



Properties and relevance of the volatile flame of an isolated coal particle in conventional and oxy-fuel combustion conditions



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ARTICLE INFO

Article history:

Received 7 March 2016

Revised 11 April 2016

Accepted 26 September 2016

Available online 11 November 2016

Keywords:

Coal devolatilization
Homogeneous chemistry
Oxy-combustion
Volatile flame

ABSTRACT

A model that accounts for the volatile matter release and its subsequent combustion in the surroundings of an isolated coal particle is presented and used to analyze the characteristics and relevance of the flame so generated in a broad range of conditions. The devolatilization kinetics were experimentally determined in a previous work; the volatile composition is given by the chemical percolation model; and the GRI 3.0 mechanism accounts for the homogeneous reactions. Both conventional and oxy-fuel combustion conditions are considered. In all the cases, three consecutive (although not fully independent) flames are identifiable around the particle, corresponding to the consumption of CH₄ and C₂H₂, first, and the oxidation of CO, further on. A more intense chemistry is generally observed in N₂ than in CO₂-rich environments; in any case, those reactions result in significant heat transfer towards the particle, and thus in an acceleration of the devolatilization, more marked for higher bulk oxygen concentrations. The predictions of the model regarding devolatilization duration and peak flame temperature and position are in good qualitative agreement with the (rather scarce) experimental data available in the literature. Finally, simulations with different particle diameters from 30 to 120 μm show that only for the finest particles an overlapping of the devolatilization and the char oxidation steps during combustion is foreseeable.

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1. Introduction

Coal combustion is still, and after a century, the subject of intense research efforts not only because of its practical relevance in the production of electric energy, but also for the complexity of the processes involved. In particular, the devolatilization of pulverized coal after injection in the combustion chamber and the subsequent combustion of the volatiles outside the particles have received considerable attention in the last decades. Regarding the volatile release from the coal particles, Kobayashi et al. [1] reviewed the experimental data available at that time, and also provided new high temperature data for pulverized coals, all fitted to the already popular single-step model

$$\frac{dV}{dt} = -A_v \exp(-E_v/RT_p)V, \quad (1)$$

where A_v and E_v are to be determined experimentally for each coal. Those authors also proposed an empirical modification of Eq. (1) to include two ‘competing’ reactions with different kinetics and thus

explain the increase in volatiles yield with temperature observed for some coals. Other researchers later developed more sophisticated models, which incorporated fundamental information on the original coal structure and different mechanisms for its progressive transformation into char, tar and non-condensable gases ([2–4] and subsequent work in these lines). Incidentally, the modeling of biomass devolatilization evolved in a similar but surprisingly unconnected way (e.g., [5]). Although some of these approaches are offered at present as options in commercial, general-purpose CFD codes (such as the chemical percolation model [3] in Fluent [6]), the model described by Eq. (1) is still, to the authors’ knowledge, the most commonly implemented in the simulation of coal devolatilization in industrial facilities, due to its simplicity and the amount of kinetic parameters available in the literature for a large variety of coals.

Once the volatiles leave the coal particle, they burn in a shell flame around the particle or as a bulk flame, depending on the local concentration of particles in the gas. This article is focused on the former case, i.e., that of an isolated particle whose volatiles encounter an oxidizing atmosphere and thus burn as they diffuse towards the surrounding gas. Timothy et al. [7,8] reported devolatilization experiments with fine, dispersed coal particles in a drop tube at high temperatures and in different oxygen concentrations, and found a reasonable fit of their data (devolatilization time and flame radius based on the distribution of soot) with a

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Nomenclature

A_v	pre-exponential factor (s^{-1})
C_p	specific heat ($J\ kg^{-1}\ K^{-1}$)
D_i	mass diffusivity of the species i ($m^2\ s^{-1}$)
d_p	particle diameter (m)
E_v	activation energy for gasification ($J\ mol^{-1}$)
H_v	heat of heterogeneous devolatilization ($J\ kg^{-1}$)
r	radial coordinate (m)
r^*	normalized radial coordinate ($2r/d_p$).
R_v	volatile release rate ($kg\ m^{-2}\ s^{-1}$)
$S_{g,i}$	source term due to homogeneous reactions in the mass balance of species i ($kg\ i\ m^{-3}\ s^{-1}$)
$S_{g,T}$	source term due to homogeneous reactions in the gas energy balance ($J\ m^{-3}\ s^{-1}$)
t	time (s)
T	temperature (K).
u	flow velocity (m / s)
V	fraction of volatile matter remaining in the particle
Y_i	mass fraction of the species i
ε	particle emissivity
λ_g	gas thermal conductivity ($W\ m^{-1}\ K^{-1}$)
ρ_g	density ($kg\ m^{-3}$)
Subscripts	
p	particle
g	gas
w	wall (actually, optical environment of the particle)

relatively simple model which considered a thin, spherical flame around the particles. Jost et al. [9] experimental and theoretical approach and conclusions were similar to those of Timothy and co-workers, but with a more limited extent. The data in [7,8] served as a benchmark for several theoretical works published in the following years: Musarra et al. [10] first used finite, global homogeneous kinetics in the description of the combustion of volatiles, simplified to two species representing heavy and light compounds; they concluded that their oxidation occurred in a broad radial range, in contrast with the sheet flame model, and that the volatile oxidation played a relevant role in the particle heat balance. However, Gururajan et al. [11] and little after also Lau and Niksa [12] found that the much simpler infinite kinetics model was in practice able to acceptably reproduce the trends observed in Timothy et al. data. Gurgel-Veras et al. [13] studied the potential overlapping of devolatilization and char oxidation in certain conditions. They developed a model for the combustion of volatiles with two global reactions (first to CO and then to CO₂, respectively), and concluded that the overlapping was possible (and relevant, according to their calculations) for the finest particles at relatively low temperatures. Higuera [14] investigated the effect of the relative motion of particles on the devolatilization rates and the heat transfer balance, by means of a model with a single thin, diffusion controlled flame; finding that a 'classical' blowing-corrected Nu-based expression for the heat transfer, modified to take the flame into account, may be used instead of the rather complex 2D computations to calculate those rates with good accuracy. Very recently, Goshayeshi and Sutherland [15] developed a model which coupled Kobayashi's or CPD's predictions for volatile release with a detailed chemical mechanism for the surrounding atmosphere (and, alternatively, a thin flame formulation), and applied it to the study of the ignition times of fine coal particles.

The relatively recent interest on the behavior of coal in CO₂-rich environments, associated to the potential implementation of oxy-fuel combustion technologies (with the final goal of reducing CO₂ emissions to the atmosphere), has motivated new experi-

ments regarding the ignition and devolatilization of coal particles in a variety of conditions. Shaddix and Molina [16], Khatami and Levedis with different co-workers [17–19] and Huang et al. [20] have reported data on devolatilization times and (the former two groups) estimates of the size and temperature of the envelope flame (based on soot observations) around coal particles of different ranks during their devolatilization, using similar experimental facilities. Their results show higher flame temperatures and generally shorter devolatilization times in N₂ than in CO₂, and the same trends with increasing oxygen concentrations; the soot cloud size is observed to decrease for greater [O₂] and to be somewhat smaller in N₂ than in CO₂. As explained later, the measurements are complex, and the data reported by the different researchers show a non negligible dispersion in some cases.

In previous articles [21–23], the authors presented a model for the oxidation of CO around an isolated coal particle and applied it to the combustion of chars from coals in very different ranks under conventional and oxy-fuel combustion conditions. In the present work, the model has been adapted to the combustion of volatiles; it is used here to illustrate the main features of this complex process, first, and then to evaluate the dependence of the devolatilization rate, flame and particle temperature, among other parameters, on the combustion conditions, namely oxygen concentration and main gas carrier (N₂ or CO₂). Finally, the results of these simulations have been compared (whenever it was possible) to the experimental data reported by the authors cited in the previous paragraphs.

2. Model. Conditions simulated

As just explained, the model used in the present work is mostly an adaptation of that recently developed for the oxidation of char particles, described in detail in [21]; for this reason it will be only briefly depicted here. It describes the heating and devolatilization of a quiescent, isolated, spherical particle immersed in a reactive atmosphere. The particle is assumed to be isothermal at any moment and the release of the volatiles at its surface is described according to the single step model described by Eq. (1) above. Its temperature, T_p , is calculated as the result of the heat balance expressed in Eq. (2), which considers radiation, conduction and the enthalpy of devolatilization. Radiative heat exchange is calculated assuming $\varepsilon = 1$ and $T_w = T_g$, which is thought to reasonably reproduce the optically thick flames generated in industrial boilers.

$$\frac{\rho_p \cdot C_p \cdot d_p}{6} \frac{dT_p}{dt} = R_v \cdot H_v + \varepsilon \cdot \sigma \cdot (T_w^4 - T_p^4) + \lambda_g \frac{\partial T}{\partial r} \Big|_{r=d_p/2} \quad (2)$$

The global volatile release rate, R_v , is calculated through Eq. (1) above. The volatile composition is estimated through the CPD model [3], which determines the fraction of tar, CH₄, CO₂, CO, H₂O and "other gases" generated at any time along devolatilization. Preliminary calculations for different particle heating rates (400–40,000 K/s) and final temperatures (1313–1673 K) showed only very minor variations in the volatiles composition, and the results corresponding to the case of 4000 K/s and 1448 K have been used as input in all the simulations. Note that although the CPD program available on the internet provides also the particle temperature evolution at the specified heating conditions, this aspect has been overridden here by the heat balance given by Eq. (2) to allow for the coupling of this sub-model with that for the gas around the particle, and only the gas composition vs. volatile content, V , has been incorporated (nevertheless, those preliminary calculations showed similar mass loss rates for both models in the absence of oxygen in the bulk gas). C₂H₂ has been assumed here to represent those "other gases" calculated by the CPD model. This species is convenient because it is included in the mechanism implemented (see below); a similar approach has been used by others recently

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