



CARBON CONVERSION PREDICTOR FOR FLUIDIZED BED GASIFICATION

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ABSTRACT

There is increased interest in biomass gasification for production of a gas which can substitute for fossil fuel. High system efficiency requires good carbon conversion in the gasifier. When a solid fuel particle is injected into a hot fluidized or fixed bed, the reactivity of the resulting char in gasification reactions (between char carbon and steam and CO₂ as well as the inhibiting reactions of product gases H₂ and CO) play a significant role in reaching good carbon conversion. In this paper, the gasification reactivity data of biomass chars, as measured in TGA experiments, is used for the determination of kinetic parameters for char carbon gasification reactivity correlations. The complicated ash-carbon interactions during char gasification are currently being studied. Laboratory measured reactivity values from TGA experiments are used in the Carbon Conversion predictor to simulate carbon conversion in a real scale fluidized bed gasifier. The predictor is a relatively simple and transparent tool for the comparison of the gasification reactivity of different fuels in fluidized bed gasification. Also a three-zone model for fixed bed gasification has been developed, based on models and parameters from the literature. Simulations with the models against some pilot-scale results show reasonable agreement.

Keywords: Fluidized bed gasification, fixed bed gasification, char reactivity, modeling, thermogravimetric analyzer

1 Introduction

The stages of gasification of a solid fuel are drying, pyrolysis and char oxidation. In most cases the slowest part of fuel conversion in a gasification reactor or gasifier, is the oxidation of the fuel char by the gasification products CO₂ and H₂O. The oxidation rate of the char is affected by process temperature, pressure, the behavior of ash, the partial



pressures of reactant gases CO_2 and H_2O and the gaseous components H_2 and CO which have some inhibitive effects [1, 2, 3].

There are many types of gasification reactors. In this paper, models for fluidized bed and fixed bed gasifiers are presented. Figure 1 shows the basic principles of these reactors.

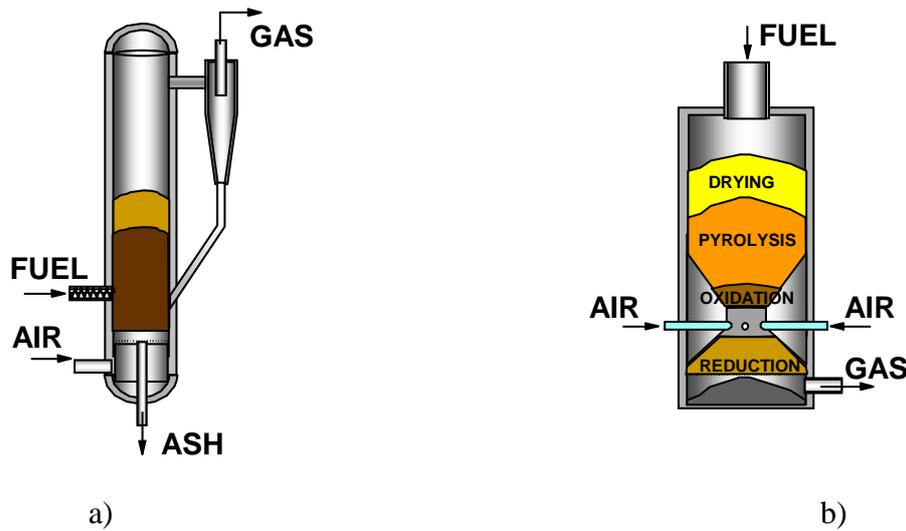


Figure 1: Schematic figures of gasification reactors, a) fluidized bed gasification and b) fixed bed (downdraft) gasification. [1]

In the Carbon Conversion Predictor model, laboratory measured reactivity numbers are converted into carbon conversion numbers relevant to a fluidized bed gasifier.

In the first version of the model, this conversion has started by extracting from the thermogravimetric analyzer (TGA) runs kinetic parameters of the following equations [3, 4]:

$$R_{\text{C-H}_2\text{O}} = \frac{k_{1f} P_{\text{H}_2\text{O}}}{1 + \frac{k_{1f}}{k_3} P_{\text{H}_2\text{O}} + \frac{k_{1b}}{k_3} P_{\text{H}_2}} \quad (1)$$

$$R_{\text{C-CO}_2} = \frac{k_{1f} P_{\text{CO}_2}}{1 + \frac{k_{1f}}{k_3} P_{\text{CO}_2} + \frac{k_{1b}}{k_3} P_{\text{CO}}} \quad (2)$$

where k_{1f} ($\text{s}^{-1} \text{bar}^{-1}$), k_{1b} ($\text{s}^{-1} \text{bar}^{-1}$) and k_3 (s^{-1}) are kinetic constants and P_{CO_2} , P_{CO} , $P_{\text{H}_2\text{O}}$ and P_{H_2} are the partial pressures (bar) of CO_2 , CO , H_2O and H_2 . These equations describe the reaction rates of biomass fuel char in gasification reactions. They are used as parts of the Carbon Conversion Predictor (“kinetic parameters for char”), Figure 2 a).

The predictor is a relatively simple and transparent tool for the comparison of the gasification reactivity of different fuels in fluidized bed gasification.



In fixed bed downdraft gasification, the gasification process is conceived to follow a particular sequence of drying, pyrolysis, oxidation and reduction process, and this notion is well comprehended in modeling of fixed bed gasification (Figure 2 b). Drying and pyrolysis that comprises of a sub-model is formulated based on empirical and stoichiometric equilibrium modeling approach. Oxidation (partial) process is also framed on stoichiometric equilibrium model, whereas the sub-model for reduction process is established on finite kinetic modeling approach. Reduction process is accredited with an essential phenomenon during gasification process and encompasses several gasification reactions. [5, 6] Thus, the model can be used to analyze the influence of moisture content and equivalence ratio on the product gas composition, heating value and carbon conversion. Moreover, the model may help in optimizing the gasification process in a downdraft gasifier.

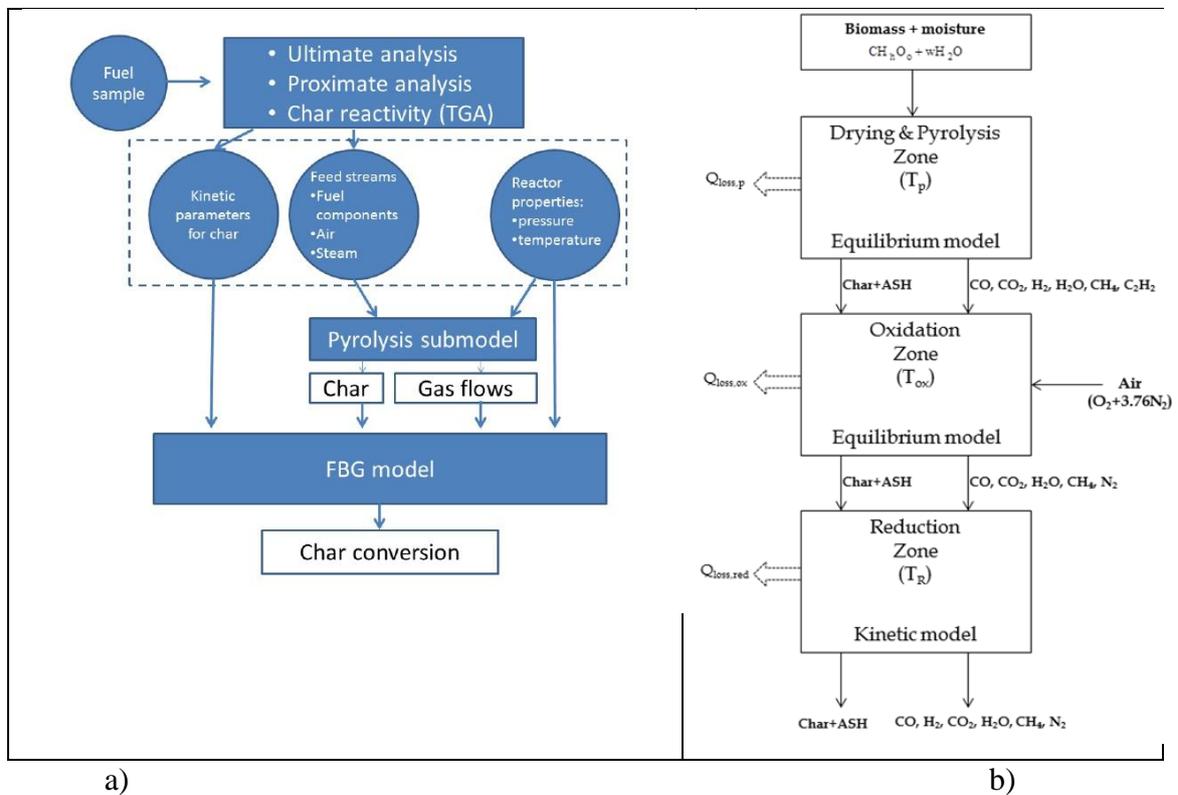


Figure 2: Principles of the a) Carbon Conversion Predictor for fluidized bed gasification and b) three-zone model for fixed bed gasification.

With the use these kind of simplified modeling approaches the problems of more complicated models can be avoided. The problems of some models based on the thermodynamical equilibrium (Gibbs energy minimization), as well as on fluidization hydrodynamics were discussed in Kontinen et al. [3].

In this paper the basic principles of the developed models for fluidized bed and fixed bed gasification are presented, as well as recent developments and examples of results.



2 Experimental / Methodology / Approach

Solid biomass and waste samples have been tested in a Thermogravimetric Analyzer (TGA) at atmospheric pressure [2, 3]. In the TGA, a solid biomass sample is heated up from room temperature to temperatures of 750-950 °C and its weight is monitored continuously. Gasification occurs by letting reactive gases H₂O or CO₂ in contact with the sample. The governing gasification reactions are the following:



Thus the solid carbon of the fuel char reacts with the gases. The measured weight loss is used to determine the rate of reaction.

For the Carbon conversion predictor, the most interesting results from the TGA tests are the instantaneous reaction rates as function of fuel conversion. Figures 3 and 4 show how the TGA data is converted to oxidation rate data.

The instantaneous reactivity values from the TGA results are determined using the following equation [2, 3]:

$$r'' = \frac{1}{w} \frac{dw}{dt} \quad (5)$$

where dw/dt is the rate of change of mass loss curve (mg/s) and w is the instantaneous ash-free weight (mg). Figure 4 shows the instantaneous char reactivities as function of carbon conversion. As carbon conversion increases above 95%, the rate for several of the fuels increases significantly, possibly due to an increased concentration of catalytic ash forming elements.

In this paper, the averaged reactivity data is used for modeling. The principle of averaging is presented in [2, 3].

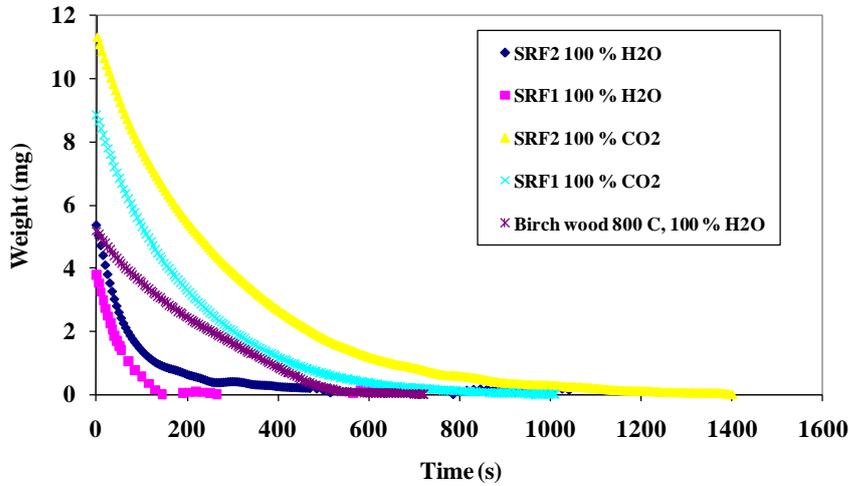


Figure 3. Mass loss curves from TGA experiments in CO₂ and H₂O atmospheres. (SRF = Solid recovered fuel). [3]

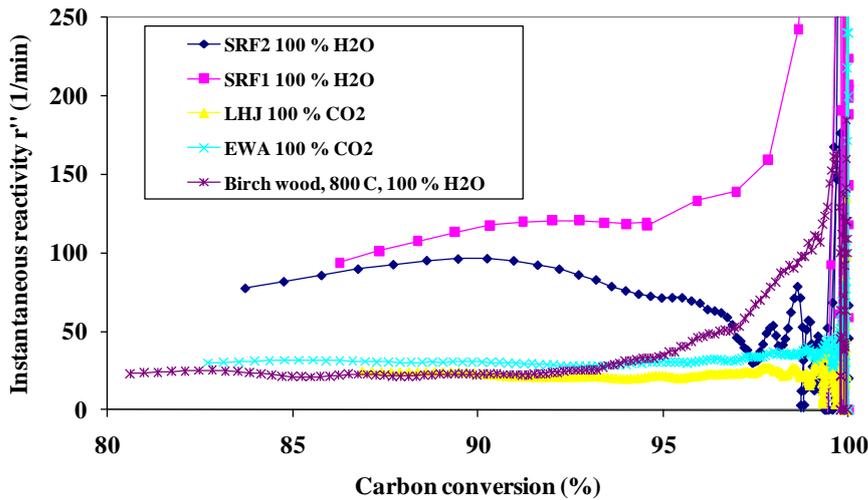


Figure 4. Instantaneous reaction rates for various fuels, obtained from the TGA data in Figure 2. [3]

2.1 Fixed bed modeling approach [5, 6]

The sub-model for drying and pyrolysis zone are established based on empirical assumptions and the composition of pyrolysis products are greatly affected by the assumptions made on association of C-H-O in a biomass. Then, the pyrolysis products are subjected to enter oxidation zone where some of pyrolysis products especially char and hydrogen are partially oxidized /combusted. It is assumed that equilibrium state exists in all kind of chemical reaction though equilibrium may not be achieved in practice. Therefore, such assumptions may elevate the degree of uncertainties of present equilibrium modeling work. The products of oxidation zone are assumed to enter the reduction zone, where several gasification reactions have been incorporated as depicted in Table 1. The reduction zone is modeled based on finite kinetic approach.



Table 1. Gasification reactions and kinetic model of associate reactions [5, 6]

Reactions	Reaction rate (mol/m ³ .s)
Boudouard reaction: C + CO ₂ ↔ 2CO	$r_1 = C_{RF}A_1 \exp\left(\frac{-E_1}{RT}\right) \cdot \left(y_{CO_2} - \frac{y_{CO}^2}{K_{eq,1}}\right)$
Water-gas reactions: C + H ₂ O ↔ CO + H ₂	$r_2 = C_{RF}A_2 \exp\left(\frac{-E_2}{RT}\right) \cdot \left(y_{H_2O} - \frac{y_{CO} \cdot y_{H_2}}{K_{eq,2}}\right)$
Methane formation: C + 2H ₂ ↔ CH ₄	$r_3 = C_{RF}A_3 \exp\left(\frac{-E_3}{RT}\right) \cdot \left(y_{H_2}^2 - \frac{y_{CH_4}}{K_{eq,3}}\right)$
Steam reformation: CH ₄ + H ₂ O ↔ CO + 3H ₂	$r_4 = A_4 \exp\left(\frac{-E_4}{RT}\right) \cdot \left(y_{CH_4} \cdot y_{H_2O} - \frac{y_{CO} \cdot y_{H_2}^3}{K_{eq,4}}\right)$

The kinetic model for the gasification reactions are of Arrhenius type and are greatly affected by the temperature (T) of the gasifier as well as equilibrium state of the reactions involved. In the reaction rate equation, C_{RF} refers to char reactivity factor, A & E are the kinetic parameters, y_i is the mole fraction of the chemical species involved in the gasification process. Then, the rate of reaction for each species can be determined. For example, the rate of formation or destruction of CO can be estimated as; R_{co} = 2r₁ + r₂ + r₄. The reduction zone is partitioned into n number of compartment. The concentration of any species at first compartment is taken from the output of oxidation zone and the concentration in the consecutive compartment is determined as:

$$n_i^n = n_i^{n-1} + \left[\frac{1}{v_{n-1}} \left(R_i^{n-1} - n_i^{n-1} \frac{v_n - v_{n-1}}{\Delta z} \right) \right] \times \Delta z \quad (6)$$

where n_i is the concentration of i species, ‘n-1’ refers to previous compartment, R_i is the rate of formation of i species, v is the gas flow rate and Δz is the length of nth compartment. Thus, the concentration of each gaseous species involved in gasification reaction can be estimated with the help of Eq. (6).

3 Modeling

3.1 Fluidized bed gasification

The Carbon Conversion Predictor results for a coal, a biomass and two solid recovered fuels (SRF1 and SRF2) are compared in Figure 5. The Figure shows the comparison as carbon conversion versus the residence time parameter (τ_C), which is defined here as [3]:

$$\tau_C = \frac{M_{Cbed}}{m_{Cf}} \quad (7)$$



where M_{Cbed} is the total carbon inventory of the gasification fluidized bed in gasification zone (g) and m_{Cf} is the carbon in fuel feed (g/s).

The results of Figure 5 show that the tested solid recovered fuels (SRF) require the shortest residence time for char particles in fluidized bed gasifier to reach reasonable carbon conversion. The longest residence time is required by coal char particles. This is largely due to high volatiles yield of SRF and biomass. When comparing the curves of wood and SRF, char gasification rates seem to have some importance, resulting in slightly lower residence times for wood to reach 100 % conversion.

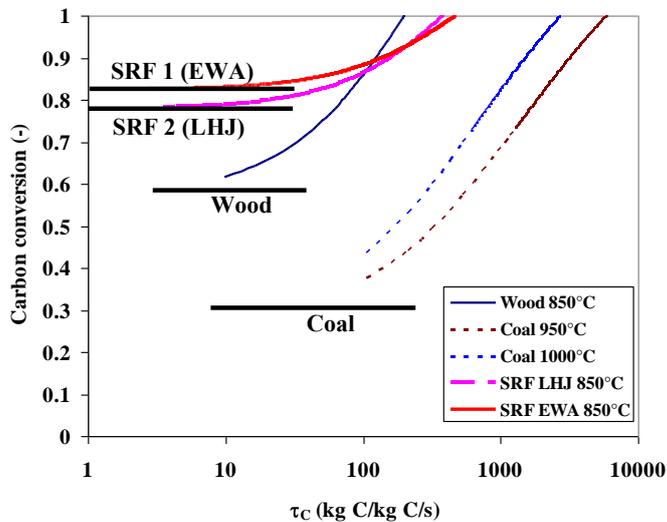


Figure 5. Carbon conversion in fluidized bed gasification as function of the carbon residence time parameter (τ_c). Wood, coal and SRF fuels at temperatures 850-1000°C, $\lambda = 0.27$ and 1.013 bar. Preliminarily reported in [3].

In the predictor, it is assumed that all volatile carbon reacts instantaneously (i.e. residence time of 0 seconds), which form the initial level of fractional carbon conversion, marked separately with a thick horizontal line in Figure 5 for wood (about 0.56), for coal (0.28) and for and SRF 1 (0.83) and SRF 2 (0.78).

Improvements to the Carbon Conversion predictor are currently being implemented. Figure 6 shows updated results from the predictor for biomass char conversion using improved residence time and conversion correlations which were developed by Gómez-Barea and Leckner [7]. These new correlations allow for the accounting of carbon lost to fly and bottom ash.

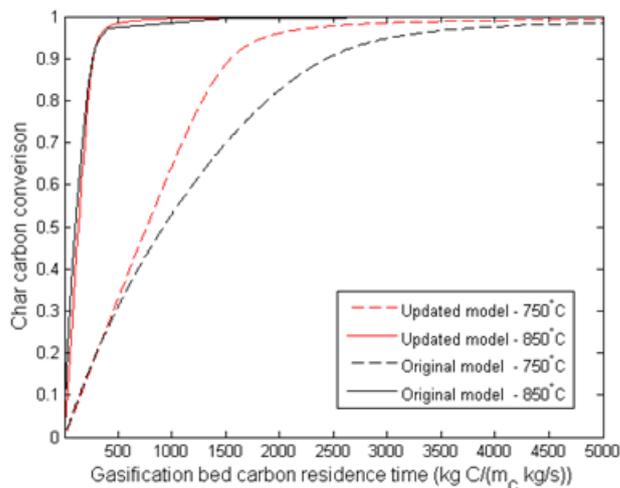


Figure 6. Char carbon conversion as a function of residence time in the gasifier. The updated model includes the residence time and conversion relations presented in [7].

Improvements to the modeling of the gasification kinetics are also underway in order to account for the effect of the interactions between char carbon and fuel ash. Dupont et al. [8] has done similar work to account for the interaction of K and Si. It can be expected that these kinds of interactions will decrease the required residence times to reach 100 % carbon conversion, from those presented in Figure 5.

3.2 Fixed bed gasification

Figure 7 shows the comparison of modeled product gas composition to the experimental results of Jayah et al. [5]. It is apparent from the Figure 7 that present model holds a good validation against experimental results, as the average accuracy for prediction of product gas composition is ~90%. The data label shown in Figure 7 refers to absolute error in prediction of corresponding gaseous species. Thus, the model may be employed to identify the optimal parameters of moisture content and equivalence ratio for downdraft gasification process.

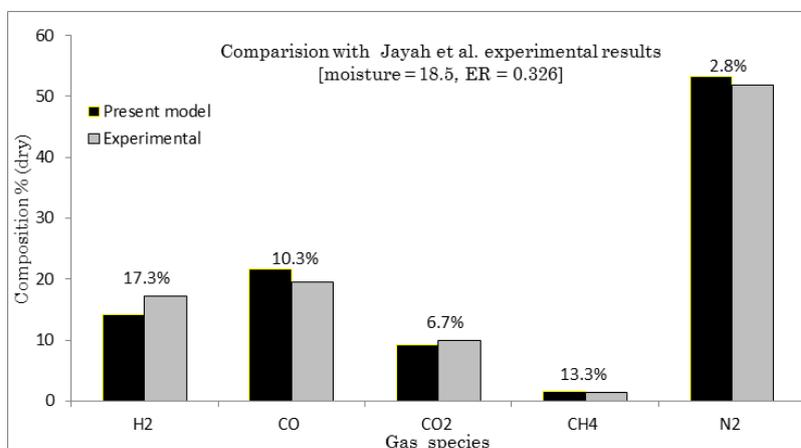


Figure 7. Composition comparisons with experimental data of Jayah et al. [5, 6]. The data label refers to absolute error in prediction of corresponding gaseous species. (ER = equivalence ratio).



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