COAL COMBUSTION MODEL FOR COUPLING WITH A CEMENT KILN CFD MODEL

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ABSTRACT

A solid fuel particle combustion model has been developed to predict flame characteristics, species evolution and concentrations and char burnout within a real cement kiln. The model was developed in a way that it is capable to be coupled with a CFD cement kiln model, while adding low computational complexity. A literature review of the state-of-the-art combustion models was conducted and the most appropriate models were chosen that can provide adequate accuracy with reasonable computational cost. Solid fuel devolatilization was modeled using a multi-step lumped species mechanism [1] to provide a realistic species composition. A kinetic diffusion model [2] was applied for the char combustion modeling. The homogeneous reactions of the devolatilized species that take place in the gas phase were included in the model together with a shrinking particle model to simulate the decreasing particle size during combustion. Experimental analyses of the actual solid fuel were performed and the data was utilized for model development. The solid fuel composition was defined by proximate and ultimate analyses. The fuel particles behavior during devolatilization and combustion was tested through thermogravimetric analysis (TGA) under various particle heating rates. The kinetic parameters of the applied mechanism and models were estimated and validated against the experiments. The in-house CFD-adapted solid fuel combustion model was written and resolved in C++ language, which was required for CFD coupling compatibility. Results from the solid fuel combustion model are presented and compared with data obtained from the experimental configurations.

KEYWORDS: Solid fuels combustion, Solid fuels devolatilization, CFD, Cement kiln

INTRODUCTION

In order to mitigate carbon dioxide emissions, which originate from both fuel combustion and thermal decomposition of calcium carbonate in the cement production industry, comprehensive simulation tools are essential for optimizing the cement production process. A digital twin CFD model of a real cement kiln is currently under development, aiming to guide the industry towards substitution of fossil fuels with alternative fuels and thereby a reduced carbon footprint. The CFD model will take into account the interactions among the main burner, the material bed, the solid fuel combustion and the kiln walls and it will be able to predict key operating parameters such as flame length, heat transfer and pollutant emissions.

The present study is a crucial step in the above methodology as it aims to develop a solid fuel combustion model capable of predicting species evolution and concentrations and char burnout.

Solid fuels combustion is characterized by two stages. The devolatilization stage, which occurs at relatively low temperatures, involves the evaporation of moisture and volatile species from the solid structure into the gas phase, followed by residual char combustion. One devolatilization modeling approach is to consider the process as a single step reaction influenced by the volatiles concentration in the solid. However, this is not an accurate approximation. Several volatiles are usually present in the solid fuel requiring different activation energies to allow their devolatilization, indicating a multi-step process. Therefore, a multi-step mechanism that includes lumped chemical species was applied in this work.

The second stage is the residual carbon char combustion, which is also considered to be the limiting step [3] of the overall process. It is safe to consider char combustion as a single-step reaction that produces carbon monoxide, which latter is converted into carbon dioxide or directly produces carbon dioxide. The porous structure of the solid fuel enhances the combustion rate, as it provides additional surface area for the heterogeneous reaction [4]. Incorporating such an effect is meaningful for developing more generic models that can be applied to a wider range of similar solid fuels, such as coals from different sources, but increasing the effort of the characterization procedure. The current model does not consider the porous structure enhancement as it is beyond the scope of this work.

MATERIALS AND METHODOLOGY

Solid fuels characterization

A comprehensive experimental campaign for solid fuel characterization has been conducted to provide the necessary information to the modeling activities. Solid fuel elemental analysis was performed using the ASTM D 5291 combustion standard. In addition, Energy Dispersive X-ray Spectroscopy (EDS) was used to identify chemical elements that could not be determined from the elemental analysis. Thermogravimetric Analysis (TGA) coupled with Differential Scanning Calorimetry (DSC) was performed to determine the kinetic parameters of volatiles release and solid residue combustion. The High Heating Value (HHV) of the fuel was also established using an isoperibol bomb calorimeter.

Solid fuel combustion model

A literature review [5] of the state-of-the-art combustion models was conducted and the most appropriate models were chosen that can provide adequate accuracy with reasonable computational cost. Although the char combustion is a rather complicated process, this model was kept simple to provide an order of magnitude approximation [3]. Solid fuel particle devolatilization was modeled using a multi-step lumped species mechanism [1] to provide a realistic species composition. Each mechanism reaction is described by the Arrhenius equation, the parameters of which were estimated using experimental data and an optimization-based algorithm in gPROMS software that minimizes normally distributed errors. The reaction mechanism is presented in

Table **1**. The solid fuel characterization procedure provides information about the elemental analysis which can be related to five initial fictitious components, named as reference components; i.e. Coal1 ($C_{12}H_{11}$), Coal2 ($C_{14}H_{10}O$), Coal3 ($C_{12}H_{12}O_5$), CharH (C_2H) and CharC (pure carbon).
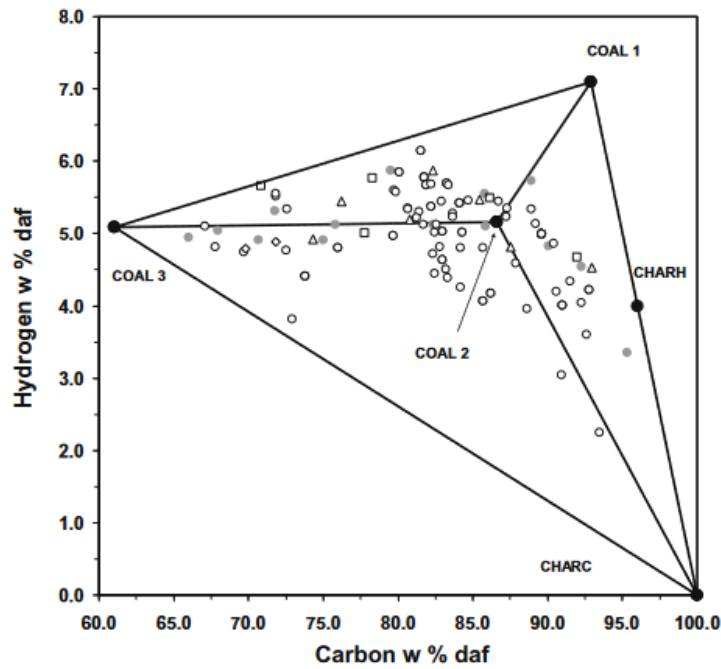
Figure 1. *Initial solid fuel reference components related to elemental analysis, as obtained from* [1] .

Table 1. *Devolatilization reaction mechanism, as obtained from* [1].

	Elements
1	Coal1 → 5 CharH + 0.1 CharC + 0.2 H_2 + 0.9 CH_4 + C_{2-5}*
2	Coal1 → Tar1*
3	Coal1 → 5 CharH + 0.25 CharC + 0.5 H_2 + 0.75 CH_4 + C_{2-5}
4	Coal1 → Tar1*
5	Tar1* → Tar1
6	Tar1* + CharH → 5.3 CharH + 3 CharC + 2.55 H_2 + 0.4 CH_4
7	Tar1* + CharC → 4.3 CharH + 4 CharC + 2.55 H_2 + 0.4 CH_4
8	Coal2 → 2 CharC + 3.94 CharH + 0.25 COAL1 + 0.04 BTX* + 0.31 CH_4* + 0.11 C_{2-5}* + 0.11 $\{COH2\}$* + 0.15 $CO2$* + + 0.41 H_2O* + 0.18 CO* + 0.265 H_2
9	Coal2 → 0.61 CharC + 4.33 CharH + 0.21 Coal1 + 0.16 BTX* + 0.27 CH_4 + 0.7 CO + 0.1 H_2O + 0.2 $\{COH2\}$* + 0.28 H_2
10	Coal2 → Tar2*
11	Coal2 → Tar2
12	Tar2* → Tar2
13	Tar2* + CharH → 1.5 CharC + 7 CharH + H_2O* + 0.5 CH_4
14	Coal3 → 2.73 CHARC + 1.8 CHARH + 0.22 COAL1 + 0.08 BTX* + 0.2 Ox–C + 0.1 CH_4* + 0.11 C_{2-5}* + 0.2 H_2 + + 0.6 $\{COH2\}$* + 2.2 H_2O* + 0.1 $CO2$ + 0.4 $CO2$* + CO*
15	Coal3 → Coal3*
16	Coal3* → 1.5 CHARH + 0.82 CHARC + 2.08 CO + 0.25 Ox–C + 0.14 CH_4 + 0.7 C2–5 + 0.5 $CO2$ + 0.47 $\{COH2\}$* + 0.16 BTX* + 0.25 COAL1 + 1.2 H_2O + 0.29 H_2
17	Coal3 → Tar3* + CO_2* + H_2O
18	Coal3 → Tar3 + CO_2 + H_2O
19	Tar3* → Tar3
20	Tar3* + CharH → 4 CharH + 2.5 CharC + 0.2 CH_4 + 2 $\{COH_2\}$* + 0.8 H_2 + 0.3 C_{2-5}
21	CH_4* → CH_4
22	C_{2-5}* → C_{2-5}
23	BTX* → BTX
24	CO* → CO
25	CO_2* → CO_2
26	H_2O* → H_2O
27	$\{COH_2$*$\}$ → CO* + H_2

A kinetic diffusion model [2] was applied to the subsequent char combustion. The model can be described by equation (1) in the model, which relates the burning particle mass flux rate with

contributions from both the combustion reaction kinetics, $\mathcal{R}$ (m/s), and the oxygen diffusion in the gas phase, D_0 (m²/s). Depending on the conditions, and especially the particle temperature, either of the above contributions can be the limiting one.

$$\frac{dm''_p}{dt} = -A_p \frac{\rho_{ox} R\, T_\infty\, Y_{ox}}{MW_{ox}} \frac{\frac{D_0}{d_p} \mathcal{R}}{\frac{D_0}{d_p} + \mathcal{R}} \tag{1}$$

$$D_0 = C_{diff}\left(\frac{T_p + T_\infty}{2}\right)^{0.75} \tag{2}$$

$$\mathcal{R} = k_0 \exp\left(-\frac{E_A}{R\, T_p}\right) \tag{3}$$

In the equations above, m''_p (kg/m²), A_p (m²) and d_p (m) are the particle mass flux, surface and diameter respectively. Also, T_p and T_∞ (K) are particle and gas phase temperature, ρ_{ox} (kg/m³), Y_{ox} (-) and MW_{ox} (kg/m³) are the oxidizer mass density, mass fraction and molecular weight respectively and R (J/mol/K) is the gas constant. Finally, C_{diff} (m²/s/K$^{0.75}$), k_0 (m/s) and E_A (J/mol) are the parameters to be estimated.

The exothermic homogeneous reactions of each devolatilized species that take place in the gas phase were considered stoichiometric.

A shrinking particle model was applied to simulate the decreasing particle size and density during combustion. To obtain the model equations simple physical assumptions have been made; the particle has a spherical shape and the particle mass is being reduced together with either the particle density or size. For two distinctive times, t_1 and t_2, it can be shown that

$$\frac{d_p(t_2)}{d_p(t_1)} = \left(\frac{m_p(t_2)}{m_p(t_1)}\right)^{\frac{1}{3}\alpha}, \text{ with } \alpha \in [\,0,1] \tag{4}$$

The parameter α (-) represents the particle size contribution to the particle mass reduction during combustion, i.e. if it is equal to 0, only the particle density is decreased with constant particle size, while vice versa is true when α is equal to 1. In the model, α was assumed to be equal to 0.75.

The solid fuel particles trajectories were modeled in a Lagrangian framework within the Eulerian continuous gas phase. Experimental analysis of the actual fuel devolatilization was performed and the data was utilized to define the physical properties and kinetic parameters required. The CFD-adapted solid fuel combustion model comprises the in-house code written in C++ using stiff solvers and a computational fluid dynamic platform code as an intermediate to translate the heat and mass exchanges information between the present model and the CFD code.

RESULTS AND DISCUSSION

Solid fuels characterization

Solid fuel samples were analyzed in terms of elemental composition and the results are shown in Table 2. The fuel behavior during devolatilization and combustion was also experimentally tested through TGA.

Table 2. Quantitative composition of solid fuel as determined by elemental analysis.

Elements	Solid Fuel (wt. %)

C	85.10
H	3.67
O	5.88
N	1.58
S	3.33
Ca	0.45
HHV (MJ/kg)	34.57

Solid fuel combustion model validation

The solid fuel devolatilization model was validated against experimental TGA measurements carried out under inert atmosphere at various heating rates. First, the multi-step reaction mechanism was performed and experimental TGA results were fed into the model to estimate its reaction kinetics. After pyrolysis of the sample, it is assumed that mainly char remains. A second TGA protocol was used for the combustion of the char residue under air atmosphere. The simulation results are presented against the experimental ones for both experimental protocols in Figure 2; (a) for the devolatilization and (b) the char combustion stage. Figure 2(a) also shows predictions of the solid fuel devolatilization at higher heating rates, i.e. 100 K/min and 10^4 K/min.
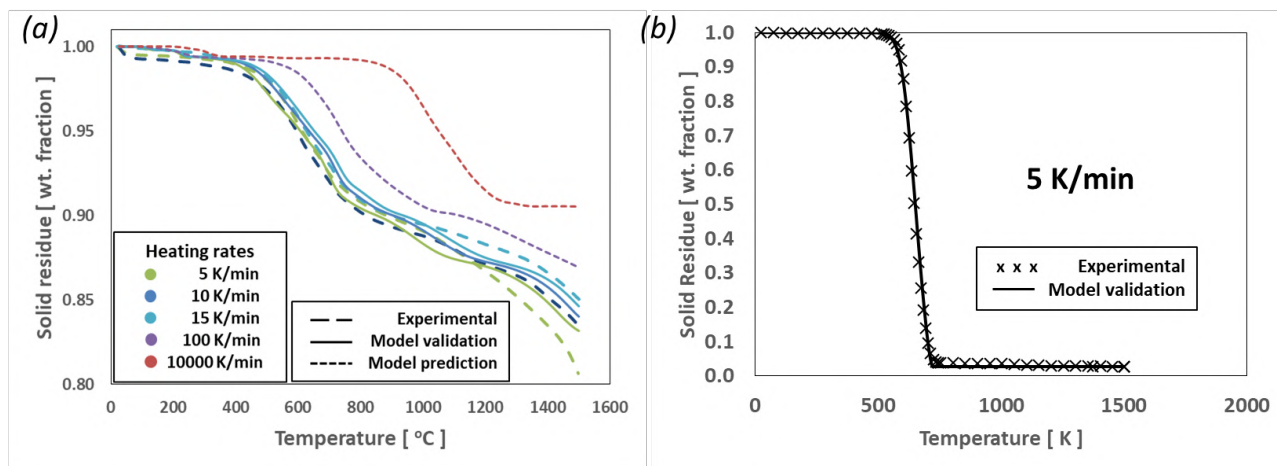

Figure 2. *Solid fuel model results compared with in-house experimental TGA measurements at different heating rates for (a) the devolatilization stage and (b) the char combustion stage.*

CONCLUSIONS AND DISCUSSION

The solid fuel combustion model is designed to integrate seamlessly with a CFD model, offering the required information on the fuel particles combustion. The model resolves physico-chemical equations, facilitating the evolution of gaseous species into the gas phase during the devolatilization stage. Additionally, the model predicts the heat generated by the heterogeneous reactions occurring during fuel particles combustion.

In comparison with TGA experiments, the model presents a good and physical behavior. Additional experiments are required for both devolatilization and char combustion at higher heating rates. With the existing instrumentation capabilities, this could be performed at heating rates up to 100 K/min. This range of heating rates is low for the real process conditions. However, the model can represent the combustion behavior in different heating rates which develops confidence about the model predictions under real cement kiln conditions. Additional experiments with different

configuration and higher particle heating rates can be taken into consideration, as similar modeling methodology can be applied.

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