

## EXPERIMENTAL MEASUREMENTS AND MODELING USING CESFAMB<sup>TM</sup> SOFTWARE OF THE PRODUCT GAS COMPONENTS ON THE 2MW<sub>TH</sub> GASIFIER PLANT

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Received 2014-09-17; Revised 2014-09-19; Accepted 2014-10-04

### ABSTRACT

The work assesses the performance of a prototype 2MW<sub>th</sub> plant as an auxiliary source of energy based on biomass gasification using wood pellets as a fuel. During steady operation, process temperature, process pressure and concentrations of components in the product gas have been measured the measurements are compared to the simulation results obtained with the CeSFaMB<sup>TM</sup> software. The underlying model in this software is also used to determine the sensitivity of the simulated concentrations to various parameters of the gasification process. The results of modeling are in general agreement with those obtained experimentally.

**Keywords:** Biomass, Gasification, Fluidized Bed, CESFAMB Modeling

### 1. INTRODUCTION

Different approaches in biomass utilization have been pursued during the past decades. For power generation, biomass can be combusted or gasified with use of the product gas for further purposes. Reviews on different aspects of biomass gasification can be found in literature (de Souza-Santos, 2004), including variations of appliances as well as variations of the fuel nature. Results of measurements presented in this study are obtained from a 2MW<sub>th</sub> demonstration plant based on biomass gasification, originally targeting the production of heat and electricity for the VUB campus. The product gas obtained from the fluidized bed gasification plant is mixed with natural gas to externally fire a 500 kWe CHP gas turbine (Marroyen *et al.*, 1999).

Long term tests have been carried out with the fluidized bed gasifier using wood pellets selected on the basis of their market potential and physical properties. During this study some important functionalities of the gasifier have been studied, such as startup and stabilization regimes, feeding system

operation and possible changes concerning those functionalities (Marroyen *et al.*, 1999). In this study the discussion is continued, but the focus is now on the modeling of the gasification process, the influence of physical and chemical properties of the fuel on the gasifier performance as well as on several aspects related to the process parameters.

The purpose of this study is to compare the experimental results to results obtained through simulations and to use the software model to analyze the influence of variations of the input parameters that characterize the gasification of wood pellets in a fluidized bed, on the product gas composition.

### 2. EXPERIMENTAL

The gasifier installation and functioning is thoroughly discussed before (Marroyen *et al.*, 1999). However the main gasifier characteristic, the process operation conditions and the measuring techniques are briefly described in this study. The gasifier has a diameter of 0.8 m and a height of 0.6 m at the fluidized bed section and

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1.2 m and 2.0 m for the freeboard. The reaction temperature and feeding rates of fuel and air passing the fluidized bed section are monitored. A feeding mechanism can deliver the fuel from a storage silo to the fluidized bed with a flow rate between 200 and 300 kg/h. The air factor is estimated in a range between 0.30 and 0.35. The gas velocity is normally set at nearly 10 times the minimum fluidization velocity which is an empirically defined value for providing better mixing and avoiding problems of fuel floating above the bed and agglomeration. With those ranges of the flow rates, steady operation of the installation is attainable producing a gas with an approximate calorific value of 3.5 to 4 MJ/kg (without tars).

The residence time and elutriation of substances are increased inside the freeboard by its expanded volume in favor of the calorific enrichment of the production gases due to the effects of chemical reactions and reduction of carbon losses.

A single cyclone with a maximum capacity of 500 mg/Nm<sup>3</sup> provides filtering of the dust. The gas pressure measured inside the cyclone is about 40 mbar. After passing the cyclone the gas has a temperature above 450°C, sufficient to prevent the condensation of volatiles.

The measuring campaign has been associated with many hours of adjustments and primarily testing. Approximately 70 h of tests with stable gasifier operation have been recorded. Amongst them, several are carried out while the concentrations of the components of the product gas are measured.

The sampling system for concentration measurements is based on the concept used by VTT (Technical Research Centre of Finland) (Ståhlberg *et al.*, 1998). The probe of the sampling line was mounted on the flange attached to the stack after the cyclone. The tip of the probe was provided with the quartz wool filter to prevent the probe duct clogging by solid particles (soot and ashes) which were not separated by the cyclone.

The gas temperature at the probe position measured by a thermocouple was in a range between 450°C and 550°C. Inside the probe, to prevent condensation of tars it has been kept in a range of 200 to 300°C (TC BT/TF 143 WI CSC 03002.4, 2004; Neeft *et al.*, 2002; Van De Kamp *et al.*, 2005).

Four wash bottles of the tar sampling train were placed in a cooling bath at -20°C to avoid losses of volatile compounds. The first bottle was empty and served to condense water. Other bottles were filled with 65 mL of dichloromethane to absorb tars from the gas bubbling through the solvent. The content of the bottles was then analyzed by gas chromatography for tar composition.

The gas sampling line consisted in two wash bottles, an empty one and one filled with sulfuric acid, for tar

and water removal, kept at ambient temperature. The gas samples were then collected downstream in glass bottles for further gas chromatography analysis.

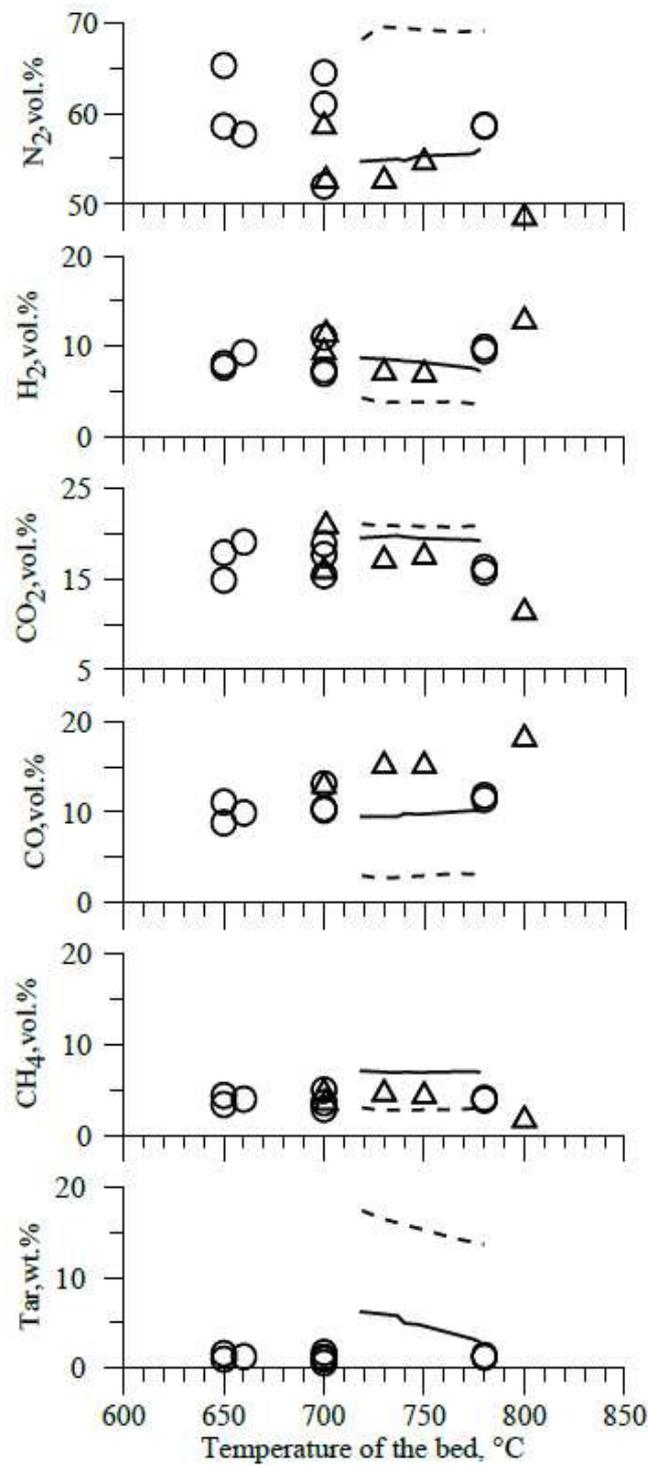
Temperature and pressure measurements with gas-flow measurements were performed in order to determine the total gas volume of the sample.

The sample flow rate was set and controlled at approximately 1 L/min with a valve adjacent to the pump. The sampling was secured by a shut-off valve. Auxiliary valves served to direct the sampling flow either to the tar or gas sampling lines. Sampling typically took 25 min: 15 min for one tar sample and 10 min for two gas samples. After the sampling the content of all bottles was collected together with a final volume of 250 mL using the solvent for rinsing the wash bottles and stored at -25°C shortly before the analysis. Immediately after collecting the samples the glass bottles with the gas free of tar and water were transported to the lab, connected to the Varian 3400 gas chromatograph via a conventional syphon system and analyzed.

### 3. MEASUREMENTS

The results of the measurements performed during the experimental campaign are shown in **Fig. 1**. Those data correspond to the range of the bed temperatures 650-780°C self-established during few hours of the stable gasifier operation which appears to be attributable for the installation throughout the operation campaign and consistent with the given air factor (Maniatis, 1986). Although the temperature is a measured output parameter, it is used on the abscissa axis for convenient comparison of various data. The results of this study are compared to similar experimental results performed by Van den Aarsen (1985) for the points measured between 700 and 800°C. The range of values and scattering of data from both sources are rather consistent with regard to the temperature. The results of Van den Aarsen (1985) obtained for a larger temperature range demonstrates that the scattering of concentration values is greater at lower temperatures. For the present measurements with a given number of data no dependence on the temperature or other observed values could be determined.

The explanations of the scattering could perhaps be found in less intensive decomposition of solid carbonaceous gasification products in this temperature range. Due to partial remaining in the cyclone section or depositing on the feeding system elements the overall carbon balance cannot be precisely determined.



**Fig. 1.** Concentration of main components of the product gas. Open circles-present measurements; open triangles-literature data (Van den Aarsen, 1985); dashed line-simulation

Another cause of the scattering could be the variation in fuel and air flow rates indirectly determined from the rotation speed respectively of the conveyor screw mechanism and the ventilator of the compressor. It could also depend on the intrinsic fuel properties. The overall uncertainty of measurements estimated from the data scattering does not exceed 16% for the gas components and 20% for tar. The conventional error of 50 K for temperature measurements should also be considered.

#### 4. MODELING

The simulation package CeSFaMB™ (formerly CSFMB®) has been used for modeling. It is a comprehensive mathematical model and simulation program for bubbling and circulating fluidized-bed as well as downdraft and updraft moving-bed equipment. Detailed description of the basic principles, assumptions, simulation outputs etc. of the package can be found in de Souza-Santos (2004). The software includes an extensive database of specific classes of solid and liquid fuels devolatilization parameters and data of kinetics for more than 90 chemical reactions comprising the great majority of cases. However, all possibilities cannot be covered because even in a single class of fuel different reaction rates are observed. Those could be due to catalyst or poisoning substances in the fuel matrix (usually in the ash) that lead to changes in reactivity. For instance, the water gas shift reaction and some others very important reactions in the process could be catalyzed by different substances present in the reaction zone from fuel components to ash as well as the reactor walls (de Souza-Santos, 2004; Bustamante *et al.*, 2002). CeSFaMB™ allows users to calibrate the simulator when dealing with such effects. 'Calibration' means that the models used are considered as valid and only model parameters need to be adjusted based on the experimental data. Once the calibration is completed, CeSFaMB™ could provide a valuable input in optimization of the design and performance of the unit.

Mostly it is essential for the gasification cases, because gasification reactions are largely affected by differences in reactivity. For kinetics calibration, the reactions considered by the simulation model can be adjusted by changing the reaction rate coefficients. Usually the pre-exponential factor needs to be adjusted through fitting with reliable experiments. Activation energies and yields of pyrolysis or devolatilization might also be modified. **Table 1** shows the potential impact of the considered reactions. The practical experience is however that many reactions interact and calibration is therefore not a straightforward task.

Stepwise corrections become complex when adjusting several components. It is therefore preferred to apply a multiple regression through least square fitting. Adjustments based on the concentrations of H<sub>2</sub>, CO, CO<sub>2</sub>, CH<sub>4</sub> and tars offer a possibility for maximum 5 parameters, preferably less. After a number of essays and discussions with the developers the calibration has been concentrated on reactions R.5 for methane, R.41 for H<sub>2</sub>/CO and R.50 for tars.

The calibration has been performed as follows. The variations of the molar concentrations  $Y$  can be written as Equation 1:

$$dY_i = \sum_j \frac{\partial Y_i}{\partial x_j} dx_j \quad (1)$$

Where:

$Y_i, I = 1, 5$  are the molar concentrations of H<sub>2</sub>, CO, CO<sub>2</sub>, CH<sub>4</sub> and tars

$x_j, j = 1, 3$  are the logarithms of the pre-exponential factors of reactions R.5, R.41 and R.50

Logarithms are used because in many cases linearity is observed in the dependency of the concentrations towards logarithms of kinetic constants. Expressing the deviation between calculated and observed concentrations can now be approached as Equation 2:

$$Y_i^{obs} - Y_i^{calc} = \sum_j \frac{\partial Y_i}{\partial x_j} \Big|_{calc} (x_j^{new} - X_j^{old}) \quad (2)$$

The derivatives are approached as Equation 3:

$$\frac{\partial Y_i}{\partial X_j} \Big|_{calc} = \frac{(Y_i^{X_j+1} - Y_i^{X_j-1})}{2} \quad (3)$$

If  $i > j$  a least square fit yields the best values for corrected pre-exponential factors through  $x_j^{new}$ . The more experiments are available, the better the fitting.

If the system is linear the optimal solution is found in one step and a recalculation of  $Y_i$  should correspond to the values calculated from Equation 2. If the system is non-linear and/or corrections are important this will not be the case and the procedure must be repeated until convergence is obtained. In practice two to three steps seem required.

The calculated concentrations of the main gaseous components and tar concentration in the product gas are compared to the experimental results in **Fig. 1**.

**Table 1.** Impact of reactions (CeSFaMB™ manual)

Reaction	No	Impact
$\text{CH}_4\text{O}_b\text{N}_c\text{S}_d + \text{H}_2\text{O} \rightarrow \text{CO} + \text{H}_2 + \text{N}_2 + \text{H}_2\text{S}$	R.3	H <sub>2</sub> /CO ratio, C conversion
$\text{CH}_4\text{O}_b\text{N}_c\text{S}_d + \text{CO}_2 \rightarrow \text{CO} + \text{H}_2\text{O} + \text{H}_2 + \text{NH}_3 + \text{H}_2\text{S}$	R.4	CO/CO <sub>2</sub> ratio
$\text{CH}_4\text{O}_b\text{N}_c\text{S}_d + \text{H}_2 \rightarrow \text{CH}_4 + \text{H}_2\text{O} + \text{NH}_3 + \text{H}_2\text{S}$	R.5	H <sub>2</sub> /CH <sub>4</sub> ratio
Tar → Char2	R.14	Tar content
$\text{CO} + \text{H}_2\text{O} \leftrightarrow \text{CO}_2 + \text{H}_2$	R.41	H <sub>2</sub> /CO ratio
Tar → Gases	R.50	Tar content
$\text{Tar} + \text{H}_2 \rightarrow \text{CH}_4 + \text{Other light gases}$	R.51	Tar, H <sub>2</sub> /CH <sub>4</sub> ratio

It can be seen that, without calibration three gaseous components H<sub>2</sub>, CO and CH<sub>4</sub> are underestimated in the simulations and the calculated tar content is much higher than the experimental values. After calibration, the CeSFaMB™ software is able to reproduce relatively well the product gas components defined in the experimental tests. The simulations have been performed under the condition of 2% of the maximum deviation for the convergence of fixed-carbon in the bed. The overall accuracy for the simulated gas components is estimated to be below relative 10%.

The simulated values correspond to an air factor between 0.3 and 0.35 covering the temperature regime 720-780°C. Deviation of few experimental temperatures from that regime could be perhaps explained by the above mentioned temperature measuring error as well as uncertainties on the indirect estimation of the air factor. In general, the simulated temperature regimes of the gasification are in agreement with the measured values. It is also seen from **Fig. 1** that the simulated values of the gas components generally correspond to the experimental results. Even though the tar concentration is reduced, it remains overestimated if compared to the experimental measurements. Throughout the routine inspection of the gasifier equipment a certain amount of solid matter has been found in the cyclone section. It consists of the fly ash and some quantities of carbonaceous compounds, which could not be measured. The tar associated with those found quantities can to some extent explain the difference between modeling and experiments. The simulation results also show that the transport disengaging height exceeds the total reactor height. This means that certain amounts of solid substances are entrained out of the reactor. Different sorts of wood pellets can be used during exploitation of the gasifier. It is obvious that the properties of the wood pellets vary from one pattern to another (ECN Phillys database) and the impact of different parameters on the simulation results can be anticipated. The recommendations on the properties of the wood pellets are defined in national

standards and their variations and margins are thoroughly described in different sources (DIN 51731, 1996; ÖNORM M7135, 2000; ASAE 269.4, 1991). However entire information for a particular fuel is not always available. Also uncertainties when defining its properties in laboratory are unavoidable (Rabier *et al.*, 2006). Therefore the sensitivity of the CeSFaMB™ modeling output to several fuel variations as well as to some process parameters has been analyzed in this study.

The considered properties were estimated according to literature data (Rabier *et al.*, 2006; Audigane *et al.*, 2012) and applied in a realistic range. They include the bulk density, apparent and true densities (densities of a pellet respectively with and without voids), size of fuel particles and moisture content. Among the gasification conditions the wall thermal conductivity responsible for the heat losses and the air factor are considered. **Table 2** represents the results of the sensitivity of the concentrations of main components in the flue gas and the gasifier temperature obtained by varying several selected parameters. Since all parameters significantly differ from zero the sensitivities are defined as ratios of the relative change of the output and input parameters,  $(\Delta y/y)/(\Delta x/x)$ . The values in the table have signs indicating the decrease or increase of simulated concentrations with the parameter change. The determined tendencies are valid however only for the particular case with this fixed set of input data. Due to the complexity of the process, another set of the input data can change the sensitivity values and their signs.

Regarding the fuel properties, a stronger impact is observed for the particle density, particle size and moisture content. The air factor, being one of the most important parameters in the gasification process, also influences the modeling results, as expected. The variations of the simulated component concentrations of the product gas and gasification temperature are consistent with the range of measured values. The impact of other parameters is rather limited or negligible. Hence, particle size and density might be

of certain importance when looking into the gasification of a biomass fuel. However the data for those parameters are often only estimative. **Table 4** shows modeling results for different representative fuels at similar gasification conditions. The characteristics of the wood pellets produced during the same time period by the same supplier have been selected from the ECN Phillys database. Parameters introduced to the modeling input

include the proximate analysis, the ultimate analysis and the Higher Heating Value (HHV) of **Table 3**.

Obviously, as seen from **Table 4** the variation in fuel composition could affect the concentrations of the product gas components. However those variations are quite noticeable, the results of modeling, as in the previous case with the fuel physical properties and the gasification parameters, correspond to the ranges of measurements.

**Table 2.** Influence of varying fuel properties and the air factor on the flue gas components concentrations and temperature of the gasifier

Input para-meter	App. density kg/m <sup>3</sup>	True density kg/m <sup>3</sup>	Size mm	Mois-ture	Air factor
Vary-ing range	1250-1350	1400-1500	4-5	7-10	0.30-0.35
H <sub>2</sub> sens.	0.3800	-0.2900	<0.01	0.01	-1.160000
N <sub>2</sub> sens.	-0.0600	0.0100	0.01	0.05	0.170000
CO sens.	0.4300	-0.3400	-0.06	-0.36	0.430000
CO <sub>2</sub> sens.	-0.1600	0.2800	0.01	0.12	-0.110000
CH <sub>4</sub> sens.	0.0700	-0.0500	-0.04	-0.16	-0.130000
Tar sens.	-0.0600	-0.09 00	0.23	0.36	-3.650000
T <sub>bed</sub> sens.	-0.0600	-0.0100	-0.03	0.03	0.570000
T <sub>fb</sub> sens.	0.0200	-0.0100	-0.03	-0.10	0.810000

**Table 3.** Ultimate and proximate analysis of the representative patterns of the wood pellets applied for the modeling input

Pattern	1	2	3
<b>Proximate analysis</b>			
Moisture, wt. %	7	7	11.00
Ash, wt. %	0.20	0.100	0.600
Volatiles, wt. %	76.4	75.80	72.70
Fixed C, wt. %	16.4	17.10	15.70
<b>Ultimate analysis</b>			
Carbon, wt. %	47.1	48.33	48.62
Hydrogen, wt. %	6.74	6.120	6.270
Nitrogen, wt. %	45.8	45.31	44.40
Sulfur, wt. %	0.15	0.130	0.100
Oxygen, wt. %	0.01	0.010	0.010
Ash, wt. %	0.20	0.100	0.600
<b>Calorific values, dry sample</b>			
HHV, kJ/kg	19315	19762	20515

**Table 4.** Influence of the fuel composition on the flue gas component concentrations and temperature of the gasifier

Pattern	1	2	3
Air factor	0.35	0.35	0.35
H <sub>2</sub> , %	7.5	7.7	7.8
N <sub>2</sub> , %	56.2	56.3	55.9
CO, %	10.0	9.0	10.2
CO <sub>2</sub> , %	19.2	20.0	19.4
CH <sub>4</sub> , %	6.8	6.7	6.3
Tar, wt.%	3.0	3.5	3.7
T <sub>b</sub> , C	778	801	798
T <sub>fb</sub> , C	677	603	596

## 5. CONCLUSION

The gas component concentrations from the simulation model and the experiments are in good agreement. The influences of several essential input data parameters on the main gas products of the fluidized bed gasification of wood pellets are examined and discussed.

Uncertainties in controlling the fuel and air feeding rates could explain the scattering of measured temperatures and concentrations of the syngas components.

Result of modeling could be useful for optimization and adjustment of gasification of biomass under fluidized bed conditions.

## 6. ACKNOWLEDGEMENT

This study was supported by the EU Seventh Framework Program, Grant agreement No TREN/FP7EN/219062 "Polystabilat". Authors are grateful to prof. M.L. de Souza-Santos for advices about the CeSFaMBTM software.

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