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# Investigation of the soot formation during wood log combustion

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**ABSTRACT**

Soot formation is an important issue in the design of modern wood stoves, as soot not only deteriorates the combustion efficiency but also poses threats to human health. Although soot formation in biomass combustion has been studied previously, the investigation at wood stove level is still rare due to its complex nature. In this paper, a preliminary numerical simulation is carried out to uncover the basic trends of soot formation during wood log combustion. The soot formation model is developed based on a virtual particle multiphase flow algorithm, where the mass fraction and the particle size of the soot are both resolved. Three wood logs combusting in a confined wood stove with a parallel stacking is studied. The coupling effect of the soot formation with the heating and the combustion of the wood logs is analyzed. This work is helpful for the design and the optimization of modern wood stoves. The predicted soot mass fraction and size distribution provide important information for a better control of particulate matter emission.

**Keywords:** Wood stove, combustion, soot formation, virtual particle method

**NONMENCLATURE**

| *Symbols* | |
|---|---|
| $T_s$ | Solid temperature, K |
| $\rho_s$, $\rho_g$ | Solid and gas phase density, kg/m$^3$ |
| $\varepsilon_g$ | Porosity, - |

## 1. INTRODUCTION

Small-scale wood combustion in fireplaces is an important part of the energy supply in some European countries such as Sweden. With the requirement of energy efficient modern houses, the design of low-nominal-load wood stoves is becoming increasingly important. However, for the low-load operation, the pollutant emission, especially nanoparticulate emission such as soot, becomes a serious problem. During insufficient combustion, tar species easily convert to soot, which causes air pollution and contamination of the stove. More importantly, these particulate species usually contain chemical species that are harmful to human health. Therefore, soot formation is a nonnegligible problem for the design of modern wood stoves.

Soot formation during biomass combustion has long been realized as a complex issue. In recent years, Trubetskaya et al. has done a lot of work on soot formation during the pyrolysis of biomass in drop tube furnaces [1]. It is found that the lignin content contributes the largest amount of soot formation compared with cellulose and hemicellulose. Deng et al. found similar trends for the soot formation during the basic biomass component pyrolysis [2]. Ferreiro et al also studied the soot formation during biomass gasification [3]. However, these experimental works are all carried out in drop tube furnaces. When it comes to larger reactors such as a wood stove, the soot formation becomes more complex [4]. Moreover, the soot formation process itself is also a complex issue that has not been fully understood, which usually follows a series

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of nucleation processes relating to not only physical but also chemical conversions.

In this paper, we aim at developing a simplified soot formation algorithm that is suitable for efficient prediction of soot formation during wood stove combustion. The mathematical model is presented in Section 2. Numerical results and discussions are shown in Section 3. Finally, some conclusions are drawn in Section 4.

## 2. MATHEMATICAL MODEL

Wood log combustion is a complex multidisciplinary problem, which includes the thermal conduction of the solid material, the flow field evolution, the pyrolysis and chemical reactions. Considering the fact that the wood log becomes a porous char material after devolatilization, it is modeled as a porous media and a virtual particle method is used to simulate the heating and the pyrolysis of the solid wood log. During the simulation, the wood log is discretized into a cluster of virtual particles. Together with the surrounding gas phase environment, the virtual particle cluster combusting in air is treated as a multiphase flow system. Table 1 presents the virtual particle heat transfer equation and the flow field governing equations.

In numerical simulations, CFD computational grid is generated both inside and outside the wood log. Based on the CFD grid inside the wood log, the porous wood structure is discretized into a cluster of virtual particles. Initially, the porosity of the wood log is set to a small value of 0.1. With pyrolysis goes on, the virtual particles shrink according to a shrinking core model, resulting in the evolution of the internal porosity. The combustion of the released pyrolysis gas further accelerates the heating process inside the wood log. Note that this is only an appropriation of the real heating and combustion process. More realistic wood combustion model will be developed in the future work.

Table 1. solid and gas phase governing equations.

| | Governing equations |
|---|---|
| Virtual particle | $\rho_s c_s \frac{\partial T_s}{\partial t} = hS'\left(T_g - T_s\right) + \frac{e_s S'}{4}\left(G - 4\sigma T_s^4\right) + Q$ |
| Gas phase | $\frac{\partial}{\partial t}\left(\varepsilon_g \rho_g\right) + \nabla\cdot\left(\varepsilon_g \rho_g \boldsymbol{u}_g\right) = S_{p,m}$ |
| | $\frac{\partial}{\partial t}\left(\varepsilon_g \rho_g \boldsymbol{u}_g\right) + \nabla\cdot\left(\varepsilon_g \rho_g \boldsymbol{u}_g \boldsymbol{u}_g\right) = -\nabla p + \nabla\cdot\left(\varepsilon_g \boldsymbol{\tau}_{eff}\right) + \varepsilon_g \rho_g \boldsymbol{g} + S_{p,mom}$ |
| | $\frac{\partial}{\partial t}\left(\varepsilon_g \rho_g E\right) + \nabla\cdot\left(\varepsilon_g \boldsymbol{u}_g (\rho_g E + p)\right) = \nabla\cdot\left(\varepsilon_g \alpha_{eff} \nabla h_{sen}\right) + S_h + S_{p,h} + S_{rad}$ |
| | $\frac{\partial}{\partial t}\left(\varepsilon_g \rho_g Y_i\right) + \nabla\cdot\left(\varepsilon_g \rho_g \boldsymbol{u}_g Y_i\right) = \nabla\cdot\left(\varepsilon_g \rho_g D_{eff} \nabla Y_i\right) + S_{p,Y_i} + S_{Y_i}$ |

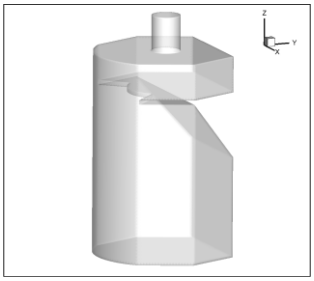
Table 2. pyrolysis, gas phase combustion and soot formation reactions.

| | Reactions |
|---|---|
| pyrolysis | $m_s = \sum \alpha_i m_s, \quad \sum \alpha_i = 1$ |
| | $i$ = $H_2O$, $H_2$, CO, $CO_2$, $C_6H_{6.2}O_{0.2}$(tar), $C_2H_2$, char, and ash. |
| Combustion | $H_2+0.5O_2=H_2O$ |
| | $CO+0.5O_2=CO_2$ |
| | $C_2H_2+O_2=CO_2+H_2O$ |
| | $C_6H_{6.2}O_{0.2}+2.9O_2=6CO+3.1H_2$ |
| Soot formation | $C_2H_2=2C+H_2$ |

Soot formation depends largely on tar and flow field evolutions during biomass combustion. Tar is a pyrolysis compound containing hundreds of chemical species such as benzene, naphthalene, anthracene and pyrene. Under high-temperature conditions, some of the tar species will convert to hydrocarbon ring structures, the so-called polycyclic aromatic hydrocarbons (PAH). With a complex nucleation process, the PAH is finally converted to soot particles [5]. However, the current paper is not aimed at a detailed description of the tar and soot formation processes. Instead, tar is simplified as $C_6H_{6.2}O_{0.2}$ and soot precursor is modeled as $C_2H_2$ [6]. Table 2 shows the pyrolysis, the combustion and the soot formation reactions. The char combustion reactions are taken from our previous work [7]. For the simulation of soot evolution, a classical two-equation model is used [7].

## 3. RESULTS AND DISCUSSIONS

The established algorithm is used to simulate the soot formation from three wood logs combusting in a wood stove. Figure 1 shows the geometry and the computational grid of the wood stove. The air comes from the bottom of the stove and is released at the top outlet boundary during the combustion. In the current simulation, three wood logs with the size of 5×5×20cm are placed parallelly near the bottom of the furnace. For simplicity, the time-varying mass flow rate of the inlet air is set to a constant value of 5.0e-4 kg/s in the current test.



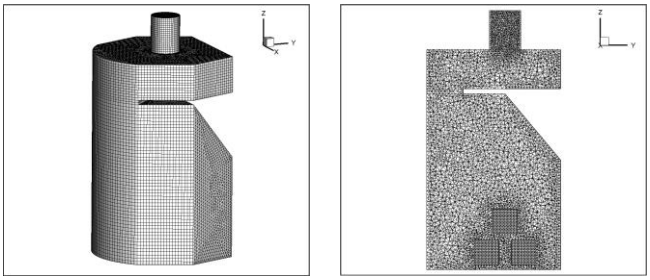


Figure 1. The geometry of the wood stove and the computational grid.

Figure 2 presents the temperature and the pyrolysis gas species distribution at the symmetry plane of the furnace 3 seconds after ignition. It is seen that the temperature inside the wood log (~600K) is much lower than the combusting environment, resulting in an unsynchronized pyrolysis process in the radial direction of the wood log. The tar species distribution is similar to that of the light gas species of CO. The mass fraction of tar reaches a maximum of 0.14 above the upper wood log. Figure 3 presents the soot mass fraction and the particle size distribution. It is shown that the maximum soot mass fraction reaches 0.05 near the flame zone where the local temperature is close to 1800K. Besides, the high mass fraction of soot is also seen in the intermediate zone between the wood logs, indicating that the soot formation is influenced by both high temperature and the stacking pattern of the wood logs. The soot particle size distribution illustrates that the primarily formed soot near the flame zone tend to concentrate in the low-speed leeward area and grows gradually. Under the tested air flow rate, the maximum soot particle size reaches 260nm.

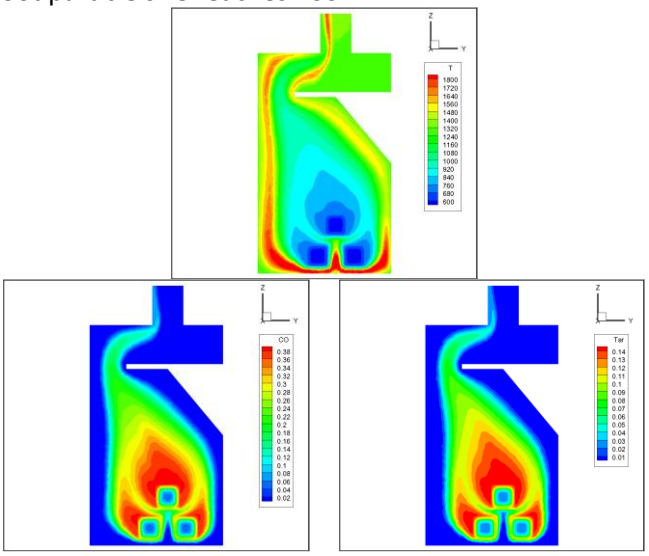


Figure 2. Temperature and pyrolysis gas species distribution during combustion.

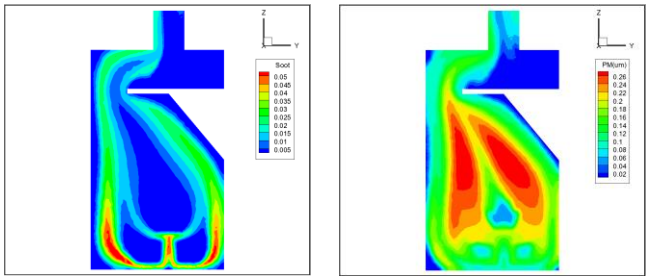


Figure 3. Soot mass fraction and particle size distribution.

## 4. CONCLUSIONS

A multidisciplinary wood log combustion algorithm together with a soot formation model is established. The tar and soot evolutions are treated in a simplified but efficient way, where tar is model as a single compound of $C_6H_{6.2}O_{0.2}$ and soot precursor is modeled as $C_2H_2$. The model is demonstrated to be a capable tool to predict the basic trend of tar and soot evolutions during wood log combustion in a three-dimensional wood stove. A preliminary numerical simulation is carried out for 3 seconds of wood log combustion. It is found that the maximum tar mass fraction reaches 0.14 during the ignition process. The corresponding maximum soot mass fraction reaches 0.05 and the largest soot particles exceed 200 nm in diameter. Numerical results demonstrate that flame temperature and the relative positions between wood logs are the potential influential factors that would cause significant impact on soot formation. Moreover, the soot particle size distribution is closely related to the flow field characteristics.

## ACKNOWLEDGEMENT

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