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DYNAMIC OF SOOT PARTICLE IN DROPLET COMBUSTION

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"A sabedoria torna bons os homens. A simulação da sabedoria torna-os péssimos."

(Juan Luis Vives)

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RESUMO

Este trabalho visa estudar alguns aspectos particulares da dinâmica de partículas de fuligem. Através da geometria do campo fluído e o tipo de combustão (não pré-misturada) a partícula é gerada. A dimensão das partículas de fuligem é da ordem de nanômetros. Nesta escala espacial as duas principais forças agindo sobre a partícula são a de arrasto e a termoforética. A primeira empurra a partícula para a chama, enquanto que a segunda puxa a partícula para perto da gota. As condições onde a força de arrasto prevalece levam à redução da emissão de partículas de fuligem na atmosfera, pois a fuligem se queima na chama. Quando a força termoforética prevalece, a combustão é fuliginosa, pois as partículas não passam pela chama. Além disso, a fuligem influencia na propagação do fogo, principalmente nas condições de micro-gravidade pois a transferência de calor por radiação pelas partículas de fuligem é o principal processo de propagação de chama. Entretanto, a descrição da dinâmica de tais partículas revelará características que serão usadas no controle de consumo de fuligem.

DYNAMIC OF SOOT PARTICLE IN DROPLET COMBUSTION

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. 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.

LISTA DE SIGLAS E ABREVIATURAS

INPE	Instituto Nacional de Pesquisas Espaciais
SID	Serviço de Informação e Documentação
TDI	Teses e Dissertações Internas
SPG	Serviço de Pós-Graduação

1 INTRODUCTION

Soot is formed by agglomeration of spherical precursor particles about 1 to 5 10–8m (nanoparticles) Glassman (1987). Therefore, by controlling the reactions forming 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 takes place for soot particles pushed to the flame. In the case of the droplet combustion, the soot formed in the fuel flame side is taking to 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,a); 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 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 the soot is not only on the pollution, but also on the droplet combustion regime. Therefore, the understanding of the 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, by 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 to reduce 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.

2 MATHEMATICAL FORMULATION

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

$$m_p \frac{d\overline{V}_p}{dt} = \overline{F}_F + \overline{F}_A \quad (1)$$

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

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

$$\overline{F}_A = -6\pi\mu R_p (\overline{V}_p - \overline{U}) \quad (3)$$

In Eqs. (1) and (2), \bar{T} is the temperature profile in the gas phase at the position of the soot particle, \overline{U} is the velocity in the gas phase at the position of the soot particle, and \overline{V}_p is the particle velocity. Consequently, the position of the soot particle \overline{x}_p is given by $\partial \overline{x}_p / \partial t = \overline{V}_p$. 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 e p represent gas, liquid and particle, μ is the viscosity, α is the momentum accommodation factor

and α_a is the thermal accommodation factor. k_n is the Knudsen number defined as λ/\bar{R}_p , with \bar{R}_p as the particle radius, \bar{c} is the velocity of the sound.

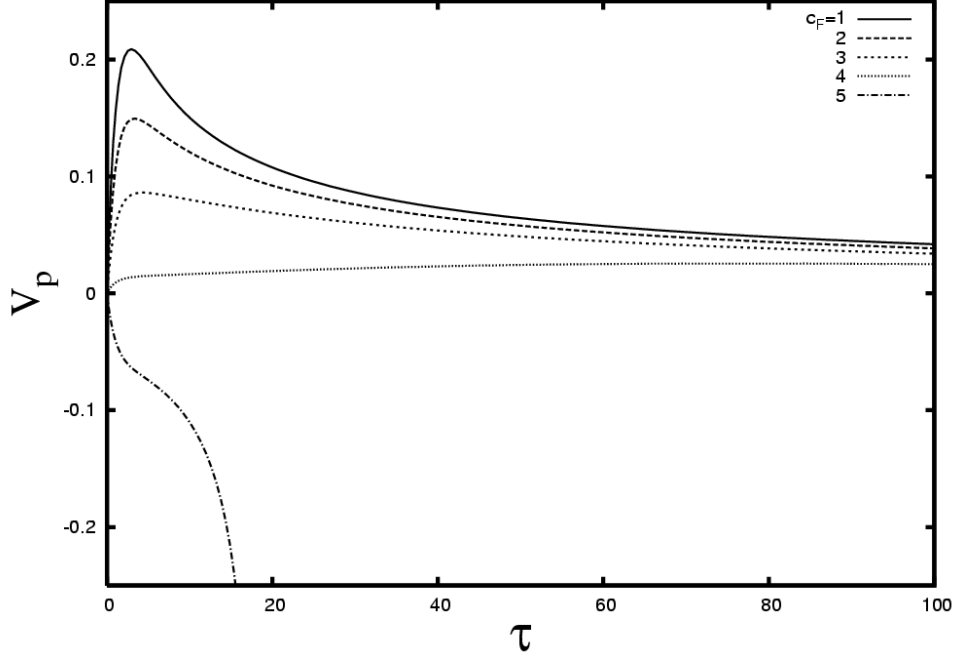


Figure 1: Soot particle velocity V_p as a function of the time τ for different values of the parameter c_F

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

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

are used to adimensionalize Eq. (1),

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

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 function 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 that appears in Eq. (4) is defined as:

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

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

3 RESULTS

Equation (4) must be integrated together with particle position equation $\partial x_p / \partial \tau = V_p$. The system of equations is solved numerically by the Runge-Kutta method.

As the problem is presented, the properties of the soot and gas phase are collected in one parameter c_F . Therefore, the problem has the same solution for different properties if 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 $V_p = 0$ as an unstable equilibrium position. It is seen that the condition $V_p = 0$ is not found. For soot being formed before the position where $V_p = 0$, $x_p < x_p(V_p = 0)$, 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 $x_p > x_p(V_p = 0)$, the soot particle is taken by the drag force to the flame. This feature is confirmed by Fig. (2).

The unstable equilibrium point is determined by imposing the condition $V_p = 0$ in the equation $c_F \cdot \nabla \theta / \theta + U = 0$. 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 in the interval $1 < x_p < x_f$, the value for c_F is determined by the above expression. The results are plotted in Fig. (3). It is found that for $c_F = 5.6$, $x_p = x_f$. Therefore, if the particle and gas properties satisfy the condition $c_F > 5.6$, it is possible to grantee qualitatively that the soot particle formed in the fuel side of the flame crossed the flame. This is a mechanism to reduce the soot emission, forcing them to oxidize in the flame.

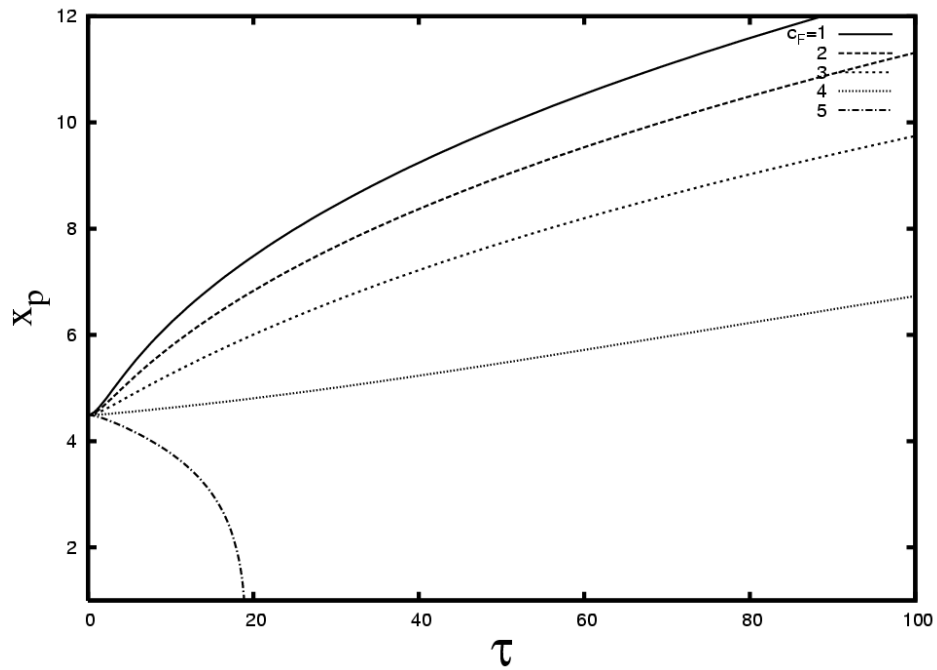


Figure 2: Soot trajectory V_p as a function of the time τ in the flow field generated by the droplet combustion. The plot corresponds to five different values of the parameter c_F

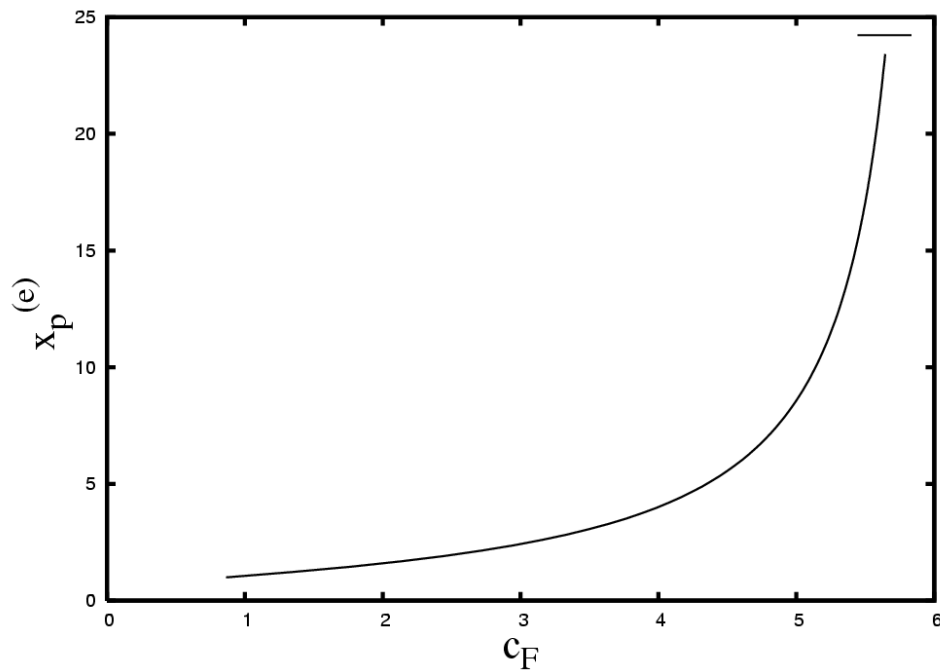


Figure 3: Equilibrium position of the soot particle $x_p^{(e)}$ as a function of the parameter c_F

4 CONCLUSION

It was 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. For soot generation zone between the droplet surface and $x_p^{(e)}$, the thermophoretic force pulls the particle to the droplet surface. 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, relates qualitatively with the particle equilibrium position $x_p^{(e)}$. Also, the present analysis exposed a characteristic time for the soot dynamics.

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