



## Transport of soot particles in droplet combustion

Rafael Pereira Bianchin<sup>1</sup>, Denize Kalempa<sup>2</sup>

<sup>1</sup> Instituto Nacional de Pesquisas Espaciais, Cachoeira Paulista, SP, Brasil  
PhD Student of Space Engineering and Technology Graduate Program, Combustion and Propulsion.

<sup>2</sup> Universidade de São Paulo, Escola de Engenharia de Lorena, Lorena, SP, Brasil

rafaelbianchin@inpe.br

---

**Abstract.** *In most practical applications, the combustion of droplets can generate large amounts of soot due to the large molecules of the fuel and the flame being of the diffusive type. The equilibrium between aerodynamic and thermophoretic effects leads to the formation of a soot shell in the vicinity of the droplet. The aim of this paper is to investigate the transport of soot and the properties of the soot shell based on the classic models for droplet combustion and thermophoresis.*

---

**Keywords:** Droplet combustion; Soot; Thermophoresis.

### 1. Introduction

Recently, much attention has been paid to the study of soot in combustion, regarding its formation, transport and oxidization in combustion of droplets. It has been observed that the soot, formed in the flame, can often form a shell around the droplet (BEN-DOR; ELPERIN; KRASOVIT, 2003). The formation of this shell is due to the equilibrium between aerodynamic and thermophoretic effects; the vaporization of the droplet pushes the soot particles away from it, but the temperature gradient caused by the flame pushes the soot towards the droplet.

A model for the transport of soot was proposed by Kumar *et al.* (KUMAR; RAY; KALE, 2002), and involves features such as fully transient behaviour, radiation, a transport equation for soot (including thermophoresis) and models for nucleation, growth and oxidization of soot. Despite using a crude approximation for the thermophoretic force, and, assuming free-molecular flow around the soot particles, the model seems to work remarkably well.

A similar yet simpler model was proposed by Ben-Dor *et al.* (BEN-DOR; ELPERIN; KRASOVIT, 2003), including the effect of diffusiophoresis, which was found to be small, yet not negligible. Ben-Dor *et al.* also used an improved model for the thermophoresis, valid for the assumption of continuum and slip flow around the soot particles, despite using old data and non-realistic accommodation coefficients of gas molecules at the soot boundary.

The present work intends to replicate Ben-Dor *et al.* results using the classic formulation for droplet combustion instead of the more complex numerical model adopted by them for droplet combustion. Different thermophoretic data will be used to identify possible improvements.

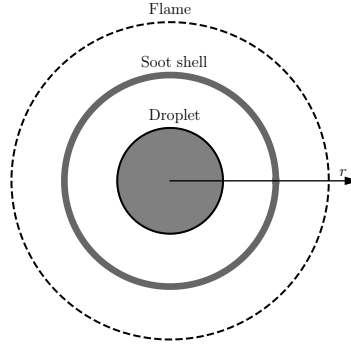


Figure 1. Representation of the problem.

## 2. Mathematical formulation

The combustion of a fuel droplet in an atmosphere of oxidizer is studied on the basis of a classic model. A flame is established around the droplet, and a soot shell between the droplet and the flame is formed, as depicted in Figure 1. Since the phenomena of droplet combustion and soot transport take place in very different scales, it is possible to model them separately.

### 2.1. Droplet combustion

For the sake of simplicity, it is assumed that: the gas phase has constant density, transport and thermodynamic coefficients; the Lewis numbers are equal to the unity; the liquid phase is much denser than the gas phase; and that the chemical reaction is infinitely fast and follows a single-step mechanism (LAW, 2010).

Due to the geometry, the problem has spherical symmetry. Thus, in nondimensional variables, the continuity, energy conservation and species transport equations are written as

$$\epsilon \frac{\partial \rho}{\partial t} + \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 \rho u) = 0, \quad (1)$$

$$\epsilon \frac{\partial(\rho T)}{\partial t} + \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 \rho u T) = \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial T}{\partial r} \right) + q\omega, \quad (2)$$

$$\epsilon \frac{\partial(\rho Y_F)}{\partial t} + \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 \rho u Y_F) = \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial Y_F}{\partial r} \right) - \omega, \quad (3)$$

$$\epsilon \frac{\partial(\rho Y_O)}{\partial t} + \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 \rho u Y_O) = \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial Y_O}{\partial r} \right) - s\omega, \quad (4)$$

in which  $\epsilon = \hat{\rho}_\infty / \hat{\rho}_l$  is the ratio between the density of the gas and liquid phases,  $\omega$  is the reaction rate,  $Y_F$  and  $Y_O$  are the fuel and oxidizer concentrations, respectively,  $q$  is the enthalpy of combustion and  $s$  is the stoichiometric coefficient. Since the liquid phase is much denser than the gas phase,  $\epsilon$  is very small, and the transient terms can be neglected, leading to the quasi-steady regime of droplet combustion (LAW, 2010).

These equations can be solved using the classic boundary conditions and with the Zeldovich formulation, yielding the velocity field around the droplet, given by (LAW, 2010)

$$U = \frac{\lambda}{r^2}, \quad (5)$$



(with  $\lambda$  being the instantaneous vaporization rate), the flame position  $r_f$ ,

$$r_f = \lambda \left[ \log \left( \frac{s+1}{s} \right) \right]^{-1}, \quad (6)$$

the temperature profile and gradient in the inner region of the flame,

$$T = 1 + \frac{q}{s} - Le^\beta \left[ 1 - \exp \left( -\frac{\lambda}{r} \right) \right], \quad \nabla T = Le^\beta \frac{\lambda}{r^2} \exp \left( -\frac{\lambda}{r} \right), \quad (7)$$

and in the outer region of the flame,

$$T = 1 + \left( q \frac{s+1}{s} - Le^\beta \right) \left[ 1 - \exp \left( -\frac{\lambda}{r} \right) \right], \quad \nabla T = - \left( q \frac{s+1}{s} - Le^\beta \right) \frac{\lambda}{r^2} \exp \left( -\frac{\lambda}{r} \right), \quad (8)$$

with  $\beta$  being the vaporization constant and  $L$  the latent heat of vaporization.

## 2.2. Soot transport

The velocity of the soot particle is affected by the gas velocity field (caused by the droplet vaporization) and by thermophoresis. Since both the velocity field and the temperature gradient point in the radial direction, the particle also has velocity only in the radial direction.

It is assumed that the particle has no relative velocity to the velocity field, except for the velocity caused by thermophoresis. Therefore, the particle is at rest if (BEN-DOR; ELPERIN; KRASOVIT, 2003)

$$u_{part} = U + u_{th} = 0, \quad (9)$$

where  $u_{part}$  is the total soot particle velocity,  $U$  is the gas velocity and  $u_{th}$  is the soot particle velocity due to thermophoresis.

The relevant parameter for the description of thermophoresis is the Knudsen number  $Kn$ , defined here as the ratio between the mean free path of gas molecules and the characteristic length of the soot particles. An adequate expression for the calculation of the thermophoretic velocity of a particle at low Knudsen numbers is (BAKANOV, 1995)

$$u_{th} = - \frac{K_{ts}}{1 + \Lambda/2} \frac{\gamma}{\gamma - 1} \nabla T (1 + Kn\Phi), \quad (10)$$

in which  $K_{ts}$  is the thermal slip coefficient,  $\gamma$  is the ratio of specific heats,  $\Lambda$  is the ratio between the thermal conductivity of the particle and the gas, and  $\Phi$  is a function of the accommodation coefficients, given by

$$\Phi = A\Lambda + \frac{B + C\Lambda}{1 + \Lambda/2} + D. \quad (11)$$

The constants  $A$ ,  $B$ ,  $C$  and  $D$  depend on the accommodation coefficients of momentum and energy of gas molecules on the soot boundary and are calculated on the basis of kinetic theory of gases or extracted from experimental data.

## 3. Results

The calculations were carried out using data for n-heptane at an ambient of 1000 K, with  $\gamma = 1.4$ ,  $K_{ts} = 1.125$ , as recommended by Beresnev *et al.* (BERESNEV; CHERNYAK, 1995) and  $\Lambda = 10$ , as calculated by Ben-Dor *et al.* (BEN-DOR; ELPERIN; KRASOVIT, 2003).



The results were obtained for the typical value of  $Kn = 0.1$ , which means that the gas flows around the particles in the so called slip flow regime. Moreover, the results are valid under the assumption of diffuse scattering of gas molecules on the boundary. Figure 2 shows the velocity profile calculated using thermophoretic data from Poddoskin *et al.* *apud* Beresnev *et al.* (BERESNEV; CHERNYAK, 1995).

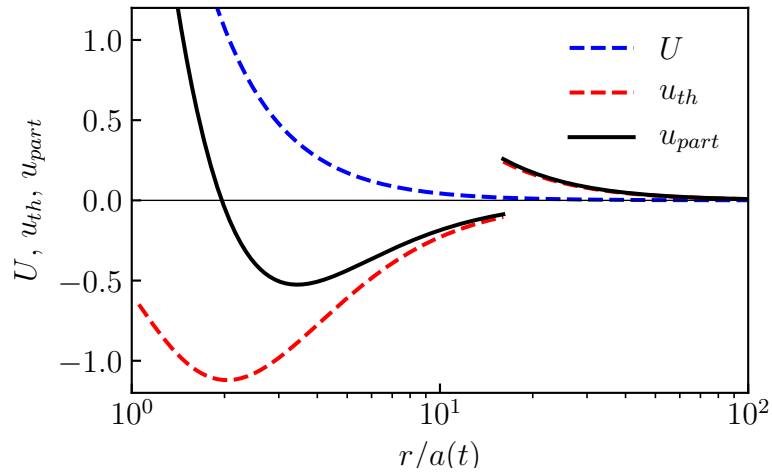


Figure 2. Velocity profiles obtained using data from Poddoskin *et al.*.

According to the figure, soot particles reach equilibrium around  $r/a = 1.95$ . This value is coherent with the results obtained by Ben-Dor *et al.*. However, while Ben-Dor *et al.* observes a second point of equilibrium, the results shown here present instead a discontinuity. This is due to the fact that, for infinitely fast reaction, the temperature gradient is discontinuous in the flame because the flame is infinitely thin. Since the thermophoretic velocity is based on the temperature gradient, it is also discontinuous at the flame. However, this second point of equilibrium is unstable and, therefore, is of no physical significance (BEN-DOR; ELPERIN; KRASOVIT, 2003).

Figure 3 shows the results obtained using more modern data from Beresnev and Chernyak (BERESNEV; CHERNYAK, 1995). As one can see from Figures 2 and 3, the results are strongly dependent on the thermophoretic data.

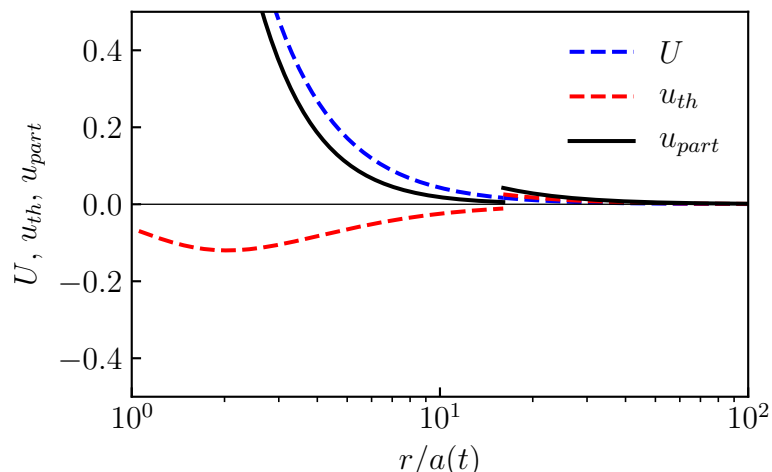


Figure 3. Velocity profiles obtained using data from Beresnev and Chernyak.



Even though the results correspond to the same case, the use of new data seems to show that no soot shell is formed; instead, all the soot is blown away from the droplet. It is clear that the results are highly sensitive to the thermophoretic data, which appears to have been overlooked by Ben-Dor *et al.*

Bakanov *et al.* observes that the expression he presents for thermophoresis is derived as a small Knudsen number expansion from the continuous ( $Kn = 0$ ) case (BAKANOV, 1995). Therefore, it is reasonable to expect that this model cannot yield coherent results for the slip flow regime, that takes place for  $Kn \sim 0.01$  to  $Kn \sim 0.1$ .

#### 4. Conclusion

A simple model for the transport of soot particles was developed, and although it appears to be able to reproduce the behavior observed in previous studies, a possible flaw in the model was found, which affects the validity of the results obtained by Ben-Dor *et al.*. An improved model shall be implemented, focusing on the interpolation of results obtained from the numerical solution of the Boltzmann equation for arbitrary values of the Knudsen number.

**Acknowledgements:** *This work was developed under support from the Conselho Nacional de Desenvolvimento Científico e Tecnológico (CNPq).*

#### References

- BAKANOV, S. Future directions for experiments in thermophoresis: A commentary. *Journal of aerosol science*, Elsevier, v. 26, n. 1, p. 1–4, 1995.
- BEN-DOR, G.; ELPERIN, T.; KRASOVIT, B. Effect of thermo–and diffusiophoretic forces on the motion of flame-generated particles in the neighbourhood of burning droplets in microgravity conditions. *Proceedings of the Royal Society of London. Series A: Mathematical, Physical and Engineering Sciences*, The Royal Society, v. 459, n. 2031, p. 677–703, 2003.
- BERESNEV, S.; CHERNYAK, V. Thermophoresis of a spherical particle in a rarefied gas: Numerical analysis based on the model kinetic equations. *Physics of fluids*, American Institute of Physics, v. 7, n. 7, p. 1743–1756, 1995.
- KUMAR, S.; RAY, A.; KALE, S. A soot model for transient, spherically symmetric n-heptane droplet combustion. *Combustion science and technology*, Taylor & Francis, v. 174, n. 9, p. 67–102, 2002.
- LAW, C. K. *Combustion physics*. [S.l.]: Cambridge university press, 2010.
- PODDOSKIN, A.; IUSHKANOV, A.; IALAMOV, I. I. Theory of thermophoresis of moderately large aerosol particles. *Zhurnal Tekhnicheskoi Fiziki*, v. 52, p. 2253–2261, 1982.