The Finite Heat Conduction Model of Single Droplet Combustion and its Verification

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1 Introduction

Two typical methods, lumped parameters model and onion-skin model, are often used to describe the heat flow through the droplet surface in the modelling of a steady single fuel droplet evaporation and combustion. The lumped parameters model regards the temperature in different positions of the droplet as the same. So the heat flux through the droplet surface could be described as [1]:

$$\dot{Q}_{i-l} = m_d c_{pl} \frac{dT_d}{dt} \tag{1}$$

Where m_d is the total mass of the droplet, c_{pl} is the specific heat capacity, T_d is the temperature of the droplet, and $\dot{Q}_{i\text{-}l}$ is the heat conducted into the droplet per second. In this model, the heat conductivity in the droplet has been regarded as an infinite value. Thus, the temperature in the droplet is uniform.

For the onion-skin model, the droplet is divided into two parts. One is the droplet surface with the temperature of T_s, the other is the inner part of the droplet with the temperature of T_0, which is the initial temperature of the droplet. So the heat flow through the droplet could be written as [1]:

$$\dot{Q}_{i-l} = \dot{m}_F c_{pl} \left(T_s - T_0\right) \tag{2}$$

Where, $\dot{m}_F$ is the mass burning rate. In this model, the heat conductivity is regarded as an infinitesimal value because the temperature in the droplet does not change. The heat assimilation only driven by the evaporation causing mass transfer.

In this study, a modified single droplet evaporation and combustion model is developed, which involves finite heat conduction with respect to the classical one [1~3]. The comparison between

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the finite heat conduction model and the onion-skin model is demonstrated. The model is also verified through comparing the calculated results with existing simulation and experiment.

2 Physical Model

The physical model is schematically shown in Figure 1. The droplet is in a spherical shape with a concentric flame surface. The environment is divided into two parts. One is the unburned area, the other is the burning area. The interface between these two areas is the flame surface, where the fuel vapor and the oxidizing agent are reacted completely. In the unburned area, there are fuel vapor and reaction product. While in the burning area, there are oxidizing agent and reaction product. The spatial variable is only the radial distance. As for the temperature, it will rise up when the radial position goes from the center of the droplet to the flame surface. While outside the flame surface, the temperature will decrease until it reaches to the value at the infinite position.

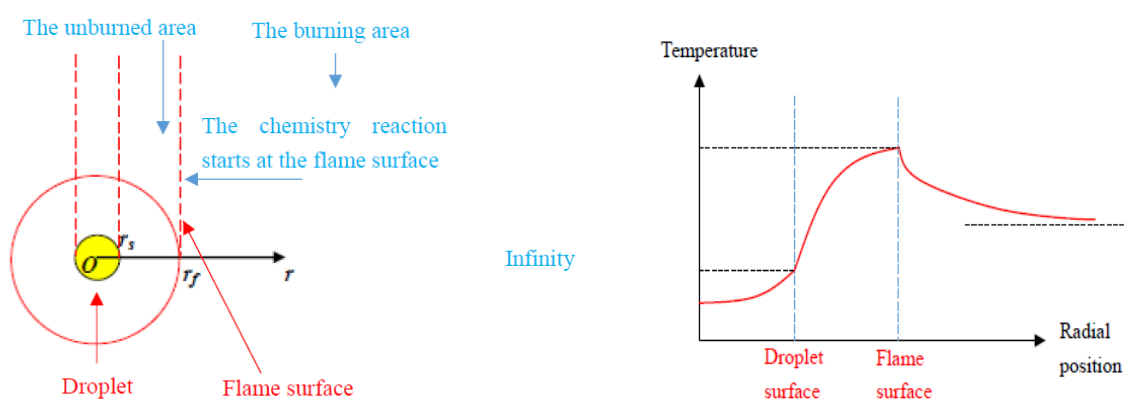

Figure.1 The physical model of the droplet combustion and a general temperature distribution

3 Finite Heat Conduction Model

To describe the heat flow through the droplet surface in another way, the heat conducted into the droplet per second has been calculated according to the temperature gradient at the droplet surface, which is obtained from the calculation of the temperature distribution in the droplet. Thus, the development of the finite heat conduction model could be demonstrated as follows.

1) Calculate the temperature gradient by the unsteady heat conduction model.
2) Describe $\dot{Q}_{i-1}$ in a new way and add it into the classical model.
3) Develop the finite heat conduction model and obtain the results.

According to the Fourier's law, the spherical one dimensional heat conduction model is written as Equation (3).

$$\frac{1}{r^2}\frac{\partial}{\partial r}(k_l r^2 \frac{\partial T_d}{\partial r}) = \rho_l c_{pl} \frac{\partial T}{\partial t} \tag{3}$$

The boundary and initial conditions are shown as follows.

$$\left.\frac{\partial T_d}{\partial r}\right|_{r=0} = 0, \qquad T_d(r_s) = f(T_s), \qquad T_d(r,0) = T_0 = 308.15K \tag{4}$$

Here $f(T_s)$ is designed to approximate the temperature increase at the droplet surface.

Thus, the calculated temperature distribution is shown in figure.2.

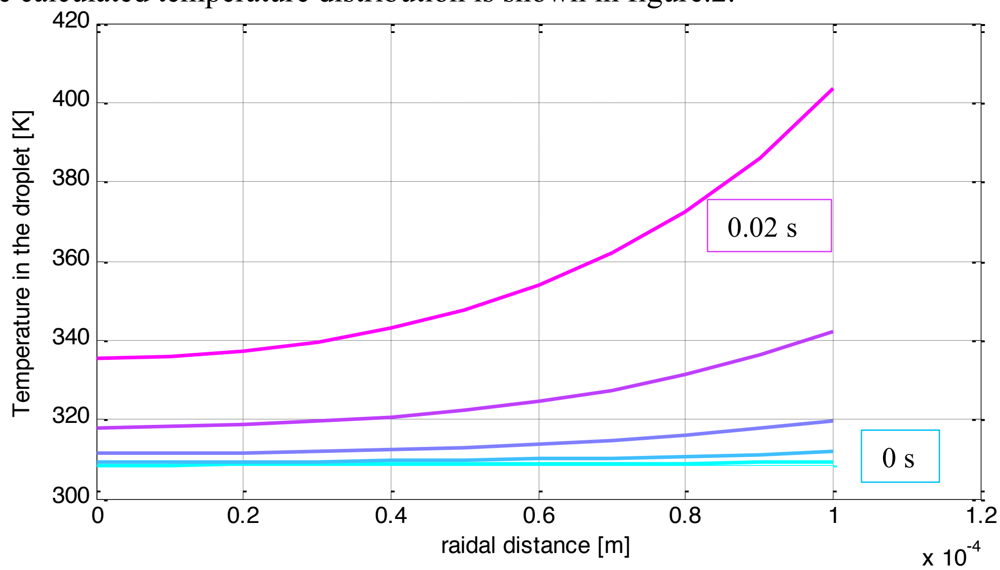

Figure2. Temperature distribution in the droplet

From the final droplet temperature distribution, $\dot{Q}_{i\text{-}l}$ can be written as:

$$\dot{Q}_{i-l} = k_l 4\pi r_s^2 \overline{\left.\frac{\partial T_d}{\partial r}\right|_{r=r_s}} \tag{5}$$

Where, r_s is the droplet radius, and k_l is the heat conductivity of the droplet. The average temperature gradient on the right side of the equation is approximated by temperature difference. This is a sort of discretization method, which is shown as:

$$\overline{\left.\frac{\partial T_d}{\partial r}\right|_{r=r_s}} = \frac{(T_s - T_0)}{r_s} \tag{6}$$

Thus, the finite heat conduction model can be written as follows.

The energy conservation equation at the droplet surface is:

$$\frac{\exp(-Z_T \dot{m}_F / r_s)}{\exp(-Z_T \dot{m}_F / r_s) - \exp(-Z_T \dot{m}_F / r_f)} = \frac{h_{fg} + \dfrac{k_l 4\pi r_s^2 \overline{\left.\frac{\partial T_d}{\partial r}\right|_{r=r_s}}}{\dot{m}_F}}{c_{pg}(T_s - T_f)} \tag{7}$$

The energy conservation equation at the flame surface is:

$$\frac{(T_s - T_f)\exp(-Z_T \dot{m}_F / r_f)}{\exp(-Z_T \dot{m}_F / r_s) - \exp(-Z_T \dot{m}_F / r_f)} - \frac{(T_\infty - T_f)\exp(-Z_T \dot{m}_F / r_f)}{\exp(-Z_T \dot{m}_F / \delta_T) - \exp(-Z_T \dot{m}_F / r_f)} = \frac{\Delta h}{c_{pg}} \tag{8}$$

The species mass conservation equation in the unburned area is:

$$Y_{F,s} = 1 - \exp(-\dot{m}_F / (4\pi\rho_{in} D_{in} r_s)) \Big/ \exp(-\dot{m}_F / (4\pi\rho_{in} D_{in} r_f)) \tag{9}$$

The species mass conservation equation in the burning area is.

$$\exp(Z_F \dot{m}_F / \delta_M) \Big/ \exp(Z_F \dot{m}_F / r_f) = v \big/ v + 1 \tag{10}$$

Finally, the Clapeyron equation at the droplet surface, modelling the evaporation process and the gas-liquid equilibrium, can be demonstrated as:

$$Y_{F,s} = \frac{A\exp(-B/T_s) MW_F}{A\exp(-B/T_s) MW_F + [P - A\exp(-B/T_s)] MW_{pr}} \tag{11}$$

Assembling these equations together with essential physical property parameters and boundary conditions, the finite heat conduction model can be obtained. Here, the main combustion parameters signified as T_s, $\dot{m}_F$, T_f, $Y_{F,s}$, r_f are droplet surface temperature, mass burning rate, flame temperature, fuel vapor mass fraction at the droplet surface, and flame radius, respectively. The distribution of the temperature and the component are also included in the model.

4 Results Discussion and Model Verification

To analyze the variation of the developed model in this study, the comparison between the convection model and the finite heat conduction model is performed. The convection model deals with the impacts of convection by setting the boundary conditions at the position of corrected film radius, instead of the position of infinity[1][4,5].

The calculation is done under the condition that the fuel is set as isooctane. The ambient pressure is set as 0.4 MPa, while the ambient temperature is 308.15 K, and the initial droplet radius is 100 μm. The airflow velocity is 10 m/s. The calculated fuel mass fraction in the unburned area and the oxidizing agent in the burning area using the finite heat transfer model and the convection model are shown in Figure 3.

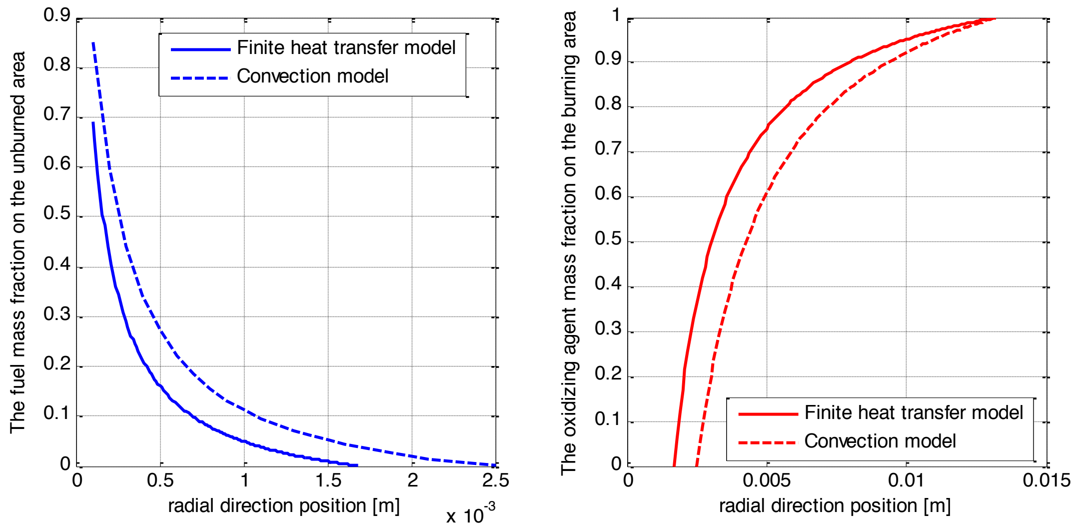

Figure 3. Component distribution from the convection model and the finite heat conduction model

The fuel mass fraction and the oxidizing agent mass fraction are more close to the droplet and the variation tendency of the curves are more rapid. At the same radial position, the fuel mass fraction calculated by the finite heat conduction model is lower and the oxidizing agent mass fraction is higher than the convection model. This may be caused by the difference of the heat transferred into the droplet. $\dot{Q}_{i\text{-}l}$ is raised by nine times from the convection model to the finite heat transfer model. Thus, more heat is absorbed and conducted into the inner part of the droplet rather than stay at the surface of the droplet. So less fuel could gain enough heat to evaporate.

The finite heat conduction model verification is performed according to the simulation results from Zhao [6] and the experiment data from Raghavan [7]. Table 1 shows the comparison between the results obtained by the convection model and the finite heat conduction model under the same conditions as the experiment, and the experimental data for three flow velocities. It is obvious that the results of the finite heat conduction model in this study are more close to the experiment than the classical convection model especially under the last two flow velocities.

Table 1. The results of the mass burning rate

Flow velocity (m/s)	Convection model ($\times 10^{-6}$ kg/s)	Finite heat conduction model ($\times 10^{-6}$ kg/s)	Experiment ($\times 10^{-6}$ kg/s)
0.4	9.638	10.032	9.2
0.6	9.676	10.071	10.0
0.8	9.713	10.110	10.9

In spite of error analysis, the mean square error between the results from finite heat conduction model and the experimental data is 0.6637, however, when it goes to the convection model, it becomes 0.7540, which shows the superior accuracy of the finite heat conduction model.

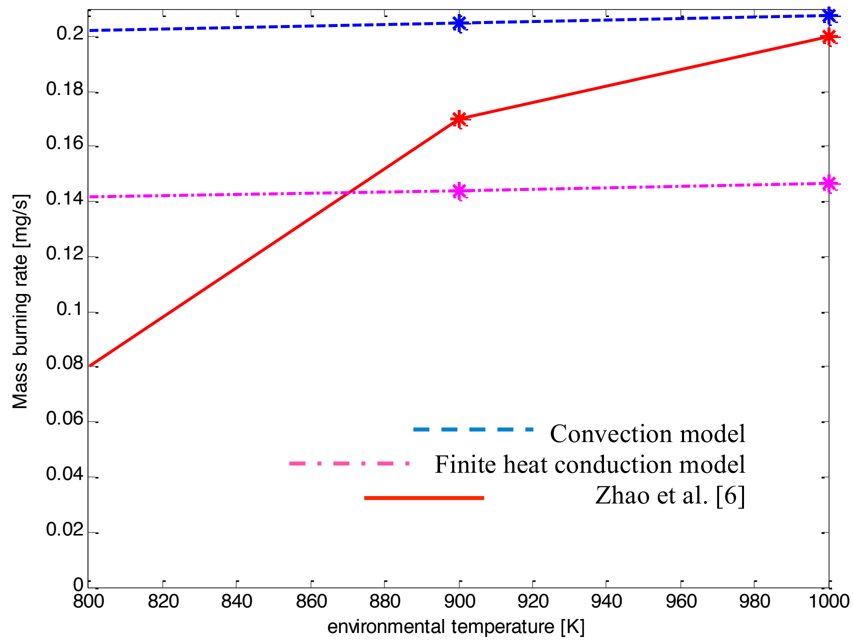

Figure 4. The results of the mass burning rate under different environmental temperatures

Figure 4 shows the mass burning rate obtained by the convection model, the finite heat conduction model and simulation results of Zhao under the same conditions with different ambient temperatures [6].

For higher temperature as 1000 K, the result from the convection model is more close to the simulation from Zhao, while for lower temperature as 800 K and 900 K, the result from the finite heat conduction model is more close to the work of Zhao.

5 Conclusions

This study tries to find a reasonable way to take into account the heat conduction at the droplet surface in a steady droplet combustion model. To achieve this target, the term describing heat transfer in the classical model is replaced by a finite heat conduction expression. This is a reasonable way to take the influence of the temperature distribution in droplet on heat transfer through its surface into consideration. It could also avoid the excessive simplification in lumped parameters model and onion-skin model, as well as improve the facticity of the model physically. In conclusion, this an economic way for calculation.

The component distribution and the mass burning rate during the combustion process of an isooctane droplet are calculated. The results under corresponding conditions are compared with the previous simulated results and experimental data, respectively. The results show that the finite heat conduction model can get closer mass burning rate to the experimental data than the classical model.

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