conversion and Biorefinery*.

Citation for the published paper:
Jie, H. (2012)
"Simulation of biomass gasification in a dual fluidized bed gasifier"
Biomass Conversion and Biorefinery, 2(1): 1-10
URL: http://dx.doi.org/DOI 10.1007/s13399-011-0030-2

Access to the published version may require subscription.

Permanent link to this version:
http://urn.kb.se/resolve?urn=urn:nbn:se:miun:diva-16182

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Biomass Conversion and Biorefinery manuscript No.
(will be inserted by the editor)

Simulation of Biomass Gasification in a Dual Fluidized Bed Gasifier

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Received: date / Accepted: date

Abstract Biomass gasification with steam in a DFBG (dual fluidized bed gasifier) was simulated with ASPEN Plus. From the model, the yield and composition of the syngas, and the contents of tar and char can be calculated. The model has been evaluated against the experimental results measured on a 150 KWth MIUN (Mid Sweden University) DFBG. The model predicts that the content of char transferred from the gasifier to the combustor decreases from 22.5 wt. % of the dry and ash-free biomass at gasification temperature 750 °C to 11.5 wt. % at 950 °C, but is insensitive to S/B (Steam to Biomass Mass Ratio). The H_2 concentration is higher than that of CO under the normal DFBG operation conditions, but they will change positions when the gasification temperature is too high above about 950 °C, or the S/B ratio is too low under about 0.15. The biomass moisture content is a key parameter for a DFBG to be operated and maintained at a high gasification temperature. The model suggests that the gasification temperature is difficult to be kept above

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850 °C when the biomass moisture content is higher than 15.0 wt. %. Thus, a certain amount of biomass needs to be added in the combustor to provide sufficient heat for biomass devolatilization and steam reforming. Tar content in the syngas can also be predicted from the model, which shows a decreasing trend of the tar with the gasification temperature and the S/B ratio. The tar content in the syngas decreases significantly with gasification residence time which is a key parameter.

Keywords Biomass · Gasification · Simulation · Tar

1 Introduction

The DFBG (also referred to as indirect or allothermal gasifier), with steam as the gasification agent, can be used to produce a syngas of 12–20 MJ/Nm^3 (LHV), which is the appropriate syngas for the downstream synthesis of transportation fuels and chemicals. The gasifier consists of two separate reactors: a steam gasifier used to convert biomass into syngas, and an air combustor used to burn the char and to provide the necessary heat for biomass steam gasification. A typical DFBG is composed of a BFB (bubbling fluidized bed) and a CFB (circulating fluidized bed). In comparison with the auto-thermal pressurised gasifier, the advantages of a DFBG are [1]:

- no oxygen demand to obtain nitrogen-free syngas
- low temperature operation
- low investment cost
- no or simple pre-treatment of biomass
- easy feeding of biomass
- suitable for the biomass-based S/M scale bio-automotive fuel plants

Reduction of tar/CH_4 in the syngas is a major challenge to the commercialization of DFBGs for synthetic fuels production. Tar condenses with decreasing temperature (below 400 °C), which leads to knotty problems to the downstream processes. The problems are *e.g.*, fouling and blocking of filters and pipeline passages, dirty working environment, heavy waste water treatment, poisoning of catalyst in synthesis reactors, *etc.* Moreover, tar results in a part of energy lost from the syngas.

For the R&D of DFBG technology, a great deal of effort has been contributed to the experimental study. Very little work can be found on the mathematic simulation, especially, the simulation on tar evolution in biomass gasification.

In coal industry, a chemical percolation devolatilization (CPD) model was developed to model coal devolatilization based on characteristics of the chemical structure of the parent coal. The direct use of chemical structure data as a function of coal properties is useful to justify the model on a theoretical basis rather than an empirical basis. Fletcher [2] made a contribution to the CPD

model development. The predictions of the amount and characteristics of syngas and tar fit well with available measurement data. The application of CPD model to biomass has not been seen to a certain extent.

ASPEN Plus is often used to simulate the coal/biomass conversion processes. Sotudeh-Gharebaagh *et al.* [3] used it to predict coal combustion in a CFB combustor regarding combustion efficiency, emission levels of CO, SO_2, and NO_x, as well as concentration profiles of O_2 and CO. Lee *et al.* [4] presented the kinetic expressions for steam–char and oxygen–char reactions in the atmospheric coal gasification in a fluidized bed reactor. These expressions were cited by Nikoo *et al.* [5] in the biomass gasification simulation with ASPEN Plus. Doherty *et al.* [6] developed a simple model with ASPEN Plus for the simulation of biomass gasification with steam and air in a CFB gasifier. Parameter sensitivity analyses, especially the effect of air preheating on gasification, were performed. The result is plausible. Corella *et al.* [7] set up a model for atmospheric biomass gasification in a CFB gasifier. In this model, the hydrodynamics and reaction kinetics aspects were considered, and the issues on the tar formation and reduction were discussed. On the basis of this model, Corella *et al.* [7] investigated the axial profiles of temperature, and the concentrations of ten different substances (H_2, CO, CO_2, tar, char $\cdots$). However, the details have not been presented.

In this work, biomass gasification with steam in a DFBG is simulated with ASPEN Plus. To deal with the simulations on biomass pyrolysis and the evolutions of tar and char, some subroutines are designed based on relevant empirical equations from literature. The submodels are set up based on the thermodynamics and reaction kinetics. The yield and composition of the syngas, and the contents of tar and char can be calculated from the model. The concerned variables are: structure of the gasifier, gasification temperature (T), steam to biomass mass ratio (S/B), biomass moisture content (M), gasification residence time (τ) and biomass/char particle size (d_p). The model is evaluated against the experimental results measured on a 150 KWth MIUN (Mid Sweden University) DFBG.

2 DFBGs AND THE MIUN GASIFIER

A DFBG consists of two beds. One is blown with steam to gasify biomass and to produce syngas. The other is blown with air to burn char to produce heat. Bed material is circulated to transfer heat from combustion bed to gasification bed. Flue gas is prevented from mixing with the produced syngas. Since air is not injected into the gasifier directly, N_2-free syngas can be obtained. The temperatures in the reactors are maintained by the char combustion and bed material recirculation. Some options for DFBG technology are possible from different combinations of the BFB and the CFB. So far, the most attractive design is supposed to have biomass gasification in the BFB and char combus-

tion in the CFB from the viewpoints of particle circulation, fuel conversion, tar cracking, *etc.* Table 1 presents some well-known DFBGs [1,8–21] and their measurement data. Similar summaries can be found [8,9]. The Blue Tower gasifier is listed for its unique design. As seen in Table 1, the measured H_2/CO ratios range from 0.45 (SilvaGas) to 3.5 (Blue–Tower). The CH_4 concentration is generally around 10.0 vol. %, but fairly low as 4.7 vol. % in the case of Trisaia gasifier. The tar contents range from 0.5 g/Nm^3 (Trisaia, Güssing) to 32.0 g/Nm^3 (MIUN, Milena). The measurement data are scattering in a wide range.

A MIUN gasifier is schematically shown in Fig. 1. The gasifier consists of an endothermic steam fluidised bed gasifier and an exothermal CFB combustor. The biomass treatment capacity is 150 KWth, *i.e.*, approx. 30 kg/h. The heat carrier is silica sand (150 μm, diameter). The bed material circulation is controlled with the air velocity in the combustor, the steam velocity in the gasifier, the total solids inventory, and the aeration in a tube connecting the bottoms of the gasifier and the combustor. The PLC-operated (Process Logic Controller) feeding system is designed for constant biomass feeding. The biomass is fed into a pneumatic oscillatory vane feeder to achieve high precision. The fluidisation agent in the gasifier is steam, and the syngas is drawn off from the top of the gasifier. The residual biomass char is transferred along with bed material into the combustor through the lower pressure lock. In the combustor, the fluidization agent is air participating in the char combustion (950–1050 °C). The hot bed material is separated from the flue gas through a cyclone and recycled into the gasifier through the upper pressure lock (loop seal pot) which is designed to prevent the gas leakage. The heights of the gasifier and combustor are 2.5 m and 3.1 m, and the inner diameters, 300 mm and 90 mm, respectively. It is 0.7 m from the surface of bed material to the distributor, and is about 0.2 m to the feeding point. The experiments were carried out at 750, 800, and 850 °C, respectively. The steam input into the gasifier was held at 4.0 kg/h. Wood pellets are from SCA BioNorr AB. The S/B ratios are 0.3, 0.6, and 0.9, respectively. The details on experiments have been reported elsewhere [8].

3 SIMULATION

ASPEN Plus consists of various sub-models simulating various unit operations. It can be used to model the complicated chemical engineering systems. Equations and data for the calculations are accessed from ASPEN Plus databases. Customized models can be created to extend capability of ASPEN Plus. Here, the module *RGibbs* was mainly adopted. *RGibbs* module performs calculation, according to the *Gibbs* free energy theory. Some subroutines are integrated for simulating biomass devolatilization and the evolutions of tar and char. Relevant empirical correlations [4,5,7,22,23] are adapted and employed in the subroutines. As illustrated in Fig. 2, this model consists of 4 sections. The bed materials are not considered in the phase and chemical equilibria calculations.

Q_{cg} denotes a stream of heat carried by bed material. With respect to tar and char, as nonconventional components, the calculations will be conducted independently from using the database in ASPEN Plus. S/B is calculated according to:

$$S/B = \frac{\dot{M}_{steam} + \dot{M}_{H_2O\ in\ biomass}}{\dot{M}_{dry\ biomass}} \tag{1}$$

where, $\dot{M}$ denotes the mass flow (kg/s). A number of hypotheses for the model are listed:

- the process is of steady state;
- the biomass feedstock and bed materials are fed at an uniform temperature;
- ash as well as bed materials are inert;
- the char particles are spherical and of uniform size;
- the mixing of solid particles is perfect;
- the combustion and gasification of biomass are described by the shrinking core model.

3.1 Drying

In ASPEN Plus, biomass is a nonconventional component. Biomass drying is assumed to be a conversion of a portion of biomass into H_2O and modeled with the modules *RStoic* and *Flash2*. ASPEN Plus assumes that every nonconventional component has a molecular weight of 1.0. 1.0 mole biomass reacts to form 0.0555084 mole water. The equation is:

$$biomass\ (wet) \rightleftharpoons 0.0555084\ H_2O \tag{2}$$

The equation (3) is derived, on the basis of the material balances.

$$CONV = \frac{M^i - M^c}{100 - M^c} \tag{3}$$

$CONV$ indicates the drying efficiency. M^i and M^c denote moisture contents of the biomass before and after being dried, respectively. It is hard to dry the biomass completely. The final moisture content is initially set as 5.0 wt. %.

3.2 Devolatilization

The modules *RYield*, *Sep*, and *Mixer* are adopted. Biomass is assumed to be decomposed into H_2O, Ash, C, H_2, N_2, Cl_2, S and O_2. Carbon partly constitutes the gas phase. A subroutine is designed to calculate the yields. The traces of N_2, Cl_2, and S are ignored in calculation. Biomass devolatilization can be expressed as [7]:

$$C_{4.2}H_{5.8}O_{2.8} \rightleftharpoons a\ CH_{0.85}O_{0.17} + b\ CH_{0.20}O_{0.13} + c\ H_2 + d\ CO + e\ CO_2 + f\ CH_4 + g\ C_2H_4 \quad (4)$$

The moisture content 5.0 wt. % was not considered in the equation (4). The coefficients a–g are not presented in calculation. The molecular formulas, in sequence, are supposed to be biomass $C_{4.2}H_{5.8}O_{2.8}$, tar $CH_{0.85}O_{0.17}$, and char $CH_{0.20}O_{0.13}$.

3.3 Steam reforming

The module *RGibbs* is used. The evolution of CH_4 is simulated with this module as well. In general, low-temperature DFBG and dry ash gasifiers gasification processes do not reach chemical equilibria, while that of high-temperature slagging gasifiers closely approach to equilibria. A function block, *Restricted Equilibrium*, in the module *RGibbs*, is used for calculating the chemical equilibria restricted. A temperature difference needs to be specified in a sub-item, *Entire System with Temperature Approach*, and is specified as 300.0 °C with an optimization route programmed. This temperature difference reflects the difference between the theoretical chemical equilibrium state and the practical state in the gasification process.

3.4 Combustion

The modules *RGibbs* and *Sep* are adopted. The reaction expressions (5) and (6) are referred to for calculating the amount of O_2 for char combustion. The excess air ratio is taken to be 1.24 for combustion.

$$C + 0.9\ O_2 \rightleftharpoons 0.2\ CO + 0.8\ CO_2 \quad (5)$$

$$H_2 + 0.5\ O_2 \rightleftharpoons H_2O \quad (6)$$

3.5 Tar

The yield of tar from biomass devolatilization is expressed as [22]:

$$C^w_{tar}\ [kg/kg\ biomass_{daf}] = 0.35 \times \exp[-3.04 \times 10^{-3} \times (T - 500.0)] \times \exp\{-4.34 \times [\frac{-2.34 \times 10^4}{R \times (T + 273.15)}] \times \tau\} \quad (7)$$

After devolatilization, tar is reformed. The reaction equation is [7]:

$$CH_{0.85}O_{0.17} + 0.15\ H_2O \rightleftharpoons 0.32\ CO + 0.13\ H_2 + 1.2\ C_xH_y \quad (8)$$

The expression (9) is obtained by fitting $r = k \cdot C_{tar}^{m} \cdot C_{H_2O}^{n}$ with the experiment results [8].

$$r_{tar}\ [mol \cdot m^{-3} \cdot s^{-1}] \ = \ 0.66 \times exp[-2904.0/(T+273.15)] \times C_{tar}^{1.31} \times C_{H_2O}^{0.30} \quad (9)$$

3.6 Char

The yield of char from biomass devolatilization is expressed as [7]:

$$C_{char}^{w}\ [kg/kg\ biomass_{daf}] \ = \ 2.09 - 3.47 \times 10^{-3} \times (T + 273.15) + 1.48 \times 10^{-6} \times (T + 273.15)^2 \quad (10)$$

After devolatilization, char experiences gasification. The reaction equation is [7,24]:

$$CH_{0.20}O_{0.13} + 0.87\ H_2O \rightleftharpoons CO + 0.97\ H_2 \quad (11)$$

The kinetic expression is [24]:

$$r_{char}\ [mol \cdot m^{-3} \cdot s^{-1}] \ = \ \frac{C_{H_2O}}{1/k_m + \frac{1}{589.0 \times (T+273.15) \times \exp[-26800.0/(T+273.15)]}} \times \frac{6 \times (1-\epsilon)}{d_p^c} \quad (12)$$

$$d_p^c\ [m] \ = \ [(1 - C_{ash}^{wp}) \times fv_{char}^{c}/fv_{char}^{i} + C_{ash}^{wp}]^{1/3} \times d_p^i \quad (13)$$

in which, $k_m = 0.15$; $fv_{char}^{c}/fv_{char}^{i} = 0.25$; $d_p^i = 0.005$; $\epsilon = 0.50$.

4 RESULT AND DISCUSSION

The variables, T, S/B, M, d_p and τ are examined for their impacts on the DFBG performance.

4.1 Gasification temperature

Fig. 3 shows the effect of the gasification temperature on the syngas quality when S/B, τ, and d_p are given. As seen in Fig. 3 a, the syngas yield increases with temperature as a result of the enhanced gasification and reforming at a higher temperature. Tar content decreases from 50.0 g/m^3 at 750 °C down to about 13.0 g/m^3 at 900 °C due to tar thermal cracking and steam reforming. Char to be combusted is regarded as an intermediate product. The char fraction decreases from 22.5 wt. % at gasification temperature 750 °C to 11.5 wt. % at 950 °C. The lower gasification temperature leads to higher char yield, and subsequently results in higher combustor temperature, hotter bed material, and higher gasification temperature, so that less char will be produced. A

temperature difference is existed between the gasifier and the combustor. The system is auto-stabilising.

As seen in Fig. 3 b, the concentration of CO increases with temperature, but that of H_2 reaches a maximum value at about 850 °C. This is because H_2 pronely takes part in the hydrogenation reactions at higher temperatures. The H_2 concentration is higher than that of CO under the normal DFBG operation conditions, but they will change positions when the gasification temperature is too high above about 950 °C. The CH_4 concentration is around 10.0 vol. % and not sensitive to temperature. CH_4 is highly stable, and much more difficult to be cracked or reformed than tar. Therefore, CH_4 concentration is far from its chemical equilibrium value which is close to zero. Significant reduction of CH_4 takes place at a temperature higher than 1250 °C or with help of catalysts, *e.g.*, nickel-based catalysts.

4.2 Steam/biomass mass ratio

S/B values were calculated with an assumption that the dry biomass has 5.0 wt. % moisture. Fig. 4 shows the effect of S/B on the syngas quality when T, τ, and d_p are given. The tar content decreases from 50.0 g/m^3 at S/B = 0.3 down to about 10.0 g/m^3 at S/B = 1.2 due to the enhanced steam reforming of tar. The char fraction is insensitive to S/B as shown in Fig. 4 a. The syngas yield is in the range of 0.8–1.0 Nm^3/kg daf biomass, and the LHV is about 11.65 MJ/Nm^3. Both calculated data are fairly close to the measurement results from a pilot DFBG plant at Vienna University of Technology [12].

The H_2/CO ratio is a strong function of the S/B ratio, which is primarily controlled by the water–gas shift reaction. The H_2 concentration is higher than that of CO under the normal DFBG operation conditions, but they will change positions when the S/B ratio is too low under about 0.15 as seen in Fig. 4 b. The CH_4 concentration is around 10.0 vol. % and not sensitive to the S/B ratio.

4.3 Biomass moisture content

For an autothermal gasifier, gasification temperature can be held by adjusting the oxygen equivalent ratio. For a DFBG, extra fuel needs to be added in the combustor. Fig. 5 shows that the gasification temperature is difficult to be kept above 850 °C when the biomass moisture content is higher than 15.0 wt. %. Gasification temperature can be raised about 50 to 100 °C when the combusted biomass is 10.0 wt. % of the total biomass feedstock, as seen in Fig. 5.

In Fig. 6, the exact amount of the combusted biomass can be found out corresponding to different biomass moisture content when the gasification temperature is held at 850 °C in 3 cases of S/B = 0.3, 0.6, and 0.9, respectively.

4.4 Biomass particle size

Biomass and coal particles have totally different behaviours, in a thermochemical conversion environment. Coal particles can be described by particle shrinking model, while biomass particles by particle shrinking core model. For a biomass particle, its size is regarded to be kept, but the mass density decreases layer by layer from the surface to the center as the volatile and water vapour flow through the out-layers of char to the outside. Gasification and reforming occur only outside the particle until biomass devolatilization is completed.

Fig. 7 illustrates that the char content in the syngas increases, when the biomass of a bigger size is used. The particle size has little influence on the syngas composition. The fine particle is carried more easily by the gas flow, which will lead to a short residence time and incomplete decomposition. The heat transfer is fast for fine particles.

4.5 Gasification residence time

Fig. 8 shows the effect of the residence time on biomass gasification. It indicates that the residence time is a key parameter. The tar content in the syngas decreases significantly with the residence time. But, char content is insensitive to the residence time. The syngas yield is therefore increased.

4.6 Tar

The prediction shows a decreasing trend of the tar with the gasification temperature and the S/B ratio. Table 2 shows the tar classification [25]. Heavy tar has a boiling point higher than 350 °C. Light tar consists of hydrocarbon compounds with molecular weights in the range of 78–300. The total tar and light tar are measured by gravimetrical analysis and SPA (Solid Phase Adsorption) method, respectively [8]. Fig. 9 shows the co-effects of the gasification temperature and the S/B ratio on the contents of light tar, heavy tar, and total tar, respectively. The total tar and heavy tar decrease with temperature and S/B. The light tar also decreases with S/B, but unlike the total tar, increases with temperature. This is because the heavy tars are cracked to increase the light tar as the temperature increases.

4.7 Model performances

The model predicts that the H_2/CO ratio is strongly dependent on S/B, T, and τ. The H_2/CO ratio is generally greater than 1.0, under normal DFBG operation conditions. The H_2/CO ratios are less than 1.0 in the cases of Chalmers, CAPE, MILENA and SilvaGas gasifiers. This might be due to an extremely low S/B ratio as illustrated in Fig. 4 b. In the case of the MILENA gasifier, the S/B is 0.12 which is low enough to give a H_2/CO under 1.0. With regard to the H_2/CO ratio, the incomplete mixing of steam with biomass volatile is one factor and difficult to be considered in the model.

The tar contents and CH_4 concentrations are low in the cases of Trisaia and Güssing gasifiers. These can be explained by the application of catalysts, which has not been considered in this model. After rough adjustment, the model can make plausible prediction for each gasifier, as described in Table 1.

5 CONCLUSIONS

A mathematic model based on ASPEN Plus is established to simulate biomass gasification in the DFBGs. The model predicts that the content of char transferred from the gasifier to the combustor decreases from 22.5 wt. % of the dry and ash-free biomass at gasification temperature 750 °C to 11.5 wt. % at 950 °C, but is insensitive to S/B. The H_2 concentration is higher than that of CO under the normal DFBG operation conditions, but they will change positions when the gasification temperature is too high above about 950 °C, or the S/B ratio is too low under about 0.15. The biomass moisture content is a key parameter for a DFBG to be operated and maintained at a high gasification temperature. The model suggests that the gasification temperature is difficult to be kept above 850 °C when the biomass moisture content is higher than 15.0 wt. %. Thus, a certain amount of biomass needs to be added in the combustor to provide sufficient heat for biomass devolatilization and steam reforming. Tar content in the syngas can also be predicted from the model, which shows a decreasing trend of the tar with the gasification temperature and the S/B ratio. The tar content in the syngas decreases significantly with gasification residence time which is a key parameter.

NOMENCLATURE

daf—dry and ash-free
LHV—lower heating value, MJ/Nm^3
a–g, k, m, n, x, y—constants
R—the gas constant
Q_{cg}—heat carried by bed material, KW
S/B—the mass ratio of steam to biomass
M—mass flow, kg/s

P—*pressure, atm*
T—*temperature,* °C
τ—*gasification residence time, s*
ϵ—*bed porosity*
K_m—*the maximum value of the mass transfer coefficient, m/s*
fv^c_{char}, fv^i_{char}—*(current and initial) char flow, kg/s*
d_p—*biomass/char particle diameter, m*
$[6 \times (1-\epsilon)]/d^c_p$—*particle density number, 1/m*
M^i, M^c—*moisture content, wt. %*
C—*concentration, mol/m*^{3}
C^{wp}_{ash}—*ash content, wt. %*
C^w_{char}, C^w_{tar}—*concentration, kg/kg biomass*$_{daf}$
r_{char}, r_{tar}—*reaction rate,* $mol \cdot m^{-3} \cdot s^{-1}$

Acknowledgements The author would like to acknowledge the project support of EU regional structure fund, Ångpanneföreningen Foundation for Research and Development, LKAB, Västernorrland Länsstyrelsen, FOKUSERA, Härnösand Kommun, Toyato, SCA BioNorr and SUNTIB.

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the Captions of the Figures and Tables

Figure 1: Schematic diagram of the 150 KWth biomass DFBG at MIUN
Figure 2: Flowsheet of the DFBG biomass gasification model
Figure 3: Effect of temperature on the gasification
(Experiment—MIUN gasifier, wood pellets, sand bed material, S/B = 0.6, τ = 5.0 s, d_p = 5.0 mm)
Figure 4: Effect of S/B on the gasification
(Experiment—MIUN gasifier, wood pellets, sand bed material, 850 °C, τ = 5.0 s, d_p = 5.0 mm)
Figure 5: Effect of biomass moisture content on the gasification temperature
(Experiment—MIUN gasifier, wood pellets, sand bed material, τ = 5.0 s, d_p = 5.0 mm)
Figure 6: Fraction of biomass combusted to hold the gasification temperature
(Experiment—MIUN gasifier, wood pellets, sand bed material, 850 °C, τ = 5.0 s, d_p = 5.0 mm)
Figure 7: Effect of biomass/char particle size on the gasification
(Experiment—MIUN gasifier, wood pellets, sand bed material, 850 °C, S/B = 0.6, τ = 5.0 s)
Figure 8: Effect of residence time on the gasification
(Experiment—MIUN gasifier, wood pellets, sand bed material, 850 °C, S/B = 0.6, d_p = 5.0 mm)
Figure 9: The tar content as a function of temperature and S/B
(Experiment—MIUN gasifier, wood pellets, sand bed material, τ = 5.0 s, d_p = 5.0 mm)

Table 1: Comparison of the simulation results with the measurement data from some DFBGs
Table 2: A typical classification of tar [25] (according to the molecular structures and dew points)