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Development of a numerical model for biomass packed bed pyrolysis based on experimental validation ☆

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HIGHLIGHTS

- A model for packed bed pyrolysis of sawdust was proposed and calibrated.
- Experimental tests were properly designed and realized to calibrate the model.
- Three temperature levels were considered to extract proper reaction kinetics.
- The model demonstrated a satisfying accuracy with the experimental tests and can be used for a compatible biomass.
- The methodology can be used for calibrating other biomass types.

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ABSTRACT

A mathematical CFD model of pyrolysis process was developed to predict the volatiles in terms of tar and light gas as well as char fraction released in a biomass packed porous bed system. In particular, phenol was considered as tar representative while the main gas species were individually considered (in particular H_2, CO, CO_2, CH_4 and steam). The model was implemented in a commercial CFD code through several original User Defined Functions (UDFs) to reproduce the source terms in the continuity, energy and chemical species mass fraction equations. Furthermore, both inertial and viscous resistances within the packed bed were modeled and coded to assess the pressure drop in the porous media. Code validation was achieved by comparing the numerical results against experimental data obtained in a small-scale biomass reactor using N_2 as carrier gas. To assess the kinetic parameters of the pyrolysis model at different operating conditions, the experiments were carried out by varying, in a wide range, the temperature of both the N_2 flux and reactor walls.

1. Introduction

To properly understand (and hence to model) the biomass combustion process, pyrolysis mechanism must be specifically addressed. Pyrolysis is an endothermic degradation process of a solid fuel occurring in total absence of oxidizing agents. It results in the formation of a great variety of chemical species usually divided into three categories: a stable mixture of synthesis gas, a liquid resulting from condensation of the condensable organic compound (tar), and a solid residue rich in carbon (char). The former is mainly composed of CO, CO_2, H_2 and light hydrocarbons, while the main components of tar are heavy hydrocarbons (C_xH_y) [1–4]. Pyrolysis process is governed by many parameters among which the most important are pressure, residence time of the fuel within the reactor, and operative temperature. In particular, the latter significantly influences the concentration of products involved. Several studies in literature show that an increase in temperature favors the formation of gas and tar resulting in a reduction of the residual char [3,5]. During pyrolysis, there is a continuous interaction among the physical processes involved, causing variations of the fuel characteristics, and among the chemical reactions causing the conversion in final products.

Pyrolysis processes are generally analyzed performing experimental campaign [1,5]. Some of them were finalized to determine reactions kinetics [6]. Application of products of pyrolysis in fuel by products are also frequent [7]. Often pyrolysis process is analyzed together with gasification process, where pyrolysis products interact with an oxidizing agent [8]. Pyrolysis and

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Nomenclature

A	pre-exponential factor (s^{-1})
C_2	inertitial resistance factor (m^{-1})
d_{eq}	equivalent diameter (m)
Ea	activation energy (J mol^{-1})
h	specific enthalpy (J kg^{-1})
h_f^0	standard enthalpy of formation (J kg^{-1})
l_b	bed depth (m)
$\dot{m}$	mass flow rate (kg s^{-1})
M	species molecular weight
R	universal gas constant (J mol^{-1} K^{-1})
S_h	specific enthalpy source (W m^{-3})
J	species diffusive flux (mol m^{-2} s^{-1})
S_m	mass source (kg m^{-3} s^{-1})
u	velocity (m s^{-1})
T	temperature (K)
V_b	bed volume (m^3)
X	volume fraction (–)
Y	mass fraction (–)

Greek

α	permeability (m^2)
γ	mass fraction in volatile gas (–)
ε	porosity (–)
μ	dynamic viscosity (kg m^{-1} s^{-1})
ρ	density (kg m^{-3})
τ	stress tensor (kg m^{-1} s^{-1})
$\dot{\omega}$	production rate of volatiles (kg/m^3 s)

gasification procedure for producing high quality syngas, can be considered a possible alternative to anaerobic digestion plant or landfill gas whose environmental impact can be deeply investigated [9,10]. Syngas produced by pyrolysis or gasification process is generally sent to a burner to produce heat in energy conversion systems [11,12].

CFD simulations are a very useful and effective tool for evaluating chemical and physical phenomena, such as those occurring during pyrolysis [13–15], gasification, or biomass combustion [16]. In particular CFD can help in detecting and quantifying fouling phenomena on the solid wall of the burner/furnace when char ad ashes were drag into the syngas flow [17,18].

However, the CFD study of combustion process requires defining reaction kinetics for the selected biomass. For such reason, experimental campaigns aiming at reconstructing such kinetics for different kind of biomass and in a wide range of temperature are required to assess the accuracy of the numerical approaches.

In this work, a mathematical model for a fixed bed reactor is presented. In the model, source terms have been added to the species equation of conservation in order to account for the formation/destruction of gaseous and liquid compounds, and water during the pyrolysis process. Furthermore, energy equation has been considered to account for temperature variation. The model was implemented in the commercial software ANSYS Fluent 13 by using appropriate User Defined Functions (UDFs).

The mathematical model has been validated comparing the simulation results with experimental data obtained in a laboratory scale reactor.

In the following the experimental set-up is presented. Then, the mathematical formulation is discussed and numerical details are described. Finally the assessment of the model is presented in the result section. Conclusions will close the present work.

2. Experimental set-up

Pyrolysis tests are performed using pine sawdust in a fixed bed quartz tubular reactor (internal diameter 4 cm; length 20 cm), equipped with a quartz frit to allow the biomass bed formation, and heated by an external cable heaters. Bed temperature is measured by a K-type thermocouple fitted in a small quartz pipe and placed at the center of the bed. Biomass enters the reactor from the top fed by a piston ensuring a feeding rate of 0.01 g/s; moreover it is fed for 10 min, forming a 10 cm bed height at the end of each test. During the tests, a nitrogen flow of 0.4 Nl/min is fed above the fuel bed to make the atmosphere within the reactor inert. Gasses produced during pyrolysis pass through a series of iced-cooled traps to condense tar and water; then, non-condensable gases are sent to an on-line gas analyzer (Siemens Ultramat 23) to measure in continuous the concentration of CO, CH_4 and CO_2. H_2 concentration is measured every 2 min using a gas chromatograph. The amounts of tar and water are determined gravimetrically. The experimental tests has been performed at three different temperatures 773, 873, and 1073 K in order to determine the kinetics of the process, and they are repeated three times to confirm the data. The experimental set-up is shown in Fig. 1.

3. Mathematical model

The model here presented was developed to simulate the pyrolysis of a solid biomass in a fixed bed reactor operating in steady state conditions.

Computational domain is divided into two identical parts, as shown in Fig. 2. The freeboard is defined as a fluid zone whereas the bed is modeled as a porous region, with a constant value of porosity. This assumption allows simplifying numerical simulations by considering this zone as a homogeneous medium in which both biomass and pyrolysis products are in thermal equilibrium [1]. The source terms, implemented in the CFD code through UDFs and described in the following paragraphs, are activated only in the porous region.

The pyrolysis model has been implemented through the definition of four User Defined Functions (UDFs) needed to specify the process kinetics. UDFs are implemented as source terms within the transport equations, in particular terms for mass, chemical species, and energy. Furthermore, an additional term has been added to take into account the pressure drop within the bed.

Transport equations thus write:

mass
$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \bar{u}) = S_m \tag{1}$$

chemical species
$$\frac{\partial (\rho Y_i)}{\partial t} + \nabla \cdot (\rho \bar{u} Y_i) = -\nabla \cdot \bar{J}_i + R_i + \dot{\omega}_i \tag{2}$$

energy
$$\frac{\partial (\rho E)}{\partial t} + \nabla \cdot [\bar{u}(\rho E + p)] = \nabla \cdot [k \nabla T - \sum_j h_j \bar{J}_j + \bar{\tau} \cdot \bar{u}] + S_h \tag{3}$$

The mass source term S_m is introduced to model volatile matter formation (namely tar and gas) due to the pyrolysis reactions. In steady state conditions, the inlet mass flow rate is considered equal to the biomass consumption rate, which can be expressed as the conversion rate of biomass into the pyrolysis products. Hence the mass source is computed using Eq. (4).

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