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Gasification of Continuous Wood Char Bed: Modelling and Experimental Approach

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The current paper presents a study combining experimentation and modelling of char gasification in a continuous fixed bed reactor. The char bed gasification was experimentally characterized using the Continuous Fixed Bed reactor (CFiB) at CIRAD (Montpellier, France). This reactor replicates the gasification zone taking place in the co-current, multi-stage gasification technology. It is instrumented to specifically allow the measurement of thermal and chemical profiles: measurements of temperature, pressure, and gas composition are performed every 10 cm along the bed. We also investigate the char bed compaction during gasification. For this purpose, a char bed sampling was carried out to measure char bed density and particle velocities along the char bed. A model of wood char gasification in a continuous fixed bed reactor was thus developed using COMSOL software. It couples heat and mass transfer phenomena with heterogeneous and homogenous chemical reactions taking place inside the bed. In particular, this model considers char bed compaction to predict evolution of char bed density and velocity. As an innovative approach, three simple functions to calculate char particle conversion rate of the heterogeneous reactions were proposed.

1. Introduction

Gasification has been shown to have a high potential for biomass energy production. Various forms of energy such as electricity, heat, or biofuels can be produced. Different types of technologies including fluidized or fixed bed, entrained flow, in single or staged reactors are now available commercially. The choice generally depends on the application and the size of the plant.

Whatever the technology used, gasification reactors involve a successive or simultaneous series of thermal processes, mainly biomass drying and pyrolysis, oxidation of pyrolysis gases, and char gasification. Achieving complete carbon conversion is mainly controlled by the heterogeneous reactions that occur between the char produced during the pyrolysis stage, and the reacting gases such as H_2O, CO_2 and O_2:

$$C + H_2O \rightarrow CO + H_2 \quad \text{Steam gasification} \quad (1)$$

$$C + CO_2 \rightarrow 2CO \quad \text{Boudouard reaction} \quad (2)$$

$$C + O_2 \rightarrow CO / CO_2 \quad \text{Combustion} \quad (3)$$

In staged gasification, pyrolysis and char gasification take place in separate reactors allowing independent control of each step. The pyrolysis gases are oxidized in a high temperature zone where efficient tar cracking can occur. The outlook for staged gasifiers is optimistic because less tar is produced compared to other processes.

At the moment, many different gasifier models are available according to the literature, i.e. (Di Blasi, 2004) and (Wang et al., 2007). Those describing the char gasification zone isolated from the rest of the reactor

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are less common, in particular (Babu and Sheth, 2006) and (Dasappa and Paul, 2001). However, such models are necessary for the precise prediction of char behaviour and syngas production.
Char gasification models consist in solving mass, energy, and momentum balance equations in the multi-phase media. Balance equations require source terms that provide local production or consumption rates of species and heat.
Regarding the heterogeneous reactions (Eq.1 to 3), the mass/heat source terms can be calculated directly from the particle conversion rate of the char particles At the present time, two types of sub-models are commonly used to calculate these particle conversion rates:

- (Mermoud et al., 2006) have developed a complex sub-model of char particle gasification that solves all the balance equations at particle scale. These sub-models allow a fine description of the phenomena involved at particle scale. Nevertheless, these codes are too time consuming. They are not thus practical for optimization or design purposes.
- (Di Blasi, 2004) and (Mandl et al., 2010) have developed a simple sub-model that is the most widely used solution to express the source terms. This solution simplifies char bed modelling as no description is required at particle scale. This approach will be applied in our work.

Furthermore, char gasification models have to consider compaction to describe the evolution of char bed density and velocity. This phenomenon is a major determining factor in terms of design and operation of the process. Indeed, when compaction occurs the char residence time increases. This change has a direct impact on the process efficiency (carbon conversion) and control (pressure drop).
The model we are developing aims to take this phenomenon into account in order to accurately describe char bed behaviour. The objective of this paper is to present the methodology set up to describe and optimize a continuous downdraft wood char bed reactor. First we present the experimental reactor and the fixed bed model. Then we discuss the experimental and numerical results.

2. Experimental

2.1 Production and characterization of Wood Char Chips (WCC)

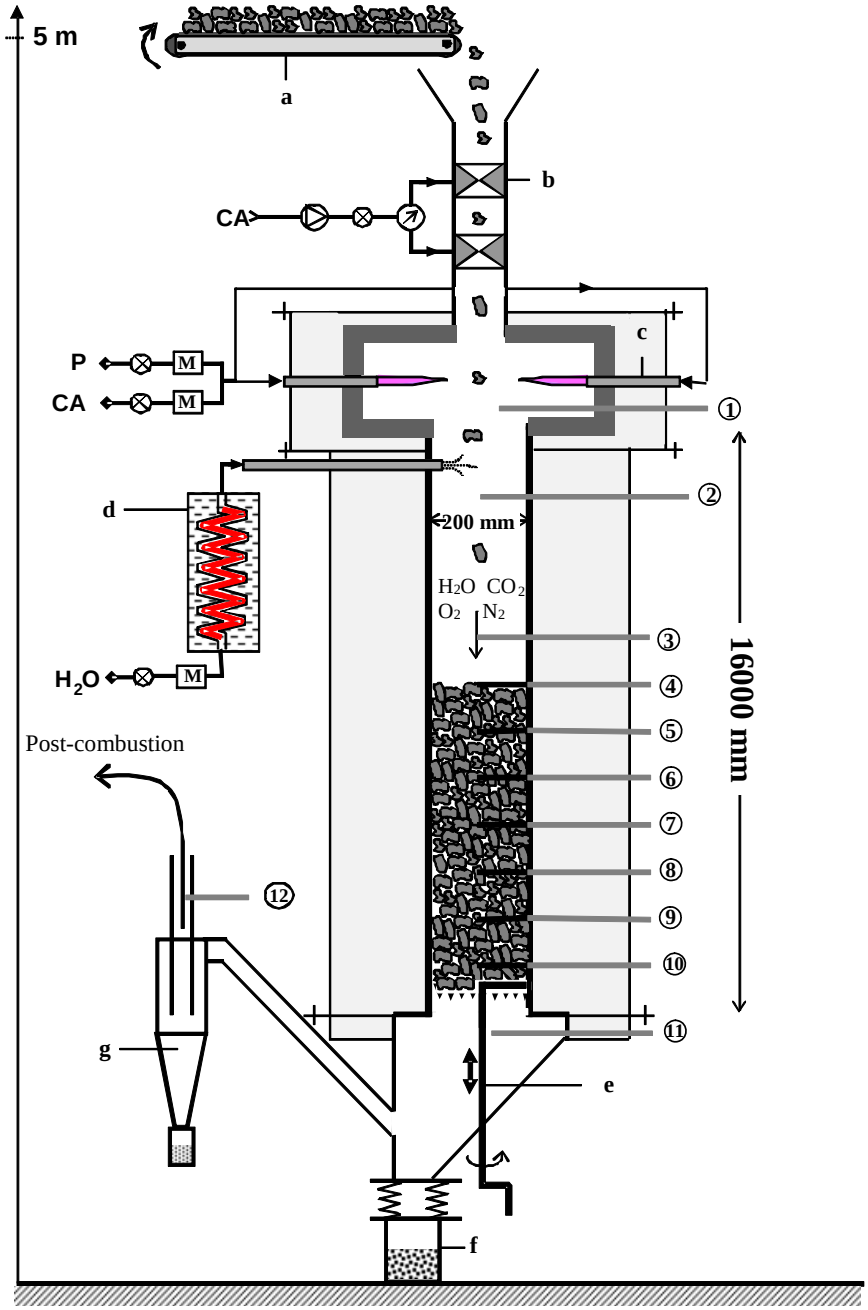
The initial sample used consisted of maritime pine wood chips delivered from the Cevennes region (France). This feedstock produced the char for the present study using CIRAD ‘s screw pyrolysis reactor (Fassinou et al., 2009). The operating conditions for the char production were as follows: residence time 1h; temperature 750 °C; flow rate 15 kg.h^{-1}. Composition and properties of the wood chips and the char produced are presented in Table 1.

Table 1: Proximate and ultimate analysis of the woodchips from maritime pine

Material	***Proximate analysis*** *(wt% dry basis)*			***Ultimate analysis*** *(wt% dry basis)*					**LHV** (MJ.kg^{-1} dry basis)	**Char bed bulk density** (g.cm^{-3})	**Particle density** (g.cm^{-3})
	Ash	Volatile matter	Fixed carbon (by difference)	C	H	O	N	S			
Wood chips	0.4	83.1	16.5	49.2	6.3	<0.1	45.2	<0.2	18.6	-	-
Char chips	1.7	4.0	94.3	92.6	1.0	0.2	3.8	<0.2	33.4	0.13	0.33

2.2 The CFIB reactor

The Continuous Fixed Bed reactor (CFiB) was designed and built at CIRAD (Fig. 1). The gasification chamber consists of a 310 type refractory steel tube (200 mm i.d., 1 600 mm long) surrounded by refractory wool insulation. The control of the process is an important point that has already been described and discussed in a previous paper (Van de Steene et al., 2010). Briefly, the gasifying stream is generated by two propane burners (c) and a superheated steam generator (d). Propane, air and water flow rates are accurately adjusted by flow meters/controllers so that the gasifying stream can be carefully controlled in terms of gas species concentration and temperature after combustion. The char mass flow rate is regulated by a conveyor belt (a). During the operation, the bed height is maintained at a constant level with the removal of the solid residue at the bottom (e), which is adjusted accordingly.
The instrumentation of the equipment is a key point. Sampling and measuring probes are located at 10 cm intervals along the length of the char bed allowing direct analysis of temperature, pressure and gas composition. A char bed sampling was brought to the apparatus allowing detailed information on char behaviour along the bed in terms of char conversion, ash content density and velocity. The sampling method is described in details elsewhere (Teixeira et al., 2012). Briefly, char bed sampling principle consists of quenching and cooling the reactor at the end of an experiment and then collecting the bed in several horizontal layers thanks to a suction system.



(a) Conveyor belt
(b) Pneumatic valve
(c) Propane burner
(d) Steam generator
(e) Ash removal system
(f) Collecting box
(g) Cyclone
ⓘ Temperature /pressure /
(CA) Compressed Air
(P) Propane
(M) Mass flowmeter/controller

Figure 1: The CFiB reactor

3. Model

A stationary model of char gasification in a continuous fixed-bed reactor was developed by the team (Teixeira, 2012). It is implanted in COMSOL version 3.5a, using 1D geometry. In the following, we present briefly the model. Modelling a continuous char bed during gasification should take into account all the phenomena involved at both bed scale and particle scale. This multi-scale approach requires a bed model and a particle sub-model. The main inconvenience is that the built-in process codes are too time consuming. For this reason, balance equations are solved at bed scale: the complexity of the

transformation at particle scale is assessed using functions for the determination of char conversion rate of the heterogeneous reactions. Char bed compaction is assessed using an empirical compaction function.

3.1 Governing equations

Momentum balance equation

The Darcy relationship was used to describe laminar gas flow through a porous medium:

$$-\overrightarrow{\text{grad}}\,\mathbf{P}_\eta = \frac{\mu_\beta}{K_\eta}\cdot\vec{\mathbf{U}}_\beta \tag{4}$$

Eq. 4 is coupled with the continuity equation, which expresses gas compressibility:

$$\text{div}(C_{\beta/\eta}\cdot\vec{U}_\beta) = St_g \tag{5}$$

The ideal gas law is used to express molar concentration of gas species $C_{\beta/\eta}$:

$$C_{\beta/\eta} = C_\beta\cdot\varepsilon_{inter} = \frac{P_\eta}{R\cdot T_\eta}\cdot\varepsilon_{inter} \tag{6}$$

Energy balance equation

Mermoud (Mermoud et al., 2006) and Van de Steene (Van de Steene et al., 2011) showed that char particle gasification was not limited by heat transfers in our operating conditions. This is why local thermal equilibrium is considered. Energy balance equation thus becomes:

$$\left((C_{\beta/\eta}\cdot\overline{Cp}_\beta\cdot\vec{U}_\beta)+(C_{\sigma/\eta}\cdot\overline{Cp}_\sigma\cdot\vec{U}_\sigma)\right)\cdot\overrightarrow{\text{grad}}\,T_\eta - \text{div}(\lambda_\eta\cdot\overrightarrow{\text{grad}}\,T_\eta) = Q_{tot} \tag{7}$$

Mass balance equation for the gas phase

For a gas species j, mass balance equation is given by Eq. 11:

$$\text{div}(C_{j,\beta/\eta}\cdot\vec{u}_\beta) - \text{div}(D^*_{j,N2}\cdot C_{\beta/\eta}\cdot\overrightarrow{\text{grad}}\,x_j) = St_j \tag{8}$$

Eq. 8 groups together 7 equations for the 7 species N_2, O_2, CO_2, H_2O, CH_4, CO and H_2 present in the gas phase.

Mass balance equation for the solid phase and char bed compaction

Compaction is the consequence of a number of coupled chemical and mechanical phenomena, which are not generally considered in existing models. The following mass balance equation was used:

$$\text{div}(C_{\sigma/\eta}\cdot\vec{U}_\sigma) = St_C \tag{9}$$

Eq. 9 is coupled with an empirical equation expressing solid phase velocity as a function of char conversion X (Teixeira, 2012).:

$$V_\sigma(X) = V_{\sigma,0}\cdot f(X) \tag{10}$$

$$f(X) = -1.03\cdot10^{-4}\cdot X^2 + 4.25\cdot10^{-4}\cdot X + 1 \tag{11}$$

3.2 Chemical reactions

For heterogeneous reactions (Eq. 1 to 3), St_i is calculated from the apparent reactivity of a char particle. This term considers all phenomena at particle scale during gasification: chemical reactions and heat/mass transfers. This apparent reactivity is calculated using a an apparent reactivity function determined from a numerical particle model, described in (Mermoud et al., 2006) ;Van de Steene et al., 2011) that enables the prediction of the char particle conversion rate under various gasifying operating conditions:

$$St_i = f(P_j, T, e_p, \varepsilon, A_i) \tag{12}$$

The char characteristics A_i, e_p and ε are supposed to take into account the influence of char's nature, size and structure on the reactivity. Detailed information are available in (Teixeira, 2012).

For a homogeneous reaction, i.e water gas shift reaction and methane reforming, St_i is classically expressed according to bibliographic data (Teixeira, 2012).

The production/consumption rate of energy for the reaction *i* is given by Eq. 13:

$$Q_i = \Delta H^T_{r,i}\cdot St_i \tag{13}$$

4. Experimental data versus numerical results

Table 2: Operating conditions at the bed surface

Reacting gas								
H_2O	CO_2	O_2	N_2	Gas velocity	Solid Char	Temperature	Gas velocity in free board	Total pressure
28 %vol;	8.2 %vol.	2.7 %vol.	61.1 %vol.	0.7 $m.s^{-1}$	28 $g.min^{-1}$	1028°C	0.7 $m.s^{-1}$	1.0 atm.

Table 2 shows the operating conditions which have been adjusted to fit with industrial gasifiers.
In Figure 2-a, the coefficient of variation (CV) – defined as the ratio of the standard deviation to the mean between experimental data and model results – is less than 2%. Given the complexity of the mechanism involved and the uncertainties in experimental measurements, this low value is quite acceptable when the aim is predicting char bed gasification. Final char conversion is reached at 38 cm and 55 cm for the model and the experiment respectively.
Concerning the profiles of temperature (Figure 2-b), the coefficient of variation was less than 2 % as well. Regarding experimental results, In the first 10 cm the bed temperature decreases to 850 °C and decreases slowly through the rest of the bed. This result confirms the presence of a highly reactive zone in the top of the bed where endothermic reactions of char gasification by H_2O and CO_2 are predominant. Below this zone, the low temperature slows down the endothermic gasification reaction by H_2O and CO_2 consequently slowing down the decrease of bed temperature.
While that of the H_2 concentration profile (Fig. 2-c) along the bed was less than 6 %. In Figure 2-d, results show that the model overestimates the CO concentration along the bed: numerical data are higher than those of the experiment of about 11%. This could be explained by the presence of volatile matter in the feedstock (4 %wt - Table 1): they are not considered in the model. This uncertainty is nevertheless acceptable since it corresponds roughly to the accuracy of the experimental results. The profiles of CO and H_2 show a decrease of CO concentration from 35 cm while H_2 concentration increases. In this zone, the model reveals that heterogeneous reactions are very slow. Only water gas shift reaction is responsible for CO consumption and H_2 production.
In Figure 2-e, the coefficient of variation, for char bed bulk density, was also less than 6 %.

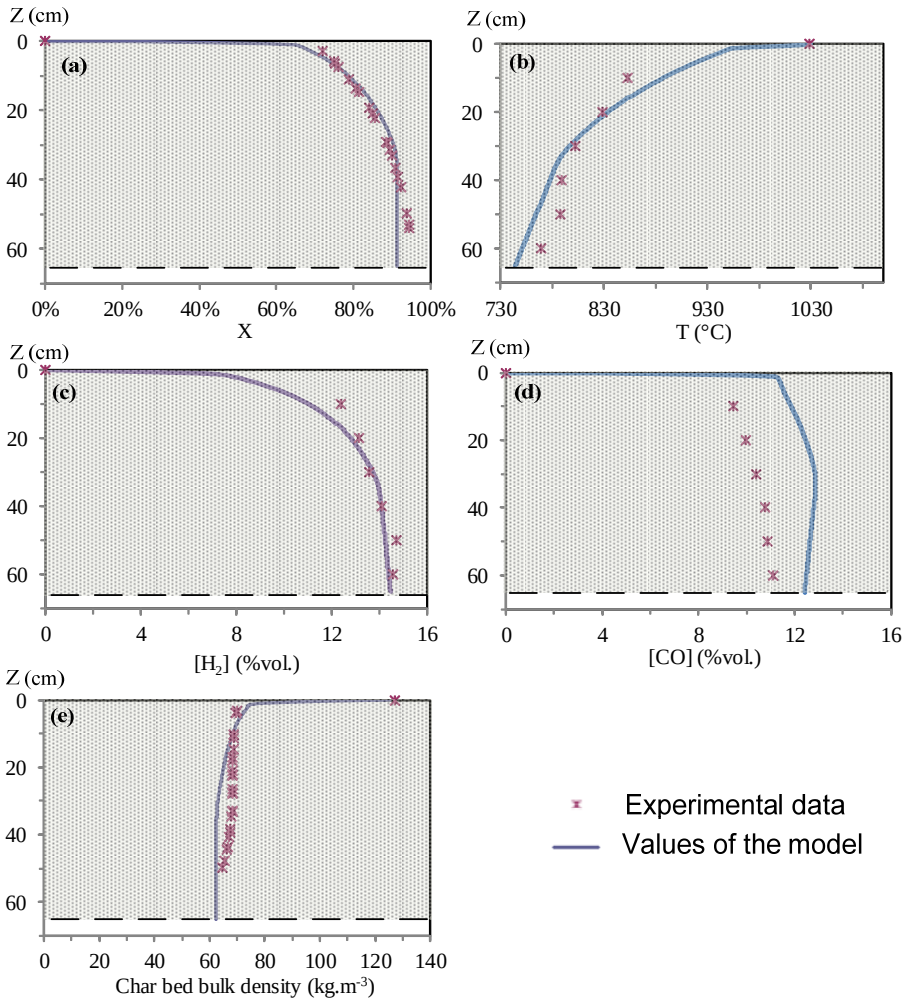


Figure 2: Comparison of model and experimental results for char conversion (a), temperature (b), H2 concentration (c), CO concentration (d) and char bed bulk density (d) along the bed

5. Conclusion

The objective of this work is to set up a methodology to characterize the wood char gasification stage in a fixed bed or staged reactor. For this purpose, an experimental reactor has been designed, built and tested. A char bed numerical model was developed and validated for many experiments and different feedstocks.
From the experimental reactor, characterization of the char bed during gasification has been performed and provides temperature, gas concentration, particle velocity, char bed bulk density and char conversion profiles along the bed. The char bed model, developed with COMSOL software, takes into account the bed compaction along the reactor, in addition to heat/mass transfers and gas flow involved in a reactive and moving porous medium. Functions were established for the rapid calculation of the St_j for the heterogeneous reactions. Char bed compaction was considered thanks to a balance equation on the solid phase coupled with an empirical compaction function calculating particle velocity from char conversion. The validation of the char bed model from experiments was carried out. In the paper, the accuracy of the model in predicting char bed gasification throughout a WCC experiment was shown. Finally, the model will be used to test new geometrical arrangements and design of char gasification reactors.

Nomenclature

A_i	Frequency factor for reaction i	[s^{-1}]
C	Molar concentration	[$mol.m^{-3}$]
C_p	Specific heat	[$J.K^{-1}$]
$D_{j,N2}$	Diffusion coefficient of a specie j in N_2	[$m^2.s^{-1}$]
e_p	Particle thickness	[m]
K	Permeability	[m^2]
P_j	Partial pressure of a specie j	[-]
Q_i	Heat source of the reaction i	[$W.m^{-3}$]
St_C	Mass source of carbon	[s^{-1}]
St_j	Mass source of a gas specie j	[$mol.m^{-3}.s^{-1}$]
U	Velocity field	[$m.s^{-1}$]
μ	Dynamic viscosity	[Pa.s]
λ	Thermal conductivity	[$W.m^{-1}.K^{-1}$]

Index

β	Gas phase
σ	Solid phase
η	Porous media
i	Reaction i
j	Species j
m	Gas compound
p	Particle phase
Inter	Inter-particular

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