NUMERICAL EVALUATION OF PARTICLE STRUCTURE EVOLUTION AND FRAGMENTATION DURING COAL COMBUSTION AT DIFFERENT HEATING RATE

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Abstract

The modification in the particle size distribution of a coal feed occurring over combustion/gasification because of particle fragmentation can significantly affect process performances. Most literature models developed in the past account only for primary fragmentation.

A mathematical model has been developed that calculates the evolution of temperature, pressure, porosity and concentration of the main chemical species within a coal particle during pyrolysis and beyond throughout char combustion. The model eventually calculates maps of internal stress and estimates the probability of particle's rupture.

Tailored computational experiments was performed with reference to a medium rank coal. Heating rates ranging from the low one typical of fluidized bed reactors (10^2 K/s) up to the very high heating rate distinctive of pulverized fire (PF) and entrained flow gasifiers (10^5 K/s) have been considered.

Introduction

A number of papers addressed fragmentation phenomena in fluidized bed combustors [1-13] over the last decades. Different models was developed to predict the fate of solid fuels in fluidized bed reactors when fragmentation reduces the feed particle size and elutriation decreases particles residence time [10-13]. The same issue has been investigated more recently for novel biomass templated sorbents for calcium looping applications [14]. In most of the cited literature, the extent and the rate of the individual fragmentation phenomena, as well as the rate of elutriation, has been assessed by purposely designed experiments following well consolidated protocols.

A first attempt to predict the fragmentation behavior of coals through modeling was done by Chirone and Massimilla [1], who developed a model for primary fragmentation of coal particles under heating conditions typical of fluidized bed combustion, i.e. large particle size, temperature around 1100 K and heating rates in the order of 100-1000 K/s [2-6]. More recently, Senneca *et al.* [6-7] published a model of primary fragmentation that also accounts for the effects of thermal stress. Lately, Senneca *et al.* [15] extended their fragmentation model, accounting for the combustion of volatiles within particle pores and for char combustion, typically associated with secondary fragmentation and percolation, in order to go far beyond the initial stage of devolatization, associated to primary fragmentation. Moreover, their model accounts for changes both in particle physicochemical properties (e.g. density, thermal conductivity, Young modulus, etc.) and in the concentration of gaseous species inside pores along burn off.

In the present work, the results of tailored computational experiments carried out on the basis of this latter model are presented with reference to a medium rank coal with two different heating rates, typical of fluidized bed reactors (10^2 K/s) and pulverized fire combustion (PF) (10^5 K/s).

Model result

The set of nonlinear-second order differential equations with associated boundary and initial conditions reported in [15] was solved in COMSOL Multiphysics® with reference to the operating conditions reported in Table 1.

Table 1. - Different operating conditions used in model simulations

Case number	**d_p, mm**	**T, K**	**Heating rate, K/s**
1	5	1123	100
2	0.1	1573	10^5

Fig. 1 reports, as a function of both particle radius *r* and time *t*, the fragmentation probability calculated in case 1. For the considered operating conditions, particle exfoliation occurs very early (1 s *circa*) while breakage at the very center occurs after about 2.5 s with a 100 % chance. Accordingly, Fig. 2 reports, for the same case, profiles of the main model variables along the particle radius just up to 3 s: no significant variation was witnessed within the examined timeframe.

Figure 3 reports computed values of model variables for a 0.1 mm diameter particle heated up to 1573 K with a heating rate of 10^5 K/s (case 2).

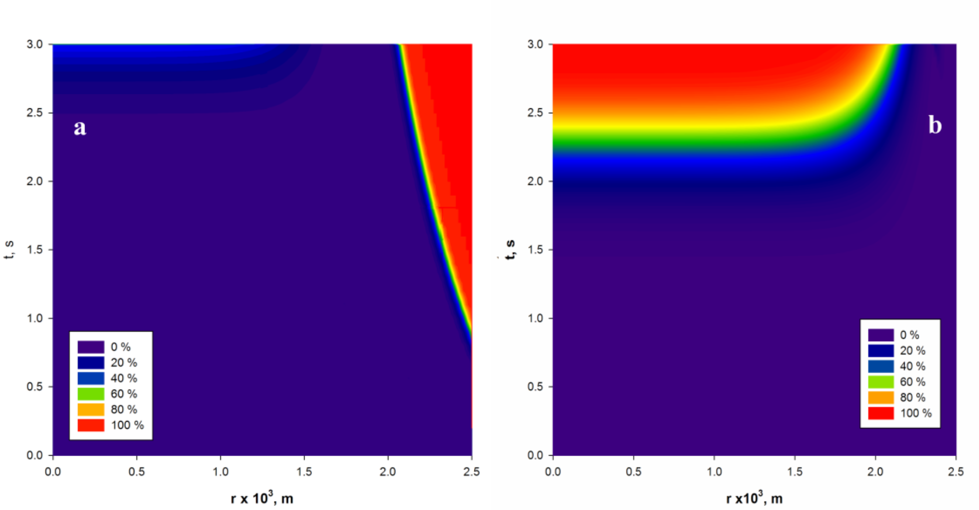

Figure 1. Model output spatio-temporal stress profiles for case 1: a) Tangential stresses; b) total radial stresses.

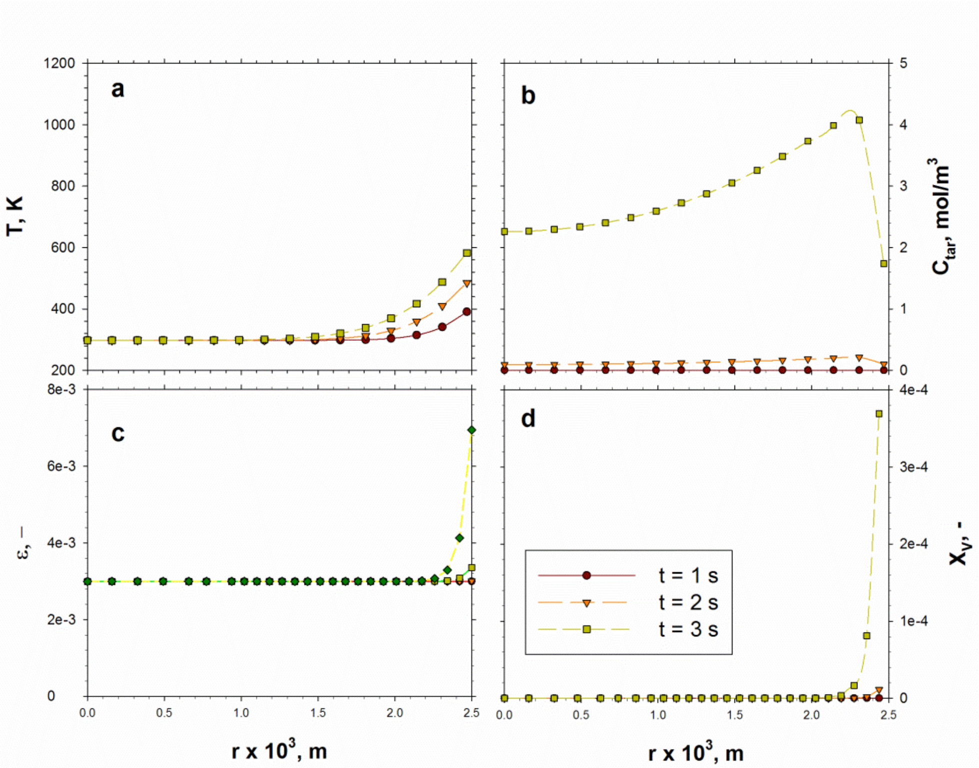

Figure 2. Model output spatial profiles at different times for case 1:
a) Temperature; b) tar concentration; c) particle voidage; d) devolatilization degree.

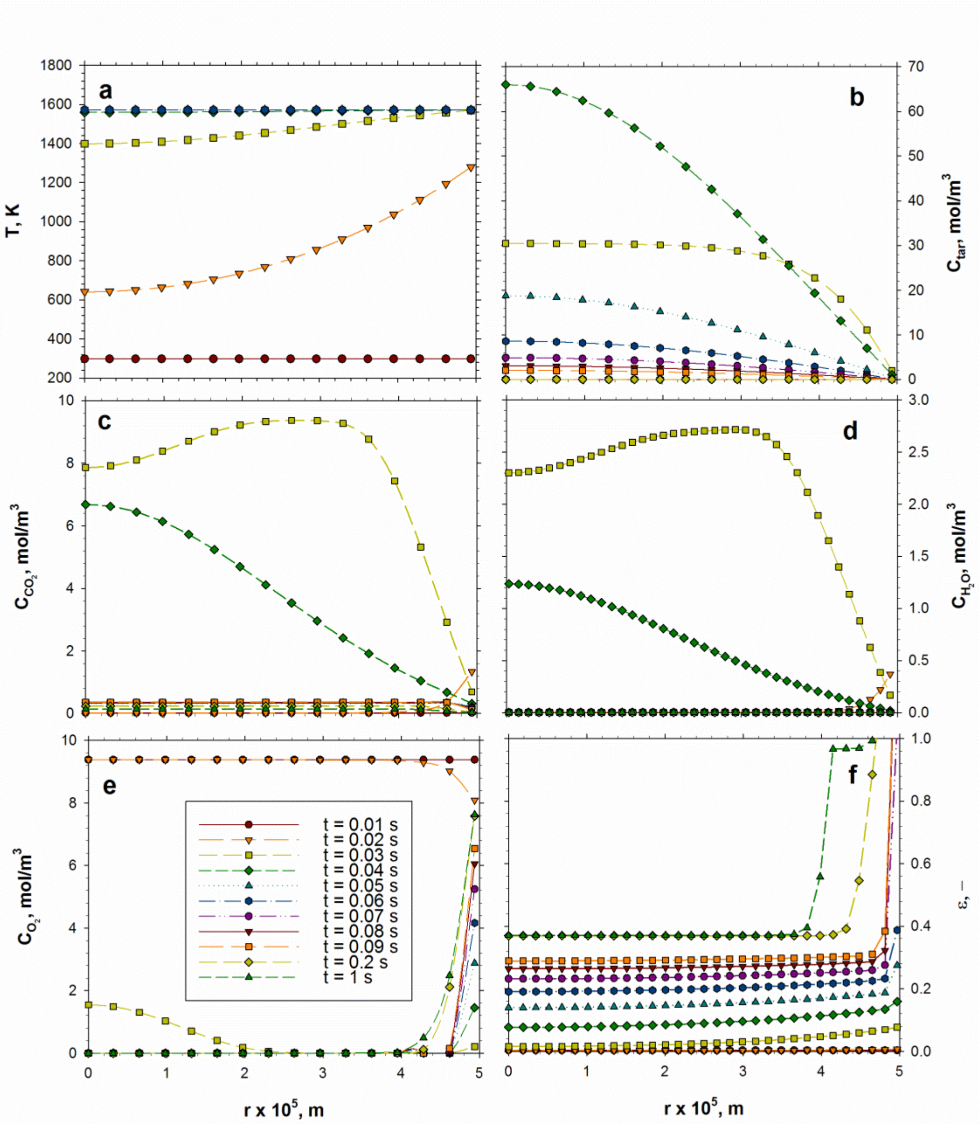

Figure 3. Model output spatial profiles at different times for case 2: a) Temperature; b) volatiles concentration; c) CO_2 concentration; d) H_2O concentration; e) O_2 concentration; f) particle voidage

For the considered operating conditions, tangential and radial breakage probabilities of respectively 5% and 30% were evaluated. Within 0.02 s, temperature gradients within the particle become noteworthy: particle surface reaches 1200 K while the center is still at 600 K. Temperature relaxes to 1573 K throughout the particle after 0.05 s. In the same timeframe tar concentration, after reaching its maximum value (65 mol/m^3) for t = 0.03 s, decreases toward lower values. Volatiles combustion also generates an increase in molar concentration of gaseous species within the particle as shown by both CO_2 and H_2O profiles (Fig. 3.c and Fig. 3.d). Particle internal porosity increases, in about 0.2 s, from the initial raw coal value up to 0.37, the value associated with complete volatiles release. Notably, for t=0.07 s, the porosity at particle shell approaches 1, meaning that char combustion is complete in the outer shells while in the inner parts of the particle the porosity is well below 0.37, suggesting that pyrolysis is not yet complete. In other words, pyrolysis, volatiles combustion, and combustion of char overlap from t = 0.07 s up to t = 0.2 s. From this time on, only char combustion occurs.

Conclusions

The work presented in the present paper reports on the application of a model developed in COMSOL Multiphysics® environment to describe the processes of heat up, pyrolysis, combustion and fragmentation of a solid fuel coal particle. The model was able to describe concentration profiles and combustion patterns of both the shrinking and internal diffusion type.

The model was used to evaluate fragmentation propensity and internal gaseous species concentration of different size particles of a medium rank coal under very different operating conditions.

Fragmentation of cm-sized particles was significant even at low heating rate: actually, for a 5 mm particle heated up to 1123 K at a heating rate of 100 K/s a 100 % breakage probability within 2.5 s was evaluated. Conversely, very small particles will have lower breakage probabilities even at higher heating rates: for a 0.1 mm particle heated up to 1573 K at a heating rate of 10^5 K/s a 30 % fragmentation probability within 1 s was calculated. Under different heating conditions and for different particle sizes, other paths may be relevant and the increase of porosity may further enhance fragmentation through percolation.

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