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AN EXTENDED ANALYSIS FOR THE DYNAMIC OF SOOT PARTICLE IN DROPLET COMBUSTION

Eduardo Melara, edumelara@gmail.com
Departamento de Engenharia Elétrica, UNESP Guaratinguera-SP
Thiago Pavan, thiago.pavan@uol.com.br
Departamento de Física, CCA - UFSCar, Araras-SP
Max A.E. Kokubun, max@lcp.inpe.br
Fernando F. Fachini, fachini@lcp.inpe.br
Laboratório de Combustão e Propulsão - INPE, Cachoeira Paulista-SP

Abstract.
This work addresses some particular aspects of the dynamic of soot particles. The analysis will be developed numerically. The dimensions of soot particles are about nanometer. In this characteristic spatial scale, the main two forces acting on the particle are drag and thermophoretic (proportional to the temperature gradient). The first one pushes soot to the flame, however the second one pulls soot away from the flame. Therefore, for conditions in which the drag force prevails the particulate emission to the ambient atmosphere is reduced, because the soot is burnt at the flame. Moreover, a reduction on soot formation can inhibit fire propagation, mainly in the microgravity condition because the heat transfer by radiation from the soot particles is an important process in the flame propagation. For conditions in which the thermophoretic force prevails lead to the sooty combustion regime because the particles do not pass through the flame. The description of the dynamic of such particles will reveal features which will be used in the control of the soot production. The model, an extension of a previous one, includes the modification on the ambient temperature gradient due to the soot displacement. The correction on the temperature gradient leads to an extra term in the thermophoretic force expression. The results of the present model do not reproduce the stable equilibrium of the soot, but are able to point out the necessary of a third force to stable the particle.
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Keywords: *Soot Particle, Droplet Combustion, Dynamic of Nanoparticle, Thermophetic Force*

1. 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.

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, 1975a; Phillips, 1975b; Talbot et at. 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, because the drag force acts on the particle in the opposite direction to the thermophoretic force. The equilibrium of these forces occurs close to the droplet surface in the gas phase, but not at the surface. Then, the soot particles find a stable position close to the droplet surface. The confirmation of this stable position is that, around it, soot is accumulated forming a stationary shield (Kadota and Hiroyasu, 1984; Shaw et al., 1988; Jackson and Avedisian, 1994; Nayagan et al., 1998; Matsumoto et al. 1999; Avedisian, 2000; Manzello et al., 2000; Bae and Avedisian, 2004; Urban et al., 2004, Yozgatligil et al., 2004; Xu et al., 2004; Manzello et al., 2004)

The experimental and numerical studies point out that decreasing the droplet initial radius, the soot formation decreases (Kitano, 1993; Jackson and Avedisian, 1996). Two mechanism are suggested to explain the soot formation reduction. By reducing the droplet initial radius, the oxygen leakage by the flame augments, increasing the oxygen concentration in the fuel side, which auçgments the soot oxidation rate. The other process responsable to the soot reduction is the decrease in the fuel pyrolysis rate 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;Nayagan 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 favour the soot transport to the flame.

Recently, the soot dynamic problem was analized considering the drag force and the thermophoretic force (Moralez and Fachini, 2008). The thermophoretic force was described by a simple model, the effect of the soot displacement on the temperature gradient was neglected (Phillips, 1975a). In the present analysis, the effect of the soot displacement is considered in the model that describes the thermophoretic force. The movement of heated soot through the flow field leads to a change in the local temperature gradient, then the thermophoretic force is changed (Phillips, 1975a).

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 acting on the particles. The evolution of the soot particle is given by the resulting force equation

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

in which m_p is the mass of the soot particle, $\bar{V}_p$ is the particle velocity and t is time.

The expressions for these forces for any Knudsen number are (Phillips, 1975a)

$$\bar{F}_F = -\frac{9}{2}\pi\beta_t \left(\frac{k_g}{2k_g + k_p}\right) K_n \mu \bar{c} \bar{R}_p^2 \frac{\nabla\bar{T}}{\bar{T}} \left[1 + \frac{A R_p^2 k_p}{\alpha_p \alpha_g k_g}(\bar{V}_p - \bar{U})^2\right], \tag{2}$$

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

In Eqs. (2) and (3), $\bar{T}$ and $\bar{U}$ are the temperature and velocity profiles in the gas phase around the droplet at the position of the soot particle. 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. K_n 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. In Eq. (2), α_p and α_g are the thermal diffusivity for particle and gas, respectively and A is a coefficient which varies with Knudsen number from $1/24$ at $K_n = 0$ to zero at $K_n = \infty$.

Since the soot dinamics depends on the temperature and velocity of the flow where is the soot particle and these properties are given in terms droplet problem, the origin of the coordinate system

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 admensionalize Eq. (1),

$$\frac{dV_p}{d\tau} = -c_{F1}\frac{\nabla\theta}{\theta}\left[1 + c_{F2}(V_p - U)^2\right] + U - V_p \tag{4}$$

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 parameters c_{F1} and c_{F2} that appears in Eq. (4) collect all properties of the problem (flowfield and particle) and is defined as

$$c_{F1} \equiv \left[\frac{9}{2}\left(\frac{\beta_t K_n}{2 + k_p/k_g}\right)cR_p\right], \quad c_{F2} \equiv AR_p^2\frac{k_p\alpha_g}{k_g\alpha_p} \tag{5}$$

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 Eq. (1) was handled to obtain Eq. (4), the parameter C_{F1} is defined as the ratio of the thermal phoretic force to the drag force. In the case of C_{F2}, the ratio is between the component of the thermal phoretic force due to the displacement of the soot particle and the drag force.

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

$$U(x_p^{(e)}) - c_{F1}\ \nabla\theta/\theta|_{x_p^{(e)}}\left[1 + c_{F2}U(x_p^{(e)})^2\right] = 0 \tag{6}$$

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 two parameters c_{F1} and c_{F2}. Therefore, the problem has the same solution for different properties provided c_{F1} and c_{F2} are kept unchanged.

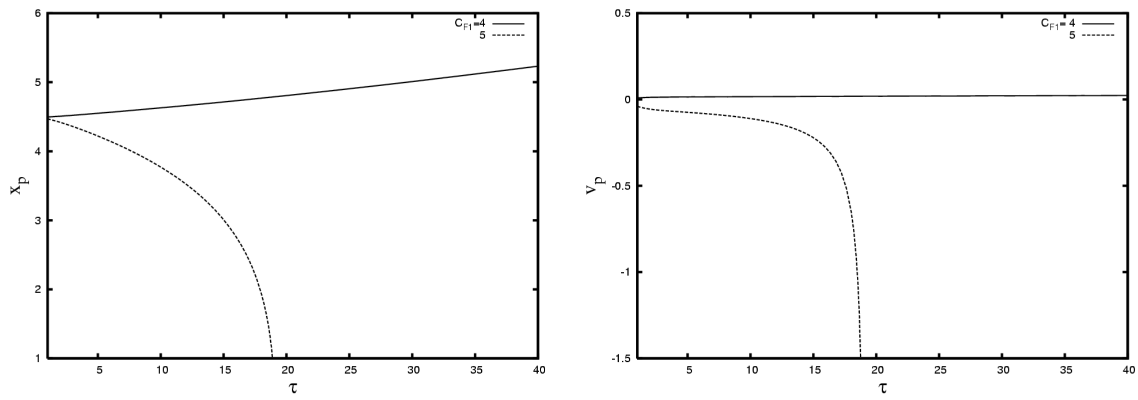
Figure 1 exhibits the soot position x_p and velocity V_p as function of time for two cases with no influence of the term corresponding to $(V_p - U).\nabla\theta$ ($C_{F2} = 0$). This picture is presented to show that the two forces system without the contribution of the $(V_p - U).\nabla\theta$ does not have a stable equilibrium ($V_p \neq 0$).

Figure 2 depicts the soot dynamic in the flow field generated by the droplet combustion. The model represented by Eq. (4) considers modification of the gradient temperature established by the droplet combustion due to the soot displacement, which is expressed by $c_{F2} \neq 0$. As seen, the cases for $c_{F1} = 5$ and $c_{F2} = 0.5, 1$ do not show a stable equilibrium position.

The results point the necessity of considering a third force. In order to check this idea, the coefficient c_{F2} is made artificially negative. The cases $c_{F2} < 0$ would correspond the presence of a third force in the same direction of the drag force. A new phoretic force in the direction of the drag force in the droplet combustion problem is the diffusiophoretic. The information exhibited in Fig. 3 confirms the necessity of a third force. For the case $c_{F1} = 5$ and $c_{F2} = -0.515$, the stable equilibrium position is found, $V_p = 0$ and $x_p^{(e)}$.

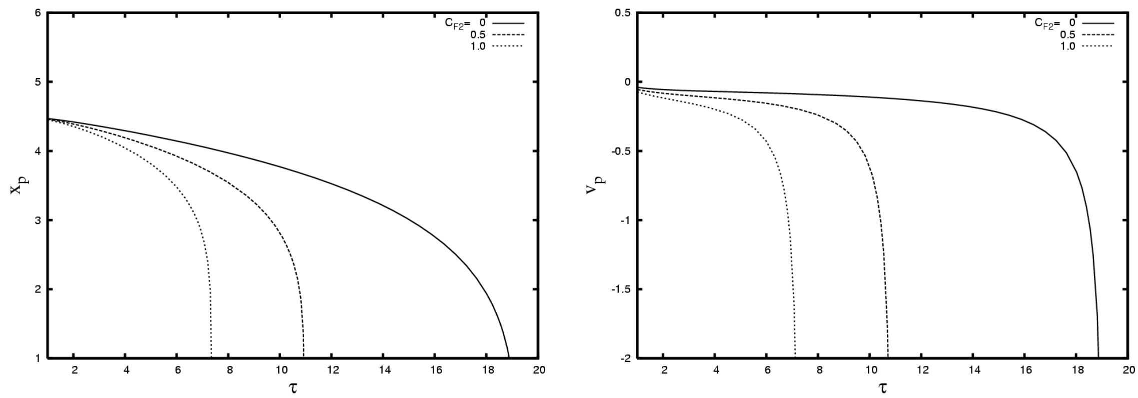
CONCLUSION

It is noted that the model with two forces (thermophoretic 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. The results point that a third force is necessary to impose stable equilibrium on the soot particle. A specific negative value of c_{F2} gives the expected equilibrium. Therefore this influence has the same direction of the drag force. A possible inclusion on the force



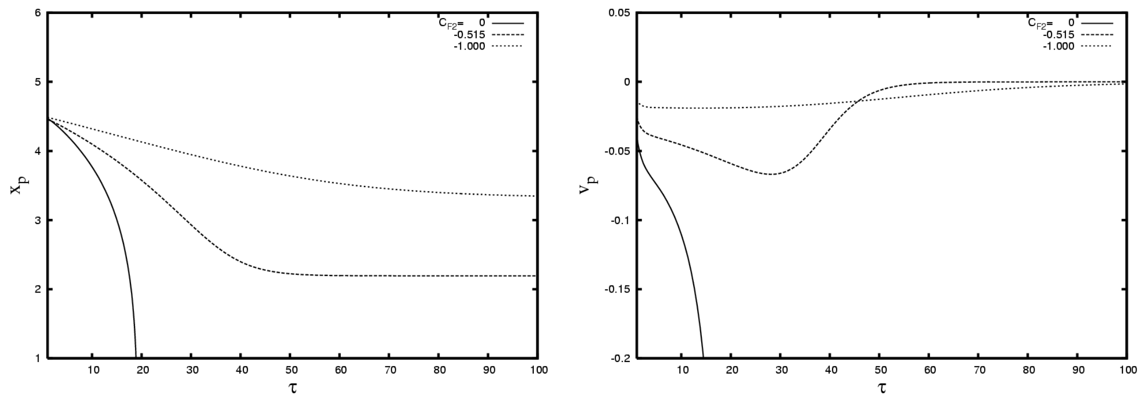
(a) (b)

Figure 1. (a) Soot particle position and (b) Soot particle velocity as a function of time for $c_{F1} = 4, 5$ and $c_{F2} = 0$.



(a) (b)

Figure 2. (a) Soot particle position and (b) Soot particle velocity as a function of time for $c_{F1} = 5$ and $c_{F2} = 0, 0.5, 1$.



(a) (b)

Figure 3. (a) Soot particle position and (b) Soot particle velocity as a function of time for $c_{F1} = 5$ and $c_{F2} = 0, -0.515, -1$.

system is the diffusiophoretic force.

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