PREDICTION OF GAS COMPOSITION IN BIOMASS GASIFIERS

Alberto Gómez-Barea[a]*, Henrik Thunman[b], Bo Leckner[b], Manuel Campoy[a], Pedro Ollero[a]

[a] Chemical and Environmental Engineering Department. Escuela Superior de Ingenieros (University of Seville). Camino de los Descubrimientos s/n. 41092-Seville. Spain
* corresponding author: Tel.: +34 95 4487223; e-mail address: agomezbarea@esi.us.es
[b] Department of Energy and Environment. Chalmers University of Technology
S-412 96 Göteborg, Sweden

Abstract

A method is proposed to estimate gas composition in biomass gasifiers. Equilibrium prediction is extended by incorporation some actions: (1) a pseudo-empirical prediction of the yields of char, tar and methane from the flaming pyrolysis processes and, (2) estimations of the unconverted fractions of these three components in the char reduction zone by means of rate models. Comparison with equilibrium predictions proves that the method improves considerably the results, showing the convenience of the method for preliminary design and simulation of biomass gasifiers.

1. Introduction

Knowledge of the main components of the gas produced in a gasifier is a key factor for preliminarily design. Modelling of biomass gasifiers (BG) is, however, a complex task, especially in fluidised beds (FB). Existing advanced models developed for BG require complex calculations and often difficult to get physical and kinetic inputs. Simple and reliable semi-empirical methods are often enough for first estimation prediction during the design phase. Equilibrium models (EM) have been widely used for this porpoise because they are simple to apply and independent of gasifier design [1]. Nevertheless EM for BG at atmospheric pressure overestimates the yield of H_2 and CO, whereas it underestimates the yields of CO_2. It predicts a gas that is nearly free of CH_4, free of tars and with no char. Therefore, this type of model does not seem to be accurate enough for design porpoises. Quasi-equilibrium models (QEM) aim at making these calculations more realistic, but in general they are difficult to apply under system conditions different from those for which the models have been developed. [2] and [3] applied this concept aiming at simplifying the process description but some essential inputs need to be estimated or correlated from pilot plant experiments. The objective of the present work is to develop a QEM with wider prediction capability for estimation of gas composition (including tar) and unconverted char in the outlet streams.

2. Model

Approach. The model is developed to calculate the gas yields of permanent (light) gases (CO, H_2, CH_4, CO_2, H_2O, N_2), char and heavy hydrocarbons from available parameters: fuel characteristics, reactor temperature, reactor design and kinetic data. **Figure 1** illustrates the procedure followed to solve the problem. The initial devolatilisation and subsequent oxidation of gas and char take place in the so-called Flaming Pyrolysis Zone (FPZ). The FPZ provides the composition of the gas entering the Char Reduction Zone/Process (CRZ), where the char gasification reactions occur, also indicated in **Figure 1**. The model is based on the following steps:

Step 1. Estimation (experimentally or by modelling) of the yield of light gases (including CO, CO_2, H_2O, H_2, CH_4, N_2), char and tar from the FDZ. With this, we can estimate the yields: $x_{char,\mathrm{FDZ}}$, $x_{Tar,\mathrm{FDZ}}$, and $x_{CH4,\mathrm{FDZ}}$.

Step 2. Development of a corrected equilibrium model: formulation of C-H_2-O_2-N_2 mass balances together with the two equilibrium relationships imposed by the WGSR and SRMR. Methane, tar and char are removed from this analysis, because an equilibrium calculation would yield almost zero concentrations for these three components under the operating conditions of interest.

Step 3. Estimation of the conversion of tar, methane and char in the CRZ: X_{tar}, X_{CH4} and X_{char}. Simple kinetic models are developed to achieve this goal. Initial conditions for these three sub-models are the estimations of Step 2.

Step 4. Here, Step 3 corrects the equilibrium results from Step 2. The heat balance over the gasifier is solved taking into account the components added in Step 3 to the composition calculated in Step 2.

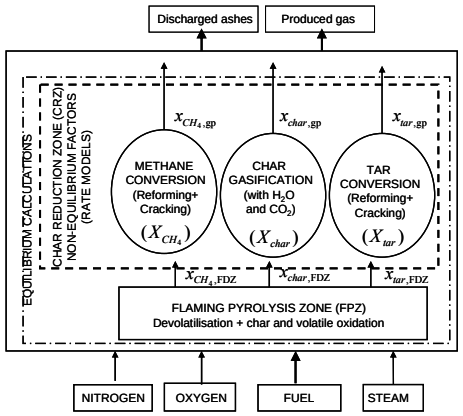

Figure 1. Schematic of the modified equilibrium model

Estimation of yields during FPZ of the fuel ($x_{char,\mathrm{FDZ}}$, $x_{Tar,\mathrm{FDZ}}$, $x_{CH4,\mathrm{FDZ}}$). Figure 2 illustrates an FB where the devolatilisation is assumed to occur in the bottom part of the bed. In the figure, both the FPZ and the CRZ are displayed. Emphasis is on showing that: (1) the FPZ includes the OZ, indicated by the dashed line, (2) the product from the FPZ is the initial condition for the CRZ, where the char reacts with H_2O and CO_2.

A simple version of a more general model [4] is used here based on the following assumptions: (1) char conversion in the oxidation zone (OZ) is neglected. The char produced during devolatilisation ends up in the CRZ; (2) Hydrogen and CO consume completely the oxygen, and methane and tar are not converted in the OZ. (3) The change of moles in the OZ is small compared with the one occurring during fuel devolatilisation. By these three assumptions the FPM can be approximately represented by devolatilisation yield from experiments reporting the yields of tar, methane and char.

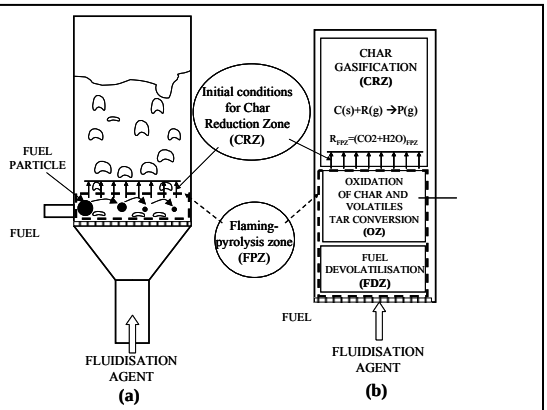

Figure 2: (a) Physical situation in an FB (b) Model representation and identification of the different zones

Methane and tar conversion models (X_{tar}, X_{CH4}). Methane and tar conversions are calculated by simple kinetic models, assuming one-phase flow of the gas in the CRZ as

$$X_i = \frac{\mathrm{Da_i}}{1+\mathrm{Da_i}} \qquad \mathrm{i}=CH_4, \mathrm{Tar}$$

$$(-r_i) = k_i \cdot C_i, \quad k_i = A_i \cdot \exp\left(-E_i / R_g T\right) \cdot C_{H_2O}^{n_i} \quad (1)$$

Table I. Kinetic parameters for equation (1)

i	A_i	E_i (kJ/mol)	n_i
tar	$1 \cdot 10^4$ (s^{-1})	100	0
CH_4	$3 \cdot 10^8$ (m^3/kmol/s)	125.5	1

The dimensionless parameter Da is Damköhler number defined as the rate of reaction over the spatial velocity in the reactor: $\mathrm{Da_i}=k_i\tau_{\mathrm{CRZ}}$. The kinetic parameters for evaluation of k_i for cracking of tar and methane are shown in Table I

Char conversion model (X_{char}). The CRZ is modelled assuming the simplified reaction system employed by [5]. H_2O and CO_2, and H_2 and CO are lumped into the same pseudo-components, R and, P

respectively. As a result, the only heterogeneous reaction in the CRZ is Char + R → P. This reaction is assumed to occur in the emulsion phase where most of char particles are found. The rest of bulk gas is regarded inert in the CRZ, since no homogeneous reactions other than WGSR are considered. The recent method for general gas-solid reactions in [6] is applied to calculate the char conversion.

3. Results: validation and discussion

The model developed was compared with experiments conducted in the 150 kW_{th} bubbling fluidised-bed gasifier (BFBG) at atmospheric pressure situated in the University of Seville. Various biomasses and gasification agents have been tested along the years and the main results have been published elsewhere: Orujillo air-blown tests [7], MBM air-blown gasification [8] and air-steam gasification tests with wood pellets [9]. Here, for illustration these latter experimental results are compared with model results. Table 1 includes the main parameters that are most useful to assess a typical gasification test. For comparison results applying EM are included. As seen the model presented here improves significantly the prediction with regard CH_4, CO, H_2 and CO_2. In addition tar and char yields are well predicted. This prediction, however, is much dependant on the kinetic model chosen for modelling the tar conversion processes in the CRZ. This must be select carefully by screening literature data. Main aspect for selection is: nature of biomass and operating conditions at which the kinetics data has been obtained, particularly the heating rate, peak temperature and residence time. The data for this simulation tests where taken from [10]. Finally note the good estimation in the carbon content in the discharged ashes and in the gas yield. This latter is poorly predicted by EQ because the char are assumed to be completely gasified. As seen this is far from being real and again, the QEM developed here give excellent agreement.

Table II. Comparison of the method (first column) with experimental results (second column) and purely equilibrium prediction (third column)

	Units	**This method**	**Equilibrium**	**Pilot results**
CO	% vv	15.0	24.5	14.3
CO_2	% vv	17.2	7.1	18.5
H_2	% vv	12.5	25.5	11.9
H_2O	% vv	12.5	5.5	11
CH_4	% vv	4.5	0.0	5.1
N_2	% vv	51	40	52
$C_kH_lO_m$ (tar)	g/Nm^3	12	0.0	12.5
$F_{gp,d}$ (Gas yield)	mole gas/kg fuel daf	2.1	2.4	2.1
$x_{C,ash}$	kg_C/kg_{da}	0.32	–	0.28
CC (tar included)	%	91.5	100	92.5

4. Conclusion and significance

A model has been developed to predict the performance of biomass gasifiers. The model adopts the framework of quasi-equilibrium models (QEM) and further uses simple rate sub-models to adjust typical deviations from equilibrium. The model improves the existing QEM in the sense that essential information, such as char, tar and methane conversion are estimated as part of the model. This aspect makes the method predictive, in contrast to other QEM.

Nomenclature

A	frequency factor, $m^3 \cdot kmol^{-1} \cdot s^{-1}$
C	gas concentration, $mol \cdot m^{-3}$
Da	Damköhler number, –
E	Activation energy $kJ \cdot mol^{-1}$
k	n^{th}-order kinetic constant, $(mol/m^3)^{1-n} \cdot s^{-1}$
n	order of reaction, –
P	gasification product is P ($P = H_2 + CO$)
R	gasification agent is R ($R = CO_2 + H_2O$)
T	temperature, K
x	mass fraction on dry, ash-free fuel, $kg/ kg_{fuel(daf)}$
X_{tar}	conversion of tar in the CRZ
X_{CH4}	conversion of methane in the CRZ
X_{char}	conversion of char in the CRZ
$x_{char,FDZ}$	yield of char from FPZ
$x_{tar,FDZ}$	yield of tar from FPZ
$x_{CH4,FDZ}$	yield of methane from FPZ
$x_{C,da}$	carbon content in discharged ash, $kg/ kg_{fuel(daf)}$.
τ	gas residence time, s

References

[1] S. A. Scott, A. T. Harris, J.S. Dennis, A. N. Hayhurst and J. F. Davidson. Gasification of biomass: the consequences of equilibrium. *17th International fluidized bed combustion conference, Jacksonville, Florida, USA* (2003).

[2] N. Jand, V. Brandani and P.U. Foscolo. Thermodynamic Limits and Actual Product Yields and Compositions in Biomass Gasification Processes. *Ind. Eng. Chem. Res*., 45 (2006), p. 834-843.

[3] X. Li, J. R. Grace, A. P. Watkinson, C. J. Lim and A. Ergüdenler. Equilibrium modelling of gasification: a free energy minimization approach and its application to a circulating fluidized bed coal gasifier. *Fuel,* 80 (2001), p. 195–207.

[4] A. Gómez-Barea, B. Leckner and P. Ollero. An engineering model for devolatilisation and oxidation in Biomass Gasifiers. *Submitted for publication* (2007)

[5] J. A. Britten. Extinction phenomena in countercurrent packed bed coal gasifiers: A simple model for gas production and char conversion rates. *Industrial & Engineering Chemistry Research,* 27 (1988), p. 197–203

[6] A. Gómez-Barea. B. Leckner and M. Campoy. Approximate prediction of gas-solid conversion in fluidized bed reactors. *Fluidization XII. May 2007. Vancouver, Canada*. Paper 78.

[7] A. Gómez-Barea, R. Arjona and P. Ollero. Pilot plant gasification of olive stone: a technical assessment. *Energy & Fuels*, 19 (2005), p. 598-605.

[8] A. Gómez-Barea, M. Campoy, P. Ollero and C. Fernández-Pereira. Pilot plant experiences with fluidised bed gasification of orujillo and MBM. *Proceedings of 19th International Conference on Fluidised Bed Combustion. May 21–24, 2006, Vienna, Austria*. Paper 66.

[9] M. Campoy, A. Gómez-Barea and P. Ollero. Gasification of wood in a fluidised bed — an assessment of autothermal operation using air and low temperature steam mixtures. *Submitted for publication* (2007)

[10] F. G. van den Aarsen. Fluidised bed wood gasifier. Performance and modelling. *Ph.D. Dissertation, Twente University Publication. University of Twente*. 1985