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Research article

Comprehensive CFD modelling of solar fast pyrolysis of beech wood pellets

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ABSTRACT

The present work focuses on the study of the solar pyrolysis of beech wood pellets. The biomass degradation process was modelled in the CFD (Computational Fluid Dynamics) platform ANSYS FLUENT 14.0. The results of simulations were compared to experimental tests conducted in a lab-scale solar reactor in order to validate the CFD model. The biomass pyrolysis was carried out at temperatures ranging from 600 to 2000 °C, at two heating rates: 10 and 50 °C/s. This new 2D single particle model represents a significant improvement of previous simpler version, not only because it allows monitoring the evolution of gas speciation but also because its formulation enables to deal with different types of biomass feedstock. The model structure comprises a multi-step complex kinetic framework that involves competitive reactions –including secondary tar reaction- along with rigorous heat and mass (species) transport inside the particle.

On this basis, char, tar and gas predicted yields are compared with experimental data. In addition, the gas composition (CH_4, CO, CO_2, H_2 and C_xH_y) is also compared. CFD results are in good agreement with the experimental values, validating this approach as a useful tool to predict the products yields and their composition when pyrolyzing biomass particles. Furthermore, the model can be used when modelling any process where pyrolysis occurs and it can even be easily coupled to any reactor scale model.

1. Introduction

In the last two decades and as a result of the growing energy demand and of the concern of greenhouse gases emissions from fossil fuel combustion, there has been an increasing interest in renewable and environmentally friendly energy sources. Biomass energy technology stands as a promising option among others [1–3]. Among the different biomass conversion methods, thermochemical treatment is often employed; and pyrolysis is considered as one of the most attractive pathways to transform biomass into condensable gas (tar and water), permanent gas (H_2, CO, CO_2, CH_4, C_2H_6) and char, that can be subsequently upgraded to fuels [4–7]. Moreover, the yields and product distribution depend on the operating conditions and feedstock properties [8–10].

Nonetheless, pyrolysis is globally endothermic and it requires heat, which is classically provided by any fossil fuel combustion in conventional processes. This drawback can be overcome by using concentrated solar radiation as the energy source of the process, which increases the energy conversion efficiency and reduces the pollution discharge [11]. In a direct heating solar reactor, fast/flash pyrolysis (high levels of temperatures and heating rates -HR-) can be achieved since the biomass directly absorbs concentrated solar radiation, tending to yield more gas products, particularly high quality syngas [12]. Solar reactors represent an interesting alternative, when compared to conventional reactors, due to its flexibility to operate for a wide range of temperature (600–2000 °C) and heating rate (5–450 °C/s) while minimizing the energy cost [13]. Therefore, direct solar pyrolysis allows to produce more combustible gas with a higher heating value than the one obtained in traditional reaction units [14], which can be then used as fuel for power generation, heat or transportable fuel production.

The transient formation of char and release of gas and tar are governed by the pyrolysis rate. In the case of a large particle – such as the pellet dealt with in this work –, the magnitude of this rate is determined either by the heat transfer in the pellet or by both the heat transfer and kinetic rates [15]. This “thermally thick” condition leads to non-uniform biomass temperatures during pyrolysis. Additionally, the intra-particle residence time in large biomass particle may be sufficient for tar decomposition reactions to occur inside the particle. Moreover, at high heating rates, the produced char layer can act as a catalyst. As a result, the intra-particle tar cracking reactions modify the product yields by reducing the amount of produced emitted tar, and they increase the amount of light gaseous products escaping the particle. Also, this secondary tar decomposition may take place in the vapor phase (homogeneous) and on the surface of the pyrolyzing solid (heterogeneous). Even more, secondary tar cracking can also happen inside (intra-particle) or outside (extra-particle) the biomass particle [16,17].

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Nomenclature

A	Pre-exponential factor, s^{-1}
C_P	Specific heat capacity, J/kg.K
d	Diameter, m
D	Diffusivity, m^2/s
e	Particle emissivity
E_a	Activation energy, J/kmol
k	Thermal conductivity, W/(m.K)
K	Permeability, m^2
M	Molecular weight, kg/kmol
P	Pressure, Pa
r	Reaction rate, kg/(m^3.s)
r	Radial coordinate, m
R	Radius, m
R	Gas law constant, 8314 J/(kmol.K)
S	Source term, kg/(m^3.s)
S_v	Specific surface area, m^2/m^3
t	Time, s
T	Temperature, K
u	Gas velocity, m/s
x	Axial coordinate, m
x_B	Biomass conversion, dimensionless
Y	species mass fraction, dimensionless

Greek letters

α	Stoichiometric coefficient
β	Heating rate, °C/s
Δh	Reaction enthalpy, J/kg
ε	Porosity
τ	Particle tortuosity
ρ	Apparent density, kg/m^3
$\hat{\rho}$	Intrinsic density, kg/m^3
σ	Stephan-Boltzmann constant, 5.67 10^{-8} W/m^2K^4
μ	Viscosity, Pa.s

Subscripts

0	Initial
B	Biomass
C	Char
eff	Effective
g	Gas
H Init	Enthalpy initial
s	Solid
sec	Secondary

Abbreviations and chemical formulas

2D-DP	Two Dimensional Double Precision solver
AR	Argon
CELL	Cellulose
CELLA	Activated cellulose
CFD	Computational Fluid Dynamics
CO	Carbon monoxide
CO_2	Carbon dioxide
CH_2O	Formaldehyde
CH_3OH	Methanol
CH_3CHO	Acetaldehyde
CH_4	Methane
C_2H_4	Ethylene
C_2H_5OH	Ethanol
C_3H_6O	Propanal
FE2MACR	Sinapaldehyde
G{CO_2}	Trapped CO2
G{CO}	Trapped CO
G{CH_2O}	Trapped CH2O
G{CH_4}	Trapped CH4
G{C_2H_4}	Trapped C2H4
G{CH_3OH}	Trapped CH3OH
G{H_2}	Trapped H2
GLYOX	Glyoxal
H_2	Hydrogen
HAA	Hydroxyacetaldehyde
HCE	Hemicellulose
HCEA1	Activated hemicellulose 1
HCEA2	Activated hemicellulose 2
HCOOH	Formic acid
HMFU	5-hydroximethyl-furfural
HR	Heating Rate
H_2O	Water vapor
LIG	Lignin
LIG-C	Carbon-rich lignin
LIG-H	Hydrogen-rich lignin
LIG-O	Oxigen-rich lignin
LIG-CC	Carbon-rich lignin 2
LIG-OH	OH-rich lignin
LVG	Levoglucosan
PHENOL	Phenol
pCOUMARYL	Paracoumaryl alcohol
UDF	User Defined Function
XYLAN	Xylose monomer

Modelling thermochemical processes at the pellet scale (local scale) can be a very useful tool for achieving a deep understanding of the interaction between chemical and physical phenomena during solid consumption, and of the influence of variables such as temperature, heating rate, particle size and biomass composition [18]. Particularly, accurate pyrolysis modelling represents a very complex and challenging task [19], not only because there are still some uncertainties regarding transcendental aspects of pyrolysis, but also because the physical and chemical phenomena as well as the aforementioned parameters have an important impact on the pyrolysis behaviour [20].

In this sense, several numerical approaches have been developed in order to study the kinetics of the thermal decomposition of biomass [21–28]. However, most previous models were developed based on experimental results at low heating rates and low temperature. Okekunle et al. [29] and Zeng et al. [30] formulated numerical models to represent biomass pyrolysis at moderate and high temperatures and heating rates, but their models were narrowed to three lumped products (tar, gas and char) and limited to only one type of biomass: Japanese cypress and beech, respectively.

In this context, the aim of this work is to develop a CFD single particle model based on competitive, multi-component kinetic mechanisms [31] -taking into account homogeneous intra-particle secondary tar reaction-, capable of predicting tar and gas species compositions when pyrolyzing “thermally thick” biomass particles. The model is validated against experimental data obtained in a lab-scale solar reactor assisted by a 1.5 kW solar furnace, for final temperatures of 600, 900, 1200, 1600 and 2000 °C and two values of heating rate (HR): 10 and 50 °C/s.

2. Experimental method

2.1. Material

The beech sawdust particles were dried in an oven to remove their total moisture content, and then compressed into cylindrical pellets with 10 mm in diameter and 5 mm thick. The beech pellet composition and its properties are given in Tables 1 and 2, respectively. In Table 1,