DYNAMIC OF SOOT PARTICLE IN DROPLET COMBUSTION

Hélio L. F. Moralez, hfmoralez@gmail.com
Departamento de Engenharia Elétrica - Unesp, 12516-000 Guaratinguetá - SP, Brazil

Fernando F. Fachini, fachini@lcp.inpe.br
Instituto Nacional de Pesquisas Espaciais (INPE), 12630-000, Cachoeira Paulista, SP, Brazil

Abstract. *This work addresses some particular aspects of the dynamic of soot particles. Due to the flow field geometry and the type of combustion (non-premixed) soot is generated. The dimensions of soot particles are about nanometer. In this characteristic spatial scale, the main two forces acting on the particle are drag and thermophoretical. The first one pushes soot to the flame, however the second one pulls soot away from the flame. To determine the conditions in which the drag force prevails lead to a reduction on the particulate emission to the ambient atmosphere, because the soot is burnt at the flame. When the thermophoretic force prevails, the combustion is sooty because the particles do not pass through the flame. Besides that, soot influences fire propagation, mainly in the microgravity condition because the heat transfer by radiation from the soot particles is the main process in the flame propagation. Therefore, the description of the dynamic of such particles will reveal features which will be used in the control of the soot consumption.*

Keywords: *Soot Particle, Droplet Combustion, Dynamic of Nanoparticle, Thermophetic Force*

INTRODUCTION

Soot is formed by agglomeration of spherical precursor particles about 1 to 5 10^{-8}m (nanoparticle) [Glassman, 1987]. Therefore, by controlling the reactions that form soot and those which cause its oxidation, it is possible to have sooting flame and non sooting flame. In diffusion flames, the soot formation occurs in presence of very low oxygen concentration, then the oxidation of the soot particles takes place only in the flame. In the case of the droplet combustion, the soot formed in the fuel flame side is taking close to the droplet surface. The soot particles form a shield around the droplet and are partially burned at the end of the droplet lifetime when the flame collapses. In the present work, an estimation of the conditions for the soot particles to move to the flame (free soot flame condition) is presented.

To determine the soot dynamics, it is necessary to know the forces on the particles. At the soot particle dimension, the forces are: drag, electrostatic, gravitational, acoustic, diffusiophoretic and thermophoretic [Phillips, 1975b, Phillips, 1975a, Talbot et al., 1980, Rosner et al., 1991, Talbot, 1980]. The thermophoretic force is responsible to push the soot particle from the fuel pyrolysis zone toward the droplet surface. The soot particles do not reach the liquid surface. The drag force acts on the particle in the opposite direction to the thermophoretic force. The soot particles find a stable position close to the droplet surface. The drag and thermophoretic forces equilibrium determines the position of the soot in the gas phase. In the droplet combustion, the equilibrium position specifies soot shield radius [Kadota and Hiroyasu, 1984, Shaw et al., 1988, Manzello et al., 2000].

The experimental and numerical studies point out that decreasing the droplet initial radius, the soot formation decreases [Kitano et al., 1993, Jackson and Avedisian, 1996]. Two mechanism are suggested to explain the soot formation reduction. The oxygen leakage by the flame augments by reducing the droplet initial radius and oxygen in the fuel side increases the soot oxidation rate. The other process is the reduction in the fuel pyrolysis time with the reduction of the flame temperature in the oxygen leaking condition [Shaw et al., 2001].

The influence of soot is not only on the pollution, but also on the droplet combustion regime. Therefore, the understanding of soot dynamics helps to improve the combustion. The presence of the soot shield around the droplet reduces the heat transfer from the flame to the droplet. By this reason, increasing the droplet radius the soot formation increases and the droplet vaporization rate reduces [Jackson and Avedisian, 1994, Nayagam et al., 1998, Manzello et al., 2000, Avedisian, 2000].

The presence of soot in the domain between the flame and the droplet is responsible for the radiative heat loss. The distance between the border of the luminous region, thermal radiation from soot, to the flame was measured [Mikami et al., 1994]. This observation indicates, at least, that large soot particles are not found in the flame.

Therefore, the control of the soot formation and oxidation permit reducing the particle emission to the ambient and to improve the combustion. The main idea to control the amount of soot, in the particular case of the droplet combustion, is to identify the processes that favor the soot transport to the flame.

In this exploratory analysis, it is considered that the presence of the soot in the gas phase does not influence on the whole droplet problem. This droplet burning condition can be found for very low soot production, which leads to very low soot concentration in the gas phase between the droplet surface and the flame. Under this hypothesis, the soot particles dynamic can be determined by knowing the velocity and temperature profiles from the classical droplet combustion analysis.

MATHEMATICAL FORMULATION

In this work, the drag ($\bar{F}_A$) and thermophoretic ($\bar{F}_F$) forces are considered acting on the particles. The evolution equation for the soot particle is

$$m_p \frac{d\bar{V}_p}{dt} = \bar{F}_F + \bar{F}_A \tag{1}$$

The expressions for these forces under the condition of small Knudsen number, $K_n = o(1)$, are

$$\bar{F}_F = -\frac{9}{2}\pi\beta_t \left(\frac{k_g}{2k_g + k_p}\right) K_n \mu \bar{c} \bar{R}_p^2 \frac{\nabla \bar{T}}{\bar{T}}, \tag{2}$$

$$\bar{F}_A = -6\pi\mu R_p(\bar{V}_p - \bar{U}), \tag{3}$$

In Eqs. (1) and (2), $\bar{T}$ is the temperature profile in the gas phase at the position of the soot particle, $\bar{U}$ is the velocity in the gas phase at the position of the soot particle, and $\bar{V}_p$ is the particle velocity. Consequently, the position of the soot particle $\bar{x}_p$ is given by $d\bar{x}_p/dt = \bar{V}_p$. The parameters in those equations are

$$\beta_t \equiv \frac{1 + N_1 K_n + N_2 K_n^2}{1 + D_1 K_n + D_2 K_n^2 + N_3 K_n^3},$$

$$N_1 \equiv \frac{k_p}{k_g} C_t - \frac{15}{4}\frac{k_p - k_g}{k_g} C_m, \quad N_2 \equiv \frac{15}{4}\frac{k_p}{k_g} C_t C_m$$

$$D_1 \equiv \frac{9}{2}\frac{k_g}{2k_g + k_p} + \frac{2k_p}{2k_g + k_p} C_t + 3C_m$$

$$D_2 \equiv \frac{9}{2}\frac{k_g}{2k_g + k_p} C_t - \frac{135}{8}\frac{k_p - k_g}{2k_g + k_p} C_m + \frac{6k_p}{2k_g + k_p} C_t C_m$$

$$D_3 \equiv \frac{135}{8}\frac{6k_p}{2k_g + k_p} C_t C_m, \quad C_t \equiv \frac{15}{4}\frac{2 - \alpha_a}{\alpha_a}, \quad C_m \equiv \frac{2 - \alpha_a}{\alpha_a}$$

Also, k_i is the thermal conductivity and the subscripts g, l and p represent gas, liquid and particle, μ is the viscosity, σ is the momentum accommodation factor and α_a is the thermal accommodation factor. Kn is the Knudsen number defined as $\lambda/\bar{R}_p$, with $\bar{R}_p$ as the particle radius. $\bar{c}$ is the velocity of the sound.

The following estimation for velocity (gas and soot particle), temperature, radius and time,

$$V_c = \alpha/a_0, \;\; T_c = T_\infty, \;\; r_c = a_0, \;\; t_c = \left(\frac{\rho_l}{\rho_\infty}\frac{a_0^2}{\alpha}\right)\frac{\alpha}{\nu}\frac{\rho_p}{\rho_l}\frac{2R_p^2}{9}$$

are used to adimensionalize Eq. (1),

$$\frac{dV_p}{d\tau} = -c_F \frac{\nabla\theta}{\theta} + U - V_p \tag{4}$$

in which $V_p \equiv \bar{V}_p/(\alpha/a_0)$, $U \equiv \bar{U}/(\alpha/a_0)$ and $\theta \equiv T/T_\infty$.

The functions θ and U depend on the soot position x_p in the flow field, $\theta = \theta(x_p)$ and $U = U(x_p)$. In the present work, the flow field is that established by the droplet combustion [Fachini, 1999].

The parameter c_F that appears in Eq. (4) collects all properties of the problem (flowfield and particle) and is defined as

$$c_F \equiv \left[\frac{9}{2}\left(\frac{\beta_t K_n}{2 + k_p/k_g}\right) c R_p\right] \tag{5}$$

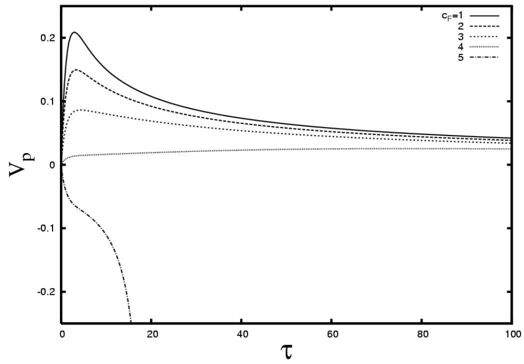

Figure 1. Soot particle velocity V_p as a function of the time τ for different values of the parameter c_F

in which $R_p \equiv \bar{R}_p/a_0$ (a_0 is the initial droplet radius) and $c \equiv \bar{c}/(\alpha/a_0)$. Note that the sound speed is considered constant, but if its dependence on temperature was considered, the first term of Eq. (4) would be $\nabla\theta/\sqrt{\theta}$.

As observed in Eq. (4), the equilibrium position of the soot particles $x_p^{(e)}$ is determined imposing the conditions $\bar{F}_A + \bar{F}_F = 0$ and $V_p(x_p^{(e)}) = 0$, which leads to

$$U(x_p^{(e)}) - c_F \; \nabla\theta/\theta|_{x_p^{(e)}} = 0 \qquad (6)$$

Note that $\bar{F}_A = -\bar{F}_F$ is found only in the flowfield inside the flame, between the droplet surface and the flame. Outside the flame, that condition is not found. The solution of Eq. (4) will show the soot particle dynamic and, at the same time, the stability condition. For any place for the soot formation region inside the flame, if the soot particles end up at $x_p = x_p^{(e)}$, the equilibrium position is stable. However, if $x_p = x_p^{(e)}$ is not achieved, the equilibrium position is unstable.

RESULTS

Equation (4) must be integrated with the particle position equation $dx_p/d\tau = V_p$. The system of equations is solved numerically by the Runge-Kutta method. Observations point out that the soot formation occur around temperature of $1400K$ [Glassman, 1987]. The initial conditions for the integration of Eq. (4) together with the equation $dx_p/d\tau = V_p$ are $x_p = x_{pi}$ and $V_p(x_{pi}) = 0$ at $\tau = 0$. The value for x_{pi} is determined by the condition $\theta(x_{pi}) = 1400/298.15$ ($T_\infty = 298.15$ is the ambient temperature), which leads to $x_{pi} = 4.492$.

As the problem is presented, the properties of the soot and gas phase are collected in one single parameter c_F. Therefore, the problem has the same solution for different properties provided c_F is kept unchanged. The present formulation provides an estimation for the soot particle characteristic time and universal parameter c_F to describe the problem.

Figure (1) exhibits the soot velocity V_p as function of time. It is observed that the set of force constituted by drag and thermophoretic describes the position where $V_p(x_p^{(e)}) = 0$ as an unstable equilibrium position. It is seen that the condition $V_p = 0$ is not found. For soot being formed before the equilibium position $x_p < x_p^{(e)}$, the soot particle is pushed by the thermophoretic force to the droplet surface; condition not observed in the experimental studies. In the same way, for $x_p > x_p^{(e)}$, the soot particle is taken by the the drag force to the flame. These features are confirmed by Fig. (2).

The unstable equilibrium point is determined by solving Eq. (6). For the present problem the flame radius is about $x_f = 23$. The inverse procedure is easy to be solved: given a value for $x_p^{(e)}$ in the interval $1 < x_p < x_f$, the value for c_F is determined by Eq. (6). The results are plotted in Fig. (3). It is found that for $c_F = 5.6$, $x_p^{(e)} = x_f$. Therefore, if the particle and gas properties satisfy the condition $c_F > 5.6$, it is possible to garantee qualitatively that the soot particle formed in the fuel side of the flame crosses the flame. This is a mechanism to reduce the soot emission, forcing them to oxidize in the flame.

CONCLUSION

It was noted that the model with two forces (thermophoretical and drag) was not sufficient to determine the soot particle dynamics. The equilibrium position $x_p^{(e)}$ imposed by the balance $F_F + F_A = 0$ with $V_p = 0$ is unstable. For soot generation zone between the droplet surface and $x_p^{(e)}$, the thermophoretic force pulls the particle to the droplet surface.

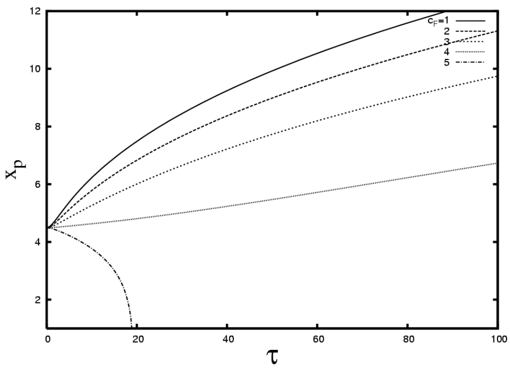

Figure 2. Soot trajectory V_p as a function of the time τ in the flow field generated by the droplet combustion. The plot corresponds to five different values of the parameter c_F

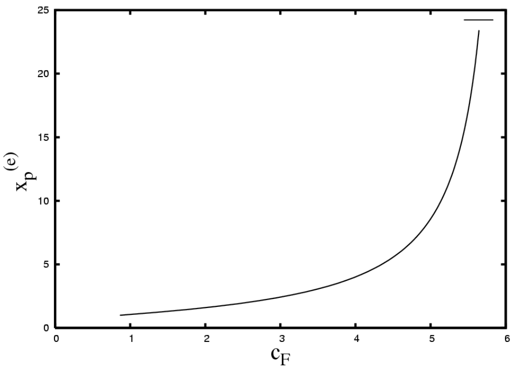

Figure 3. Equilibrium position of the soot particle $x_p^{(e)}$ as a function of the parameter c_F.

For soot generation zone between $x_p^{(e)}$ and the flame, the drag force pushes the particle to the flame. Although the model is not properly defined, a parameter c_F, that includes all properties (particle and gas phase) of the problem, is qualitatively related with the particle equilibrium position $x_p^{(e)}$. Also, the present analysis exposed a characteristic time for the soot dynamics.

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