

Effect of Radiation Reabsorption in Droplet Combustion

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Abstract. *In this article the effect of radiation in droplet combustion is investigated. In particular, the impact of the reabsorption of nonluminous radiation by the gas is studied. For gases with small absorption coefficients, i. e., gases with small optical thickness, the effect of reabsorption can be neglected, which is convenient, since the calculation of the reabsorption is considerably costly. The analysis is evaluated in the quasi-steady regime of droplet combustion in the infinitely fast reaction limit. It was observed that the effect of reabsorption is negligible in small droplets and that, therefore, the assumption of optically thin gas is acceptable.*

Keywords: Diffusion flames; Droplet combustion; Radiative heat transfer.

1. Introduction

The combustion of isolated droplets is possibly the most important problem in the study of diffusion flames (WILLIAMS, 1973). There are two reasons for that: the combustion of droplets is ubiquitously present in all areas of mobility engineering, since the combustion of liquid fuels still is the most common form of vehicle propulsion. However, the combustion of an isolated droplet is extremely simple both in the mathematical and in the computational sense, and even the most trivial analytical solutions provide valuable insights into the problem.

As computational power became increasingly available, numerical studies of droplet combustion began to include a variety of effects. Nonluminous radiative heat transfer, in particular, was first studied extensively by Marchese and Dryer (MARCHESE; DRYER, 1997). They used the expressions obtained from the equation of transport of radiant energy (VISKANTA; MERRIAM, 1968) for the radiative heat transfer in spherical symmetry with a participant gas, which means a gas that can emit, absorb and scatter radiation. As a result, the balance of energy in the gaseous phase includes a sink of heat due to the radiation emitted by the gas, according to the Stefan-Boltzmann law, and a source of heat, due to the radiation that is reabsorbed by the gas.

The emission and absorption of radiation by a gas depends on its absorption coefficient κ , which describes the interaction between gas and radiation. In the context of combustion of hydrocarbons, air and fuel are transparent to radiation, and only the products of combustion are relevant to radiation. However, as observed previously (MARCHESE; DRYER, 1997), if the absorption coefficient is small, i. e., if the gas is optically thin, the reabsorption is negligible in comparison to emission and, therefore, can be neglected. That would be particularly convenient since, as it

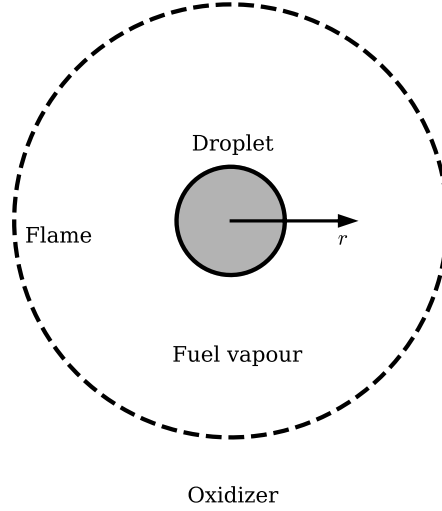


Figure 1. Representation of the problem.

will be shown later, the computation of the reabsorption term in the energy conservation equation is particularly costly. In this article the effect of the reabsorption is studied in the context of the quasi-steady droplet combustion in order to determine whether the assumption of optically thin gas is appropriate.

2. Mathematical formulation

The combustion of a single droplet is considered. The droplet is spherical, with uniform temperature equal to its boiling temperature. It vaporizes fuel into the ambient, creating a velocity field. Far from the droplet, it is assumed that the ambient is composed of air at ambient temperature. Fuel vapour and oxidizer meet at the flame, that is established around the droplet. If the droplet is sufficiently small, the effects of gravity can be neglected, and the problem has spherical symmetry. Figure 1 illustrates the geometry of the problem.

Assuming constant density, constant thermal and mass diffusivities and equal diffusivities, the nondimensional governing equations are (LAW, 2010)

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

$$\frac{1}{\rho_l} \frac{\partial T}{\partial t} + \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 u T) = \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial T}{\partial r} \right) + \nabla \cdot \mathbf{q}_R + q\omega, \quad (2)$$

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

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

where r is the radial coordinate, u is the velocity, ρ_l is the liquid phase density, t is the time variable, T is the temperature, \mathbf{q}_R is the radiative flux, q is the combustion heat, ω is the combustion

rate, Y_F is the mass fraction of fuel, Y_O is the mass fraction of oxidizer and s is the stoichiometric coefficient. The nondimensional variables are related to their dimensional counterparts by

$$t = \frac{\hat{\alpha}_\infty}{\rho_l \hat{\alpha}_0^2} \hat{t}, \quad r = \frac{\hat{r}}{\hat{a}_0}, \quad T = \frac{\hat{T}}{\hat{T}_\infty}, \quad Y_F = \hat{Y}_F, \quad Y_O = \frac{\hat{Y}_O}{\hat{Y}_{O_\infty}}, \quad u = \frac{\hat{a}_0}{\hat{\alpha}_\infty} \hat{u} \quad (5)$$

where $\hat{\alpha}$ is the diffusivity and \hat{a}_0 is the initial droplet diameter. The subscript ∞ indicates the condition far from the droplet. Moreover,

$$\rho_l = \frac{\hat{\rho}_l}{\hat{\rho}}, \quad q = \frac{\hat{q}}{\hat{c}_p \hat{T}_\infty}, \quad \mathbf{q}_R = \frac{\hat{a}_0}{\hat{k}_\infty \hat{T}_\infty} \hat{\mathbf{q}}_R, \quad s = \frac{\hat{s}}{\hat{Y}_{O_\infty}}, \quad (6)$$

where \hat{c}_p is the specific heat of the gas phase and \hat{k} is the conductivity of the gas phase.

2.1. Zeldovich formulation and quasi-steady assumption

The reaction rate can be written as

$$\hat{\omega} = \hat{B} \hat{T}^a \hat{Y}_F^b \hat{Y}_O^c \exp\left(-\frac{\hat{E}_a}{\hat{R} \hat{T}}\right), \quad (7)$$

where \hat{B} is inversely proportional to the characteristic reaction time, \hat{E}_a is the activation energy and a , b and c are constants. In the limit of infinitely fast reaction one has a very large \hat{B} , which requires $Y_F Y_O \ll 1$. This condition implies that fuel and oxidizer cannot coexist, as they are completely consumed at the flame. In that case, the use of Equations 2 to 4 is redundant, for one can define (LAW, 2010)

$$Z = s Y_F - Y_O + 1, \quad H = s T + s Y_F + (q - 1) Y_O, \quad (8)$$

and rewrite the equations without the reaction term. At the flame, $Y_O = Y_F = 0$, and $Z > 1$ corresponds to the region between the droplet and the flame (where there is only fuel vapour) and $Z < 1$ corresponds to the region outside the flame (where there is only oxidizer). Therefore, the temperature and species mass fractions can be recovered by

$$Y_F = \frac{Z - 1}{s}, \quad T = \frac{H - Z + 1}{s}, \quad Z > 1 \quad (9)$$

and

$$Y_O = 1 - Z, \quad T = \frac{H - (q - 1)(1 - Z)}{s}, \quad Z < 1. \quad (10)$$

The integration of Equation 1 gives

$$u = \frac{\lambda}{r^2} \quad (11)$$

where $\lambda(t)$ is the droplet vaporization rate, as it will be shown later. Furthermore, if the liquid phase is much more dense than the gaseous phase, i. e., if $\rho_l \gg 1$, the transient term can be neglected. Finally, it is more convenient to rewrite the equations in terms of the normalized $x = r/a$, with $a(t)$ being the droplet radius, giving

$$\beta \frac{dZ}{dx} = \frac{d}{dx} \left(x^2 \frac{dZ}{dx} \right), \quad (12)$$

$$\beta \frac{dH}{dx} = \frac{d}{dx} \left(x^2 \frac{dH}{dx} \right) + s a^2 x^2 \nabla \cdot \mathbf{q}_R, \quad (13)$$

where $\beta(t)$ is the vaporization function, given by

$$\beta = \frac{\lambda}{a}. \quad (14)$$

2.2. Boundary conditions

From the balance of mass at the droplet surface, λ can be written in terms of the droplet radius as

$$\lambda = -a^2 \frac{da}{dt}, \quad (15)$$

which is proportional to the droplet vaporization rate, since the droplet mass is proportional to a^3 . Moreover, the balance of energy and fuel mass fraction at the droplet surface gives

$$\frac{dZ}{dx} = \beta[Z - (s + 1)], \quad (16)$$

$$\frac{dH}{dx} = \beta[H + s(L - T_b - 1)] + saq_{R,s}, \quad (17)$$

where L is the latent heat of vaporization, T_b is the droplet temperature and $q_{R,s}$ is the flux of radiation at the droplet surface. Since β is unknown, a further condition must be imposed, namely, the temperature of the gas at the droplet surface, assumed to be equal to the droplet temperature, it is, the boiling temperature of the fuel, giving

$$H = sT_b + Z - 1. \quad (18)$$

After β is known, the droplet radius can be calculated using

$$\frac{d}{dt}(a^2) = -2\beta. \quad (19)$$

Far from the droplet, one has, from Equation 8,

$$Z = 0, \quad H = s + q - 1. \quad (20)$$

2.3. Radiative heat transfer

The radiative heat flux is given by (VISKANTA; MERRIAM, 1968)

$$\nabla \cdot \mathbf{q}_R = -2\sigma_B \left[2\kappa T^4 - \frac{1}{ax} (T_b^4 g_1(x) + g_2(x)) - \frac{\kappa^2 a}{x} \int_1^\infty \xi K(x, \xi) T^4 d\xi \right], \quad (21)$$

where

$$\sigma_B = \frac{\hat{a}_0}{\hat{k}_\infty} \hat{T}_\infty^3 \hat{\sigma}_B, \quad \kappa = \hat{a}_0 \hat{\kappa} \quad (22)$$

are the nondimensional Stefan-Boltzmann constant and the absorption coefficient of the gas, respectively. The first term of Equation 21 corresponds to the radiative heat emitted by the gas, after the Stefan-Boltzmann law. The term with g_1 correspond to the radiation absorbed by the gas from the droplet surface and g_2 describes the radiation absorbed from the infinity. Finally, the last term accounts for the radiation emitted by the gas and then reabsorbed. The kernel K and the functions g_1 and g_2 are given by (VISKANTA; MERRIAM, 1968)

$$K(x, \xi) = E_1(\kappa a |x - \xi|) - E_1(\kappa a (\sqrt{x^2 - 1} + \sqrt{\xi^2 - 1})), \quad (23)$$

$$g_1(x) = \kappa a E_2(\kappa a (x - 1)) - E_3(\kappa a (x - 1)) + E_3(\kappa a \sqrt{x^2 - 1}), \quad (24)$$

$$g_2(x) = \kappa a x_\infty \left[E_2(\kappa a(x_\infty - x)) - E_2(\kappa a(x_\infty + \sqrt{x^2 - 1})) \right] + E_3(\kappa a(x_\infty - x)) - E_3(\kappa a(x_\infty + \sqrt{x^2 - 1})), \quad (25)$$

where E_n is the exponential integral functions of order n , given by

$$E_n(x) = \int_1^\infty e^{-x\xi} \xi^{-n} d\xi \quad (26)$$

and x_∞ corresponds to the position at which the boundary condition for the infinity is set.

The radiative flux at the droplet surface is (VISKANTA; MERRIAM, 1968)

$$q_{R,s} = -2\sigma_B \int_1^\infty \xi J(\xi) T^4 d\xi, \quad (27)$$

with

$$J(\xi) = -\kappa a E_2(\kappa a(\xi - 1)) + E_3(\kappa a(\xi - 1)) - E_3(\kappa a \sqrt{\xi^2 - 1}). \quad (28)$$

If the governing equations are discretized along x with N points, the number of mathematical operations in the evaluation of the finite differences is proportional to N , it is, the evaluation of a time step is $\mathcal{O}(N)$. The evaluation of the radiative heat flux, however, involves the computation of an integral across the whole domain (which itself is $\mathcal{O}(N)$) for each point along x . Therefore, the evaluation of the radiative heat flux is $\mathcal{O}(N^2)$. That means the calculation of the absorption term is the most expensive part of the numerical solution of the problem.

2.3.1. Optically thin limit

In the optically thin limit, i. e., if $\kappa \ll 1$, Equation 21 can be rewritten as

$$\nabla \cdot \mathbf{q}_R = -2\sigma_B \left[2\kappa T^4 - \frac{1}{ax} (T_b^4 g_1(x) + g_2(x)) \right], \quad (29)$$

where terms of order κ^2 were neglected. Since the absorption term disappeared, the computation of the radiative heat flux in the optically thin limit is $\mathcal{O}(N)$.

2.4. Solution for the adiabatic case

If the effect of radiation can be neglected, it is, if $q_R = 0$ and $q_{R,s} = 0$, Equations 12 and 13 can be readily integrated with the boundary conditions, giving

$$Z = (s + 1) \left[1 - \exp\left(-\frac{\beta}{x}\right) \right], \quad (30)$$

$$H = [q + s(L - T_b) - 1] \exp\left(-\frac{\beta}{x}\right) - s(L - T_b - 1). \quad (31)$$

Applying the expressions to the droplet surface gives

$$\beta = \ln \left(1 + \frac{q/s - T_b + 1}{L} \right), \quad (32)$$

which is a constant. Therefore, the droplet radius is given by

$$a^2 = 1 - 2\beta t, \quad (33)$$

it is, the square of the droplet radius decreases linearly with time. This result is known as the d^2 law for droplet vaporization (LAW, 2010).

3. Numerical implementation

The Equations 12 and 13 are solved by the finite differences method. The value of β is initially estimated at the beginning of each iteration, and its correct value is obtained by the secant method until the condition 18 is satisfied. After β is obtained, the droplet radius is updated by Equation 19. The radiative heat terms are calculated using the temperature profile from the previous step, and the calculations are repeated until the droplet has completely vaporized, i. e., until $a = 0$.

4. Results

It was chosen to study the combustion of a droplet of ethanol in air at ambient temperature. The stoichiometric coefficient, the combustion heat and the latent heat were calculated as $s = 9.93$, $q = 99.17$ and $L = 3.06$. The droplet temperature was calculated as $T_b = 1.17$, and the absorption coefficient was calculated based on a mixture of carbon dioxide and water vapour, giving $\kappa = 6.6 \times 10^{-3}$. The nondimensional Stefan-Boltzmann constant is $\sigma_B = 0.1$.

The initial droplet diameter was chosen as $\hat{a}_0 = 10^{-4}$ m. It was observed that larger initial diameters greatly affected the accuracy of the numerical method, requiring small time steps and fine meshes in order to avoid spurious results. Moreover, smaller droplets are less affected by radiation (MARCHESE; DRYER, 1997). The initial condition corresponds to the adiabatic case.

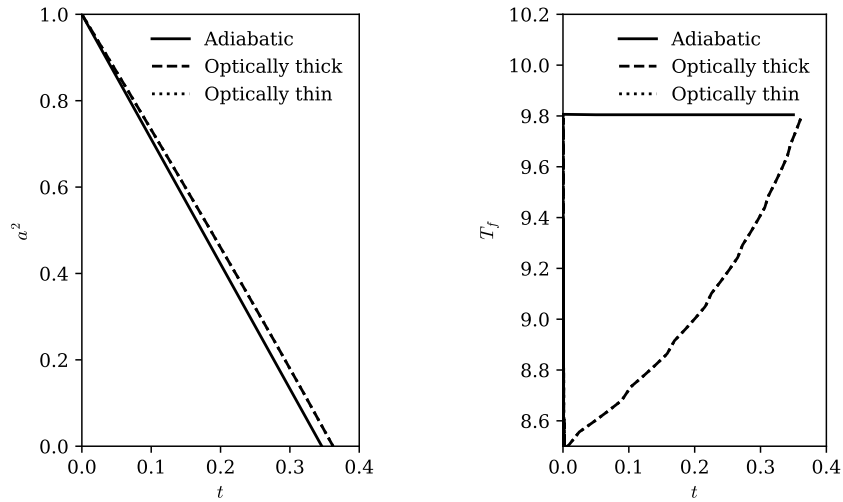
Figure 1 shows the behaviour of the droplet radius and the flame temperature along time. It can be seen from Figure 1.a that the radiation seems to have very little impact over the vaporization rate, since the droplet was completely vaporized around $t = 0.35$ in all cases. Moreover, the solution obtained for the optically thin case appears to be indistinguishable from the solution obtained for the optically thick case. It is clear that the radiative case presents a slightly lower vaporization rate, which is in agreement with results obtained previously (MARCHESE; DRYER, 1997), it is, that the effect of radiation is more pronounced in larger droplets. From the nondimensionalization of the radiation parameters, Equation 22, the radiative heat flux must increase with the square of the initial droplet radius, since both coefficients are multiplied in the final expression, Equation 29. Since the radiation removes temperature from the gaseous phase, the droplet receives less heat from conduction, decreasing its vaporization rate.

Figure 1.b shows the flame temperature along time. While the temperature is constant in the adiabatic case, the temperature in the radiative case is lower, as expected. It must be observed that the curves corresponding to the optically thick and optically thin cases are indistinguishable in the graph. One can see that the flame temperature increases with time in the radiative case. Equation 29 shows that the radiative flux is proportional to the droplet radius, which decreases with time, weakening the influence of radiation. This reflects the fact that as the droplet gets smaller, the flame gets closer to the droplet, decreasing the surface area of the flame and, therefore, the heat emitted by radiation.

It can be noticed that the effect of reabsorption appears to be irrelevant. Figure 3 shows the ratio between radiative emission and absorption evaluated with the temperature profile obtained in the adiabatic case for $a = 1$. It is clear that the emission is much more relevant than absorption and, therefore, the assumption of optically thin gas can be justified.

5. Conclusion

The effect of nonluminous radiation was studied in the case of quasi-steady droplet combustion. Despite the simplified nature of the analysis, the results were found to agree with the literature.



(a) Square of the droplet radius as function of time.

(b) Flame temperature as function of time.

Figure 2. Comparison between the adiabatic, optically thick and optically thin cases.

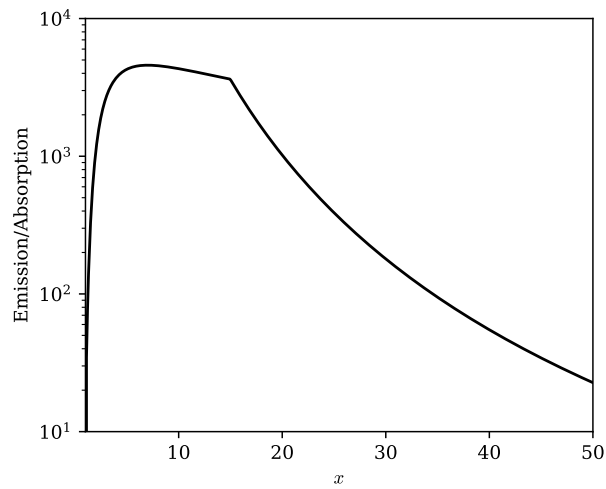


Figure 3. Ratio between radiative emission and absorption.

It was observed that the effect of reabsorption of radiation by the gas is insignificant and can, therefore, be neglected. This result is convenient to the modelling of droplet combustion because the reabsorption is particularly costly to compute.

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