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Sensitivity analysis of different kinetic factors for numerical modeling of Serbian lignite devolatilization process

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ABSTRACT

Numerical modeling is widely used tool for prediction of combustion processes. Computational Fluid Dynamics – CFD models use three kinetic rates for description of the coal combustion processes: coal devolatilization, volatile combustion and char combustion. Reported rates for coal devolatilization vary considerably among the authors depending on the type of experimental systems used in describing the phenomenon. Accurate representation of devolatilization process is necessary in order to perform successful CFD calculations of pulverized coal combustion and gasification. The subject of this work is numerical modeling of Serbian lignite pulverized coal devolatilization in drop tube type laboratory scale reactor. The aim of this study is to evaluate the influence of different devolatilization kinetic factors on total devolatilization time in numerical modeling of pulverized Serbian lignite devolatilization. Nine different devolatilization kinetic rates mostly used in devolatilization numerical modeling are compared in the presented work.

1. Introduction

Over the last 20 years CFD became powerful predictive and design tool in combustion research and development. CFD is commonly used for gaseous [1] and solid fuel (coal and biomass) burner's utilities, [2,3], and for test furnaces design and optimization [4,5], as well as for investigation of novel pulverized coal combustion technologies [6–9]. With increase of computational power CFD is also being successfully applied for combustion modeling of full scale industrial furnaces and whole boilers [10–14]. devolatilization process plays an important role in pulverized coal combustion and gasification processes. Thus, accurate representation of devolatilization process is necessary in order to perform successful CFD calculations of pulverized coal combustion/gasification.

Volatiles can account for up to 70% of the coal mass loss during combustion process, significantly increasing surrounding gas temperature in short period of time as a result of released volatiles combustion. Devolatilization has impact to combusting coal particle features from its injection to burnout. It influences particle ignition, trajectories, and eventual fragmentation as well as char intrinsic reactivity.

The two main theoretical approaches are used in devolatilization modeling: network devolatilization models and empirical devolatilization models. Models from the first group describe devolatilization behavior of the coal by approximating the breakdown of the macromolecular coal network structure. While network devolatilization models offer detail information about volatile species evolution they are not commonly used in commercial CFD codes that become restrictively slow if large coal network matrix programs were included in main solver body [7,15]. Because of this, network devolatilization models are usually employed as pre-processor routines in order to calibrate simpler empirical devolatilization models used for CFD analysis [15].

It is important to underline that in several studies, despite their higher computational demand, network models were fully utilized to predict particle devolatilization behavior during CFD combustion modeling. As example, A. Silaen and T. Wang in their work [16] investigated influence of different turbulence and devolatilization models on coal gasification simulation in entrained-flow gasifier. They compared totally four different deviolatilisation models among which one was Coal Percolation and devolatilization (CPD) network model. Authors concluded that empirical single rate model and CPD model produce consistent devolatilization rates. Recently, Jovanovic et al. compared performance of different devolatilization models in predicting ignition point position during pulverized coal combustion in O_2/N_2 and O_2/CO_2 atmospheres with different compositions [17]. Authors used two empirical models (single rate and two competing rates) and two network models (CPD and Functional Group – FG). Although, in general, better

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Nomenclature

$A[1/s]$	pre-exponential factor
d	diameter [m]
E_a	activation energy [J/kmol]
f	species mass fraction
k	kinetic reaction rate [1/s]
m	mass [kg]
T	temperature [K]

Greek symbol

α	weighting factor

Subscripts

a	ash
g	gas phase
P	coal particle
v	volatile species
0	initial content

agreement with experimental results was achieved using network models their high computational demand was pointed out.

Second group models are empirical devolatilization models that utilize global kinetics for modeling of complex devolatilization processes. Arrhenius expressions are used to correlate rates of weight loss caused by devolatilization with temperature. Since empirical devolatilization models require significantly lesser computational resources in compare with network devolatilization models they are widely used in comprehensive CFD codes [18]. However, empirical nature of these models makes them difficult for use for fuels and heating rates beyond those for which Arrhenius parameters were derived. Comprehensive reviews of devolatilization kinetic rates were reported by several authors [19–21]. Even though empirical devolatilization models require careful selection of relevant Arrhenius parameters for their successful application, reported results from relevant literature showed that when this condition is met they can predict particle devolatilization with satisfying accuracy. Hart et al. in their work modeled pyrolysis in lab-scale reactor at elevated pressures and high heating rates. Comparing numerical simulations with experimental data they showed that single reaction model could be appropriate for coal combustion CFD modeling as it as long as heating rates for the coal are comparable to the values found in industrial boilers [22]. Wendt and coauthors suggested numerical model for devolatilization and ignition of single coal particles. Particle devolatilization rate was calculated using empirical single rate model in this work. The obtained numerical results showed good agreement with the experiments for all investigated particle shapes [23]. Hashimoto et al. suggested novel devolatilization model – Tabulated-Devolatilization-Process (TDP). This model, similarly to other empirical devolatilization models (single rate model and two competing rates model), uses global kinetics based on Arrhenius expression to correlate particle temperature and mass loss. The main novelty lies in the fact that Arrhenius parameters, which are constant in case of single rate model and two competing rates model, change their values during simulation based on each particle temperature history. Arrhenius parameters database is prepared either based on experimental values or based on information obtained from network devolatilization models. Performed numerical simulations employing the TDP model are in better agreement with the experiments than that predicted by the other empirical models, with a slight increase in computation time [24,25].

Although significant efforts to determine the most appropriate Arrhenius kinetic parameters for number of different fuels and combustion conditions [17,26,27] were performed, no information's were found on influence of different devolatilization kinetic factors on overall combustion model for modeling of the Serbian lignite combustion. The subject of this work is numerical modeling of Serbian lignite pulverized coal devolatilization in drop tube type laboratory scale reactor. The aim of this study is to evaluate the influence of different devolatilization kinetic factors on total devolatilization time in numerical modeling of pulverized Serbian lignite combustion.

2. Mathematical model

ANSYS FLUENT version 12.1 [28] was used to model pulverized coal devolatilization inside drop-tube furnace. Overall model dimensions and geometry are shown in Fig. 1(a). This code uses an unstructured, collocated, finite volume discretization scheme to solve the fluid flow equations in computational space. The Finite volume grid was generated using ANSYS GAMBIT 2.4.1 pre-processor. Particular care has been given to the grid quality, since the numerical grid is crucial in order to achieve reliable CFD predictions. Even though triangular meshes are easy and time-efficient to construct, use of quadrilateral meshes is preferred in order to minimize numerical diffusivity.

Because of this computational grids consisting of all quadrilateral elements were employed in the presented work, Fig. 1(b). In order to obtain grid independent solution the four different computational meshes were constructed splitting each computational cell of previous grid into two new cells, thus obtaining very coarse, coarse, medium and fine grids consisting of 12,800, 25,600, 51,200, and 102,400 computational cells, respectively. devolatilization of 90 μm pulverized lignite coal particles using Single Rate devolatilization model with default FLUENT kinetic parameters was calculated on each grid. The obtained results, in terms of particle volatile fraction – particle path length dependency, showed that average relative difference between particle volatile mass fraction values calculated on medium and fine grids is less than 0.2%, Fig. 2. Based on this study medium grid with 51,200 computational cells was adopted for all further simulations.

The turbulent multi component flow field was calculated using Eulerian approach solving set of Partial Differential Equations (PDEs) for continuity, momentum, turbulence kinetic energy, turbulent dissipation rate, enthalpy, and volatile species mass fraction. Mass fraction of nitrogen, being dominant species, was determined by subtracting volatile species mass fraction from unity.

The standard k–ε turbulence model with default parameters, that was found to be satisfactory approach [29], is used to describe turbulent dynamic of the flow. Additional sources for kinetic turbulent energy k and turbulent dissipation rate ε are used to calculate the effects of particle-to-gas turbulence flow. The standard k–ε model was developed using the assumption that the fluid flow is fully turbulent, and the effects of molecular viscosity are negligible. Therefore this model is not valid in near-wall regions. In order to resolve flow characteristics in near-wall region, standard wall functions were used. In this approach, analytical expressions are used to calculate the velocity and temperature values from the wall to the nearest point in the computational grid. In this way,