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ZERO-DIMENSIONAL MODELING  
OF INDIRECT FLUIDIZED BED  
GASIFICATION

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# ZERO-DIMENSIONAL MODELING OF INDIRECT FLUIDIZED BED GASIFICATION

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## ABSTRACT

Zero-dimensional models has been developed to investigate mass balance and fuel (biomass) conversion in Chalmers 2-4 MW<sub>fuel</sub> indirect fluidized bed gasifier. The result from this work is that more than 95%<sub>mass</sub> of the tars is converted in the gasifier and that the water gas shift reaction is far from equilibrium.

## INTRODUCTION

Gasification is used to convert solid fuel, such as biomass, into a combustible product gas. The main components of the product gas are H<sub>2</sub>O, H<sub>2</sub>, CO, CO<sub>2</sub>, CH<sub>4</sub> and N<sub>2</sub>. This can be used in downstream processes for the production of, for example, various biofuels. The type of gasification concept investigated in the present work is the indirect fluidized bed gasification technique, where the gasification reactor is heated indirectly, see Fig.1a. At Chalmers a 2-4MW indirect bubbling fluidized bed (BFB) gasifier has been installed in connection to the 12 MW Chalmers circulating fluidized bed (CFB) boiler (1), see Fig.1b. The CFB boiler provides hot bed material to the gasifier through a particle distributor and a particle seal. Another particle seal is located after the gasifier, before the bed material reenters the boiler. The bed material flow through particle seals (fluidized with steam), while mixing of gas between the two reactors are prevented.

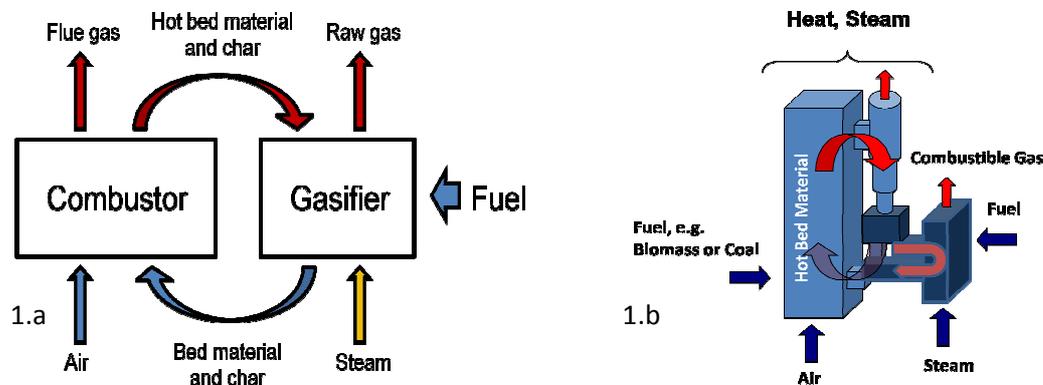


Figure 1.a(Left): Principle of indirect gasification. 1.b(Right): Scheme of the Chalmers gasifier and its integration with the previously existing CFB boiler.

The present work is focused on the use of zero-dimensional modeling to investigate the performance of this type of gasifiers. Here, Chalmers gasifier is compared with the 8 MW gasifier in Güssing (2) and the 100 kW research gasifier at Vienna University of Technology (3). A major difference between Chalmers gasifier and the other two is that the Chalmers gasifier is a retrofit on an existing boiler. The boiler can still be operated as a standalone boiler for heat production only or, with the gasifier in operation, for combined heat and gas production. The combustion part of the system is in this configuration much larger than is needed for the production of the heat for the gasification process, which leads to a more stable operation.

## CHAR CONVERSION

To determine the char conversion, measurements of the gas composition at the surface of the bed were carried out. No fuel (other than char entering from the boiler) was fed to the gasifier; hence the measured gas composition is a result of char gasification. This gives the ratio of char conversion per mass unit of steam. Thus, knowing the mass flow of steam an average rate of char conversion in the gasifier can be estimated, from the measurements performed in this work it was estimated to  $0.05 \text{ kg}_{\text{char}}/\text{kg}_{\text{steam}}$ .

The external solid flux is estimated to  $3 \text{ kg}/\text{m}^2\text{s}$  (corresponding to 25,000 kg/h) based on a correlation (4) where the solid flux is related to primary air flow in Chalmers CFB. The char content in the circulated flow is estimated to 0.25% mass percentage. This is based on measurements from the cyclone leg in experiments using similar fuel and operating conditions as the one used here (5). With this, the char flow entering the gasifier corresponds to 60 kg/h, the steam flow was 270 kg/h, which lead to a char conversion of around 20%.

## MASS BALANCE OVER THE GASIFIER

A mass balance of the gasifier has, here, been established. This mass balance is calculated through a system of equations based on measured and calculated compositions of in and out going flows, as illustrated in Fig.2. The char composition is taken from Thunman *et al.* (6). Furthermore, the composition and mass flow of the dry raw gas and the steam content are measured. Also, leakage into the gasifier is indicated by the presence of nitrogen in the raw gas. These leakages, which can consist of air and/or flue gas, are estimated from the mass balance.

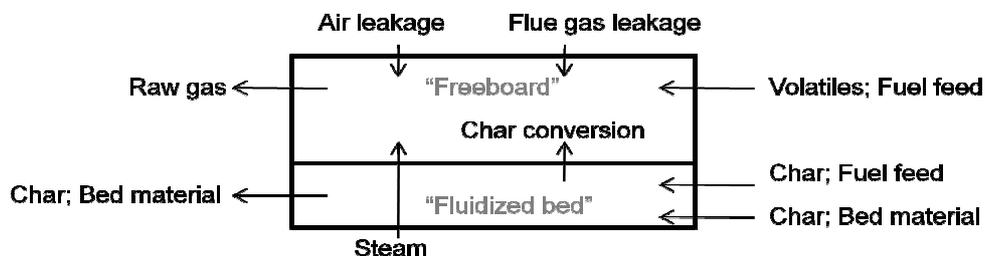


Figure 2. Mass input/output scheme for the Chalmers gasifier. The fuel feeding is illustrated as two streams; one for volatiles and one for char.

## GASIFICATION MODEL

A gasification model has been developed to be used to investigate the performance of the Chalmers gasifier. The model is built on three submodels covering respectively: the conversion of a biomass particle, the composition of the volatiles originated from the fuel particles and the homogenous reactions.

### Particle model

The particle model is based on the conversion of a moist (> 10%) thermally large particle. The rate of the release of volatiles and moisture are given from known input parameters. For further details see (7).

### Volatile Composition

The submodel for the volatile composition is based on the elemental species C,H,O balances together with the energy balance. The product distribution is outlined by means of dry ash free (daf) char and daf volatiles. The volatiles are characterized by CO<sub>2</sub>, CO, H<sub>2</sub>O, H<sub>2</sub>,CH<sub>4</sub>, C<sub>x</sub>H<sub>y</sub> (other light hydrocarbons than CH<sub>4</sub>) and C<sub>n</sub>H<sub>m</sub>O<sub>k</sub> (tars). Input data to this submodel are the C,H,O dry ash free (daf) contents and the heating value of fuel and pyrolytic products. The lower heating value (LHV) of tar is calculated from the C,H,O composition (8). The elemental composition of C<sub>x</sub>H<sub>y</sub> is set to concur with the measured raw gas composition from the Chalmers gasifier.

To close the system of equations the four balance equations are complemented with three empirical correlations.

$$Y_{H_2} = 1,145 \cdot (1 - \exp(-0,0011 \cdot T))^{9,384} \quad (i)$$

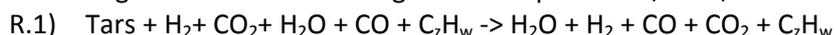
$$Y_{CO} = Y_{H_2} / \left( 0,0003 + 0,0429 / (1 + (T/632))^{-7,228} \right) \quad (ii)$$

$$Y_{CH_4} = -0,0895 + 0,1445 \cdot Y_{CO} \quad (iii)$$

These correlations are derived from data presented by Neves et al (9). The first two correlations are based on the mass ratios H<sub>2</sub> to CO and CH<sub>4</sub> to CO. These two ratios has been found to only depend on the temperature in the range of 700-900°C, hence, independent of particle size, heating rate and reactor type (10). The correlation of the mass ratio of CH<sub>4</sub> to CO is in accordance with data presented in (11). The third closure equation is given by an empirical correlation for the yield of H<sub>2</sub> as a function of temperature (9).

### Homogenous Reactions

The global homogenous reaction of the gasification process is, here, described by:



The above global reaction is here broken down into three parallel reactions:

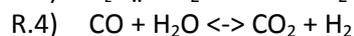
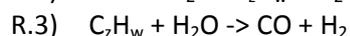
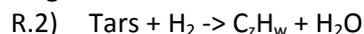


Table 1. Input data gasification model.

Input data	Used value
<u>Process parameters</u>	
Fuel feed	340 kg/h
Steam feed	270 kg/h
Mean bed temperature	791 C
Mean freeboard temperature	766 C
<u>Fuel properties</u>	
Proximate analysis	
Moisture	8.0 %mass (wet fuel)
Char	18.0%mass (dry fuel)
Volatiles	81.7%mass (dry fuel)
Ash	0.3%mass (dry fuel)
Ultimate analysis	
C	49.9%mass (daf)
H	6.1%mass (daf)
O	43.9%mass (daf)
Mean particle size:	8.2 mm
Initial temperature	25 C
Density, wet	1125 kg/m <sup>3</sup>
Thermal conductivity	0,12 W/m K
Specific heat capacity, dry	1000 J/kg K
Emissivity	0,9
<u>Bed material</u>	
Mean particle size	0.27 mm
Density	2650 kg/m <sup>3</sup>
<u>Other</u>	
Fluidization velocity	0.5 m/s
Char conversion	20 %
Leakage	-
C <sub>2</sub> H <sub>w</sub>	C <sub>1,6</sub> H <sub>4,6</sub>
<u>Leakage</u>	
Mass flow flue gas	24 kg/h
Mass flow air	19 kg/h

Table 2. Assumptions for the gasification model.

Assumption;
• the temperature of the bed is uniformed.
• the temperature of the freeboard is homogenous.
• the process operates at steady state.
• the particle size can be represented by an equivalent diameter of a spherical particle.
• fuel nitrogen, sulfur and other minor components are neglected.
• perfect mixture of the gases leaving the gasifier.
• fuel particles undergoing drying and devolatilization float on the bed surface.
• heat transfer reduction due to gases leaving through a particle are neglected
• the composition of volatiles are constant with time.
• longer hydrocarbons C <sub>4</sub> -C <sub>8</sub> around 10g/Nm <sup>3</sup> dry raw gas.

The reactions are controlled by the degree of conversion denoted  $\eta_{tar}$ ,  $\eta_{C_2H_w}$  and  $\eta_{WGSR}$  for R.2, R.3 and R.4 respectively. R.2 describes the conversion of tars and R.3 describes the conversion of C<sub>2</sub>H<sub>w</sub>. Reaction R.4 describes the water gas shift reaction (WGSR). It also balances the products of R.2 and R.3. The degree factors of conversion ( $\eta_{tar}$  and  $\eta_{C_2H_w}$ ) are defined as the ratio of the mass yields of tar and C<sub>2</sub>H<sub>w</sub> in the gas to those predicted in the devolatilization submodel denoted  $Y_{tar,0}$  and  $Y_{C_2H_w,0}$  *i.e.*:

$$\eta_{tar} = 1 - \frac{Y_{tar}}{Y_{tar,0}} \quad (iv)$$

$$\eta_{C_2H_w} = 1 - \frac{Y_{C_2H_w}}{Y_{C_2H_w,0}} \quad (v)$$

The degree of conversion of the WGSR is defined as the degree of equilibrium:

$$\eta_{\text{WGSR}} = \frac{C_{\text{CO}_2, \text{eq}} - X}{C_{\text{CO}_2, \text{eq}}} \quad (\text{vi})$$

where  $X$  represents the mol fraction to be shifted to reach equilibrium and  $C_{\text{CO}_2, \text{eq}}$  is the mol fraction of  $\text{CO}_2$  at equilibrium. The mole fraction  $X$  is calculated from the equilibrium constant,  $K_p$ , of the WGSR reaction as follows:

$$K_p = \frac{(C_{\text{CO}} - X) \cdot (C_{\text{H}_2\text{O}} - X)}{(C_{\text{CO}_2} - X) \cdot (C_{\text{H}_2} - X)} = 33.7 \cdot e^{\left(\frac{-4094}{T}\right)} \quad (\text{vii})$$

where the empirical correlation for  $K_p$  is based on data from (12).

### Input Data and Assumptions for the Gasification Model

Input data for the gasification model are listed in Table 1. The determination of the conversion of char is described above. The composition of  $\text{C}_2\text{H}_w$  is estimated from measured amount of C1 to C3 hydrocarbons in the raw gas, complemented with an approximated amount of longer hydrocarbons ( $\text{C}_4\text{-C}_8$ ). Assumptions made in the model are listed in Table 2.

## RESULTS AND MODEL PREDICTION

The mass balance over the gasifier was closed according to the above-described procedure. The output of the closure was that the leakage mass flows of flue gas and air were 24 kg/h and 19 kg/h respectively. With the input data from Table 1 the composition of the devolatilization products was predicted. The resulting mass fractions in percentage of the volatiles released from the fuel particles are as following;  $\text{H}_2\text{O}$  19.5,  $\text{CO}$  25.0,  $\text{H}_2$  0.9,  $\text{CO}_2$  10.2,  $\text{C}_x\text{H}_y$  3.7,  $\text{CH}_4$  3.7, and "tars" 37.0. The measured composition of the raw gas in mole and mass fraction, with operating conditions according to Table 1, is given in Table 3. The thermo-gravimetric tar analysis gave a tar content of 7 g/Nm<sup>3</sup>.

Table 3. Measured gas composition of the raw gas in percent of volume and percent of mass

Species	$\text{H}_2\text{O}$	$\text{CO}$	$\text{H}_2$	$\text{CO}_2$	$\text{C}_2\text{H}_w$	$\text{N}_2$
Vol %	58.9	12.7	10.0	6.4	6.4	4.2
Mass %	53.8	18.0	1.0	14.3	7.7	5.1

The conversion factors were calculated for the measured raw gas composition in regard to the predicted composition of the devolatilization products, yielding:

$$\eta_{\text{tar}} = 97 \%$$

$$\eta_{\text{C}_2\text{H}_w} = -200 \%$$

$$\eta_{\text{WGSR}} = 42 \%$$

This means that more or less all of the tar compounds leaving the virgin fuel particle were converted to lighter hydrocarbons,  $\text{H}_2$ ,  $\text{CO}$ ,  $\text{CO}_2$  or  $\text{H}_2\text{O}$ . The conversion of the light hydrocarbons is negative, which is due to a larger production of light hydrocarbons from the conversion of tars, here, described by reaction R.2. This production is much larger than

the consumption described by reaction R.3. The conversion factor of the WSGR is a measure of temperature, mixture in the freeboard and residence time of the gases. The value indicates that the gas is rather far from equilibrium, which means that the gas is rich of CO and H<sub>2</sub>O.

## SENSITIVITY ANALYSIS

The closure of the mass balance was found to be very sensitive for variations of the hydrogen content of the fuel and the hydrogen content of the light hydrocarbons (value of  $w$  in C<sub>2</sub>H<sub>w</sub>). In Fig.3 it can be seen how the estimated leakage flows of air and flue gases are influenced by a change of  $\pm 1\%$  of these two input data. The sensitivity of the degree of conversion factors,  $\eta_{tar}$ ,  $\eta_{C_2H_w}$ ,  $\eta_{WSGR}$  was in comparison to these very low, a 10 % change resulted in less than a 10 % response.

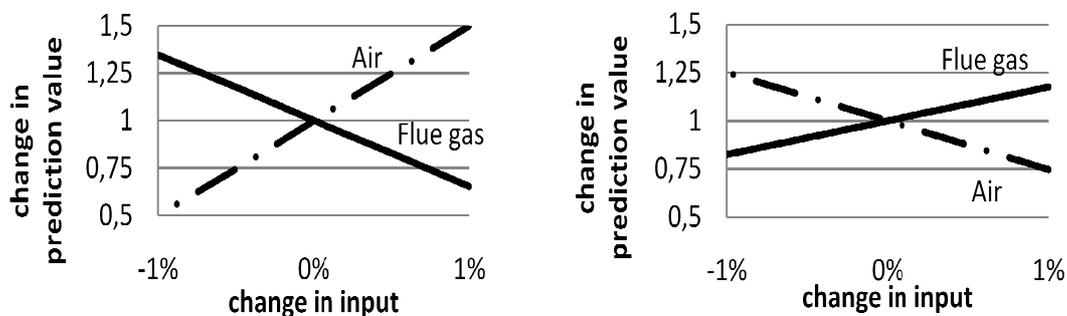


Figure 3. Sensitivity of the mass flows of the leakage of air and flue gas for changes in the H contents of the fuel (left) and composition of C<sub>2</sub>H<sub>w</sub> (right).

## DISCUSSION

The system of equations describing the closure of the mass balance is solvable only within very limited value ranges for some parameters. The most critical parameters identified were the H contents of the fuel, the total amount of H and  $w$  in C<sub>2</sub>H<sub>w</sub>. The composition of the lumped light hydrocarbons is approximated from measurements of CH<sub>4</sub>, C<sub>2</sub>, and C<sub>3</sub>. However, longer hydrocarbons (C<sub>4</sub>-C<sub>8</sub>) are not detected in these measurements, due to the present measurement setup. Therefore, subindices in C<sub>2</sub>H<sub>w</sub> should have slightly higher values than those given by the measurement of C<sub>1</sub> to C<sub>3</sub> as species such as benzene and other hydrocarbons not defined as tars should be included. The strict range of values of the hydrogen contents of the fuel and the light hydrocarbons point out the need for special attention to these parameters. For example, a 0.1% deviation in the content of hydrogen in the fuel will have a significant influence on the mass balance. Also the hydrocarbons should be carefully measured.

From the calculated conversion factors of tars and light hydrocarbons it could be noticed that there are a high conversion of the tars, above 95%. The increase of light hydrocarbons by 200% shows that the major part comes from conversion from tars. It also indicates a slower conversion of the light hydrocarbons than the tars.

Table 4. Comparison of the degree of conversion of the WGSR and values used for calculation.

Species	Chalmers (% mol wet)	100 kW (% mol wet)	Güssing (% mol wet)	Chalmers (% mol dry)	100 kW (% mol dry)	Güssing (% mol dry)
H <sub>2</sub>	10.0	21.6 <sup>3</sup>	24 <sup>3</sup>	24.5	36 <sup>1</sup>	35-45
CO <sub>2</sub>	6.4	11.4 <sup>3</sup>	15 <sup>3</sup>	15.8	19 <sup>1</sup>	20-30
CO	12.7	16.8 <sup>3</sup>	12 <sup>3</sup>	31.2	28 <sup>1</sup>	15-25
CH <sub>4</sub>	4.7	6 <sup>3</sup>	6 <sup>3</sup>	11.6	10 <sup>1</sup>	8-12
N <sub>2</sub>	4.2	<3 <sup>2</sup>	2,4 <sup>3</sup>	10.3	<5 <sup>1</sup>	3-5
H <sub>2</sub> O	58.9	40 <sup>1</sup>	40 <sup>2</sup>	-	-	-
Temperature, (C)	791	800-850 <sup>1</sup>	>800	791	800-850 <sup>1</sup>	>800 <sup>2</sup>
$\eta_{\text{WGSR}}$ (%)	43	65	76	-	-	-

<sup>1</sup> From the work of H.Hofbauer and R.Rauch (3) with a steam-fuel ratio of 0,63 and recalculated to include the water content.

<sup>2</sup> Based on the assumption that the Güssing plant reaches the same water contents as the 100kW research facility using the same steam-fuel ratio 0.6(2), (3).

<sup>3</sup> Recalculated from the mean values for the composition of the dry gas

Finally, the performance on the bases to reach WGSR equilibrium of the Chalmers gasifier was compared with the 100 kW research gasifier at Vienna University of Technolog (3) and the gasifier in Güssing (2). To do the comparison the water content in raw gas from the gasifier in Güssing was assumed to be the same as the one in 100 kW unit. The  $\eta_{\text{WGSR}}$  values are calculated at 800 °C and the results show that the WGSR has gone at least 20 %-units further towards equilibrium in the 100 kW and the gasifier in Güssing than in the Chalmers gasifier, see Table 4. This difference is a consequence of reactor temperature, char conversion, residence time at high temperature for the gas, difference in gas solid contact, difference in bed material and difference in fuel. However, the largest influence is expected to be due to differences in gas solid contact and differences in bed material.

## CONCLUSIONS

The conclusions drawn from this work are

- The presented zero-dimensional models are power full tools to evaluation the indirect gasification process
- The char conversion in the gasifier is approximately 20%
- The leakage of air or flue gas can be estimate by the established mass balance
- The closure of the mass balance is most sensitive to the composition of lumped hydrocarbons and the hydrogen content in the fuel
- The degree of conversion from the predicted volatiles was above 95%<sub>mass</sub> for tars.
- The degree of conversion predicted for the light hydrocarbons is -200%<sub>mass</sub>. The negative value implies an increase of the amount of light hydrocarbons resulting from the conversion of the tars.
- The degree of equilibrium for the WGSR was 42%.
- The WGSR at the Chalmers gasifier is shown to be significant further from equilibrium than has been reported from comparable gasifiers in the litterature

## ACKNOWLEDGEMENT

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## REFERENCES

1. Thunman H, Seemann M, C. First Experience with the new Chalmers gasifier. Proceedings of the 20th International Conference on Fluidized Bed Combustion: 659-663. Xi'an, China, 2009.
2. Hofbauer H, Rauch R, Bauch R. Biomass CHP plant Guessing—a success story. Pyrolysis and Gasification of Biomass and Waste, 2003: p. 371-383.
3. Hofbauer H, Rauch R. Stoichiometric water consumption of steam gasification by the FICFB-gasification process. Progress in thermochemical biomass conversion, 2001: p. 199.
4. Edvardsson E, Åmand L-E, Thunman H, Leckner B, Johnsson F. External Solids Flux Measurements in a CFB boiler. Proceedings of the 19th International Conference on Fluidized Bed Combustion. Vienna, Austria, 2006.
5. Åmand L-E, Lyngfelt A, Karlsson M, Leckner B. Fuel Loading of a Fluidized Bed Combustor Burning Bituminous Coal, Peat or Wood Chips. Report A97-221, Department of Energy Conversion, Chalmers University of Technology, Goeteborg, Sweden, 1999.
6. Thunman H, Niklasson F, Johnsson F, Leckner B. Composition of volatile gases and thermochemical properties of wood for modeling of fixed or fluidized beds. Energy & Fuels 2001;15:1488-1497.
7. Palchonok G, Dikalenko V.I, Kovensky V.I, Leckner B. Mechanisms of Drying and Pyrolysis in Combustion of Wood Cylinder. Proceedings of Nordic Seminar of Thermochemical Conversion of Solid Fuels, Gothenburg, Sweden, 1997.
8. Channiwala SA, Parikh PP. A unified correlation for estimating HHV of solid, liquid and gaseous fuels. Fuel 2002; 81:1051-1063.
9. Neves D, Thunman H, Seeman M, Ideias P, Matos A, Tarelho L, Gómez-Barea A. A database on biomass pyrolysis for gasification applications. Proceedings of the 17th European Biomass Conference & Exhibition: 1018-1028. Hamburg, Germany, 2009.
10. Funazukuri T, Hudgins RR, Silveston PL. Correlation of volatile products from fast cellulose pyrolysis. Ind. Eng. Chem. Process. Des. Dev. 1986;25:172-181.
11. Scott DS, Piskorz J, Radlein D. Liquid products from the continuous flash pyrolysis of biomass. Ind. Eng. Chem. Process Des. Dev. 1985;24:581-588.
12. Kanury A.M. Introduction to Combustion Phenomena, Gordon and Breach Science Publishers, New York, 1977.