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Modeling and simulation of biomass fast pyrolysis in a fluidized bed reactor

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ABSTRACT

This paper presents a phenomenologically based mathematical model for biomass fast pyrolysis process in a bubbling fluidized-bed. The model was developed in transient state, is one-dimensional and is based on the two-phase theory. A semi-global reaction mechanism in two stages was used, considering the primary formation of products and the secondary reactions of the vapors. Also, population balances for the density/temperature distribution of the particles and distribution of the bubble size were proposed. The model can predict the temperature of the phases, the distribution and yields of the products, the heating rate of particles, and the residence time of gases. Finally, a solution algorithm for the model was proposed, which was programmed in MATLAB 7.0, being able to find a good fit between simulation results and the experimental data.

1. Introduction

The growing concern about climate change and the depletion of fossil fuels has stimulated the study of potential sources of renewable energy and the development of technologies for efficient and environmentally sustainable utilization of these. Biomass fast pyrolysis is a promising energy conversion process, where waste material can be used without further pre-treatment, and with short processing time [1]. It is a thermochemical process at moderate temperature (~500 °C) in which biomass is rapidly heated in the absence of an oxidizing agent. The biomass decomposes generating condensable and non-condensable gases, and char. After gases have been cooled, a brown viscous liquid with a calorific value of approximately half of conventional fuel oil is obtained. The yield of the liquid is between 60 and 75% depending on the raw material used, the temperature and operating pressure, the heating rate and the particle size of biomass. One of the main technologies used for the fast pyrolysis process is the fluidized-bed, as it is a mature and well-studied technology, with good temperature control and a good heat transfer coefficient. The liquid production yield reported for this technology is 70–75% [2]. The residence time can vary between 0.5 and 2 s and the particle size is recommended to be less than 2 mm [3,4].

The design and scale of these reactors has been based on experimentally obtained parameters in pilot equipment, which are valid for particular conditions and systems, losing generality. Therefore, models have been proposed to describe the process behavior. Many of these combine a kinetic model with the mass, momentum and energy conservation equations, allowing evaluating the influence of design and operating parameters in the yield of the process. However, these are not detailed models, and they do not describe phenomena on the solid phase.

Di Blasi [5], Luo et al. [6] and Kaushal and Abedi [7]. developed models aimed at predicting the formation of products coupling a particle model with a heat transfer model in the bed, focusing on phenomena within the particle. Moreover, Lathouwers and Bellan [8] presented a model based on transport equations, describing the dynamics of a solid-gas reactive mixture applied to the prediction of process yield. In later work [9], they coupled a model of superimposed cellulose, hemicellulose and lignin kinetics. Similarly, Rabinovich et al. [10] and Sudhakar and Kolar [11] developed fluidized bed hydrodynamic models applied to the biomass fast pyrolysis process coupling global kinetic models.

Papadikis et al. [12] developed a CFD model for the transport of momentum between the fluidizing gas and the sand particles of the bed. This model is applied to fast pyrolysis integrating a comprehensive semi-global kinetic model and conservation equations to predict products yield. In subsequent work, they studied the impact of particle size reduction [13] and particle size in the particle-bed heat transfer coefficient [14]. Finding that for small particles, around 500 μm, particles of constant size may be consid-

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Nomenclature

A_b	Area
C^p	Specific heat capacity
D	Diameter
f_b	Bubbles distribution function
f_p	Distribution function (number of particles of each density)
G	Gravity
H	Heat transfer coefficient
H	Enthalpy
h_m	Mass transfer coefficient
k_o	Thermal conductivity
M	Mass
N_p	Number of particles
Nu	Nusselt number
Pr	Prandlt number
Q	Heat
R	Radius
r1, r2 . . . r5	Reaction rate
Re	Reynolds number
T	Time
T	Temperature
U	Velocity
V_{bz}	Volume
Z	Height

Greek letters

$\in$	Emissivity
σ	Stefan–Boltzmann constant
ΔH_{rxn}	Enthalpy of reaction
ρ	Density
γ	Mass fraction
μ	Viscosity
δ	Bubble phase fraction

Subscripts

p	Particle
g	Gas
e	Emulsion
b	Bubble
biom	Biomass
g	Gas
tar	Tar
char	Char
in	Inlet
out	Output
o	Initial condition
t	Terminal
mf	Minimum fluidization

ered and that the heat transfer mechanism depends on the particle size, smaller sizes reduce the effect of side reactions because the temperature profile is uniform within the solid.

Xue et al. [15] presented a CFD model, coupling a multi-stage kinetics and modeling biomass as a mixture of cellulose, hemicellulose and lignin. Unlike other models of this type, it takes into account the volume change of the particles in the bed having varying porosity thereof. Similarly, Boateng and Mtui [16] and Mellin et al. developed CFD models based on transport equations and global devolatilization kinetics, oriented to the monitoring of the biomass fast pyrolysis products.

In general, the studies focus on predicting bio-oil yield and the effect of temperature and the size of the biomass particles.

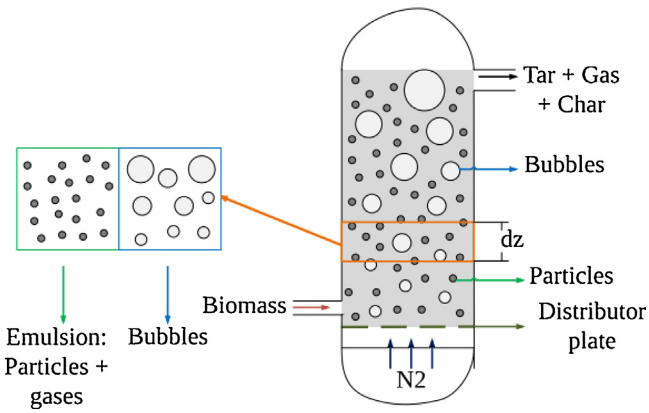

Fig. 1. General scheme of the fluidized bed reactor to be modeled.

However, these models have not explicitly studied the heating rate, which is a determining factor in the process and one of the main characteristics of fast pyrolysis process [2]. In addition, just a few of them studies the effect of bubbles in calculating the residence time of the gases and in the progress of side reactions which is an important design variable, especially for fluidised bed fast pyrolysis reactors. An accurate calculation of this variable allows guaranteeing required biomass conversion and minimizing cracking in the designed reactor. It is the reason why in this work a phenomenologically-based mathematical model that accounts for the heating rate, the particle size and bubbles distribution and its effect on the residence time of gases and process performance is proposed. This, through the incorporation of population balances to the two phases model.

2. Mathematical model

A model capable of describing the behavior of a bubbling fluidized bed reactor for the production of bio-oil by fast pyrolysis of biomass was developed. In the proposed model, biomass particles enter the reactor and are suspended in the fluidizing gas (nitrogen) entering from the bottom through a distributor plate. The gas in excess of what is required for minimum fluidization, forms bubbles rising along the reactor. A general diagram of this system is shown in Fig. 1.

The main characteristics and assumptions made during the model development are:

- The model was developed in transient state and is unidimensional, changes in the bed occur in the axial direction only.
- The existence of two phases was considered, emulsion and bubble. The emulsion is formed by gas and particles, while the bubble is formed by solid-free gas.
- The heat and mass transfer occurs between the particles and the emulsion gas, and between the bubbles and the gas from the emulsion.
- A two-stage semi-global reaction mechanism is used, in which the primary product formation and the side reactions of formed tar are considered.
- Population balances for the distribution of particle density/temperature and size distribution of the bubbles were proposed.

In order to evaluate the effect of particle size and heating rate, a model for a biomass particle in a fluidized bed was developed, which was subsequently coupled to the bed model. In the model, the energy balance of the particle, plus the balance of species to monitor biomass, non-condensable gases, volatiles and char