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Evaluation of global biomass devolatilization kinetics in a drop tube reactor with CFD aided experiments

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ABSTRACT

A procedure coupling experimental characterization and computational fluid dynamics (CFD) is developed for providing valuable global kinetic parameters to large applications of biomass fuels (fast pyrolysis, co-combustion and gasification). This is based on an advanced lab-scale apparatus (drop tube reactor), reproducing high heating rates and low residence times at different nominal temperatures (400–800 °C) for particle size of practical interest. Although the relative simplicity of the operation, a detailed and accurate evaluation of the particle residence time and effective thermal history is needed to elaborate suitable global devolatilization kinetics, which differ significantly from low heating rate kinetics (for instance in thermogravimetric balance) and also from those obtained assuming strong hypotheses (e.g. constant particle temperature in the reactor). The developed procedure gives kinetic parameters which are not the intrinsic devolatilization kinetics but global kinetics at high heating rates. These global kinetic parameters are useful to simulate practical systems (characterised by high heating rate) with comprehensive codes (CFD), since detailed particle kinetics require additional sub-models (e.g. of external and internal heat transfer) which may be time consuming and need many data, often known only with uncertainty. In this work CFD is used as both diagnostic and predictive tool; its potentials and drawbacks in aiding advanced experimentation on biomass/coal pyrolysis are discussed.

1. Introduction

Biomass fuels are a renewable energy source and may be abundant in specific local areas. Their use in co-combustion plants is limited at present but represents a short-time option for reducing CO_2 emissions [1]. The increase of the biomass/coal ratio can be achieved by optimizing the operating conditions. To this purpose, data are required for conditions similar to large plants, which operate at high heating rate and short residence time. The basic mechanism (in combustion as well as gasification reactors) is a fast pyrolysis with release of volatile species. The behaviour of biomass is much different with respect to fossil fuels and the effects of the operating conditions on pyrolysis parameters are known to be important [2].

Conventional analysis (e.g. thermogravimetry) on lab-scale can give only a fingerprinting of the fuel, because the thermal conditions are far from those of practical applications. For instance, pyrolysis kinetics change substantially when varying the heating rate (see among others Wiktorsson and Wanzl [3]). Therefore, advanced experimental facilities and elaboration procedures should be developed to provide fundamental data under operating conditions similar to those of the industrial scale.

A drop tube reactor (DTR) is a relatively simple apparatus to study the fast pyrolysis of biomass fuels. High heating rates (on the order of 10^4 °C/s) and low residence times (0.1–1 s) can be reproduced [4–7], while different analyses can be carried out on the gaseous products (speciation) and solid residues (char properties) [8–11]. However, most literature works are limited to the determination of particle conversion in different conditions, only few being actually devoted to elaborate kinetics. This is because the effective thermal history of the fuel particles in the DTR is difficult to be measured. A direct characterization would require sophisticated and intrusive experimental techniques, e.g. particle image velocimetry, and optical accesses to the DTR interior, which are hardly practicable. Letho [5] provided measurements of particle velocity and position in the outlet section of a DTR by means of optical techniques and used this information to extrapolate data on the residence time in the whole DTR. Alternatively, the effective thermal history may be deduced from either simple hypothesis or theoretical models on the particle behaviour. The easiest

Abbreviations: CFD, computational fluid dynamics; DD, size distribution of diameter; DTR, drop tube reactor; FC, fixed carbon; KIN, kinetics; MD, monodimensional class; VM, volatile matter.

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Nomenclature

A	pre-exponential factor, s^{-1}
A_p	particle area, m^2
Bi	Biot Number, $Bi = \frac{h_{rad} \cdot d}{\lambda}$
C_D	drag coefficient, –
C_P	specific heat at constant pressure, J kg^{-1} K^{-1}
d	characteristic system dimension, m
d_p	particle diameter, m
D_{32}	Sauter mean diameter, m
E	activation energy, J mol^{-1}
e_p	particle emissivity, m
f_i	mass fraction of the i-th particle dimensional class, –
g	gravitational constant, m s^{-2}
h	heat exchange coefficient, J s^{-1} m^{-2} K^{-1}
I	radiating flux to the particle surface, J s^{-1}
k	first order kinetic constant, s^{-1}
k_f	thermal conductivity of the fluid, J s^{-1} m^{-1} K^{-1}
m	mass, kg
n	fluid refraction index, –
Nu	Nusselt number, $Nu = \frac{dh_{conv}}{k_f}$
p_p	particle perimeter, m
Pr	Prandtl number, $Pr = \frac{C_p \mu}{k_f}$
Py'	Pyrolysis number, $Py = \frac{h_{rad}}{kC_1 \rho_p d_p}$
Q_c	convective heat flow, J s^{-1}
Q_m	mass heat flow, J s^{-1}
Q_c	radiating heat flow, J s^{-1}
R	ideal gas constant, J mol^{-1} K^{-1}
Re_p	particle Reynolds number, $Re_p = \frac{d_p \lvert u_g - u_d \rvert \rho_g}{\mu}$
Re	gas Reynolds number, $Re = \frac{d u_g \rho_g}{\mu}$
RF	Roundness factor, $RF = \frac{4p_p}{A_p}$
t	time, s
t_{pr}	particle relaxation time, s $t_{pr} = \frac{\rho_p d_p^2}{18\mu}$
T	particle temperature, K
T_g	gas temperature, K
Tn	electric heater nominal temperature, K
u_g	gas velocity, m s^{-1}
u_p	particle velocity, m s^{-1}
V	volatiles mass released, –
V^∞	maximum volatile mass released, –
x_i	pyrolysis conversion for the i-th particle dimensional class, –
X_{ash}	ash mass fraction, –
z	axial coordinate from the DTR entrance downwards, m

Greek letters

α	stoichiometric coefficient related to volatiles, –
β	stoichiometric coefficient related to char, –
δ	mass fraction of a dimensional class, –
ΔH_m	specific enthalpy variation associated to mass transfer, J kg^{-1}
$\lambda\lambda$	particle thermal conductivity, J s^{-1} m^{-1} K
μ	gas dynamic viscosity, kg m^{-1} s^{-1}
ρ_g	gas density, kg m^{-3}
ρ_p	gas density, kg m^{-3}
σ	Stefan Boltzmann constant, J s^{-1} m^{-2} K^{-4}
τ	residence time, s
χ	global pyrolysis conversion for a single run, –

Subscripts

conv	convective
rad	radiation
p	particle
g	gas
i	index
r	relaxation
1, 2, 3	indexes
Low$T$	low temperature interval
High$T$	high temperature interval

hypothesis is to assume a constant particle temperature equal to the DTR nominal temperature [7], but significant errors may arise from this procedure.

Therefore, detailed models of the particle behaviour in the DTR are required and to this purpose computational fluid dynamics can be taken into consideration. Indeed most of the commercial CFD codes allow treating multi-phase and reactive flows, so that the CFD poses itself a less expensive and time demanding tool for the investigation of biomass/coal pyrolysis devices. In addition, it can be adapted to full-scale plants, while extensive experiments are not always feasible in industrial devices.

Brown et al. [6] used CFD to model the gas and particles flow in a laminar entrained flow reactor. The CFD model did not account for reactions on the particles, which were assumed to be non reactive. The simulated particle trajectories, temperature and time were used in a bespoke spreadsheet where reactions were integrated appropriately. Consequently, in the procedure it was assumed that the impact of solid particles and product gases on the flow and temperature of the bulk flow is negligible; this makes sense when the flow of the solid fuel is significantly lower than that of the bulk flow. Fletcher et al. [12] investigated numerically through CFD an entrained flow gasifier, the fuel injections generating a swirl flow. The authors highlighted the complexity of the model, due to the numerous equations involved and the need of validation with experimental results.

Meesri and Moghtadieri [13] evaluated the capability of a CFD code to predict sawdust combustion conversions. They developed a model by introducing global kinetic parameters obtained through experiments. The agreement between predicted and experimental results was good but data were obtained only for very high conversions. Ballester and Jiménez [14] proposed a methodology for measuring the oxidation parameters for pulverised coal from drop-tube and thermal histories obtained with CFD; they pointed out that the consideration of a particle-size distribution instead of a single representative diameter is effective in reducing the error of the CFD conversion predictions.

In this work

- experiments on biomass pyrolysis are performed on a lab-scale drop tube reactor;
- an Eulerian/Lagragian CFD model of the apparatus is used as a diagnostic tool for obtaining the effective thermal history of the particles;
- a procedure is developed to elaborate global kinetics by combining experiments, direct characterization of the apparatus and CFD model results.

The use of CFD is discussed also as a predictive tool, as it poses difficulties and modelling choices to be addressed for the particular application, requiring the use of a combined approach between experiments and modelling.

2. Methodology

The methodology used in this work is illustrated in the scheme of Fig. 1. Details will be provided in the next sections.