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# Transient model for soot formation during the combustion of single coal particles

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## Abstract

A transient mathematical model was developed to describe soot formation during the combustion of single coal particles based on the static semi-empirical model presented by Fletcher and coworkers. Sensitivity analyses of the model parameters show that soot emissivity and mass diffusivity of tar play an important role in predicting soot volume fraction ($f_v$) and flame temperature ($T_f$). The model was applied to simulate the combustion of single bituminous coal particles with initial diameter ($2r_0$) of 83 μm in a drop tube furnace and air atmosphere. It was found that soot is only formed within the first ~ 5 ms after the appearance of the volatile flame. Although most of the soot is oxidized during the volatile flame phase, a small portion of soot still remains during the char combustion. Due to the soot presence, the volatile flame duration is extended by 2.6 ms. Compared with the soot-free flame, the sooting flame has remarkable lower $T_f$ and its peak $T_f$ value is ~ 410 K lower. As a consequence, char combustion starts at a temperature that is ~ 125 K lower than that of the soot-free case. Spatially, the peak $f_v$ at 16.6 ms appears at 4.5 $r_0$ and soot oxidation zone spans to ~ 10 $r_0$. The model was validated by comparing the predicted $T_f$ and $f_v$ under different $O_2$ mole fractions ($x_{O2}$) with recent experimental results reported by Khatami and coworkers. The predicted trends are consistent with those of the experimental results. With increasing $x_{O2}$, $T_f$ increases, but the increase rate becomes more gradual at a large $x_{O2}$. While for $f_v$, a non-monotonic variation is observed, where soot first increases and then decreases with a peak value occurring at $x_{O2} \approx 40\%$.


*Keywords:* Coal combustion; Soot formation; Transient model; Flame temperature; Single particle

## 1. Introduction

Studies on soot formation have been undertaken for several decades, but most of them focus on the gaseous hydrocarbon flames [1–3,24]. In fact, during combustion process of solid hydrocarbon fuels,

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such as coal, soot could be also massively produced [4,5] and plays a critical role in flame temperature, radiative heat transfer, and pollutant formation in pulverized coal fired boilers [6–8]. Well understanding and modeling the soot formation in coal combustion are of great significant.

So far, a few models on soot formation in coal combustion have been developed and they can be classified into empirical [6, 9], semi-empirical [7,8] and detailed [10] types. The empirical models [6,9] directly correlate soot volume fraction ($f_v$) to local equivalence ratio ($\phi$) and the amount of volatile carbon. The models are convenient to use for CFD modeling, but with low accuracy and generality, since they barely account for the physical and chemical processes of soot evolution. On the contrary, the detailed mechanisms (e.g., [10]) use detail kinetics to describe the secondary reactions of coal volatiles revealing more insights on soot formation, but with rather large computational cost.

Against the empirical and the detailed models, the semi-empirical models consider the major sub-processes such as nucleation, oxidation, and agglomeration [7,8], and approximately describe the essential characteristics of soot evolution in coal combustion with rather low computational cost. For example, with a semi-empirical model, Lau and Niksa [7] showed that soot reduced the flame temperature $T_f$ by up to 300 K and radiated 8–14% of the heat from volatile combustion. However, in the model, volatile combustion and conversion of tar into soot were assumed to be infinitely fast and thus flame is infinitely thin. Kinetic effects on soot formation are therefore neglected. However, as reported by Thomas et al. [11] that the thickness of the volatile flame can be several times of the coal particle radius. More recently, Fletcher and co-workers presented an improved semi-empirical model for soot formation [5,8]. In the model, the kinetics of soot formation is considered and the pyrolysis behavior of coal particles is described with the Chemical Percolation Devolatilization (CPD) model. Thus, this model is regarded to be more promising in predicting $f_v$ and $T_f$.

However, the parameter sensitivities in the model of Fletcher and co-workers [5] and Brown and Fletcher [8] were not evaluated. Furthermore, the model was developed for steady condition, and thus not valid for studying the soot evolution in coal flames. Since soot evolution is strongly coupled with the flame structure and the intermediate species distribution [2,3], a transient model to describe the soot evolution is demanded.

Therefore, in the present study, based on the study of Fletcher and co-workers [5] and Brown and Fletcher [8], a transient formulation is developed to describe soot formation during combustion of single coal particles. Sensitivity analyses of the model parameters are conducted. Moreover, the interactions between the flame temperature, structure, and soot formation are assessed. To validate the model, the predictions on soot formation and flame temperature are compared with the recent experimental results measured in a drop tube furnace by Khatami et al. [12].

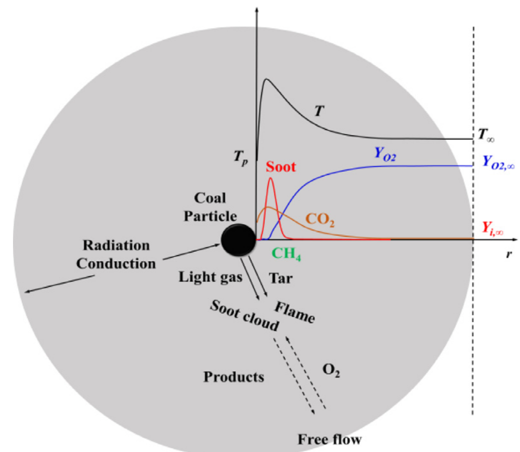


Fig. 1. Schematic of the energy and species transport in the model.

## 2. Model description and formulation

### 2.1. Problem description

Figure 1 schematically depicts the typical temperature and species mass fraction profiles around a coal particle burning in a free, high temperature environment. The coal particle is heated up by thermal conduction from the hot gas and radiation from the hot wall. Once the particle reaches a certain temperature, pyrolysis takes place and volatile matters including light gases and tar are released from the particle. Soot particles are formed in the rich regions during the combustion of volatile matter.

Figure 2a further depicts the reaction pathways for soot formation during coal combustion, similar to those described by Brown and Fletcher [8]. Three species (gases, tar, and char) are produced during the primary pyrolysis. Tar is considered the only precursor of soot, but can also undergo cracking into light gases or oxidation by $O_2$ under high temperature [8,13]. The corresponding reactions are given in Fig. 2b. Soot is assumed to be pure carbon, and the products of soot oxidation are assumed to be $CO_2$. The agglomeration of primary soot particles is calculated using Ulrich's model [14], based on the collision frequency for uncharged spherical aerosols of varying sizes.