AN INTEGRAL SOLUTION FOR TRANSIENT DIFFUSION FLAMES

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Abstract. *Transient diffusion flames are important in several combustion processes, specially in turbulent flows that occur in a number of practical devices, such as in burners and flame holders. Turbulent flames can be studied locally considering the burning of small diffusion flames, i.e., laminar flamelets. If fuel and oxidizer present different diffusion coefficients the flamelet structure can be significantly affected. This work analyses the effects of differential diffusion of fuel and oxidizer on a single plane diffusion flame separating two semi-infinite regions. Approximate solutions are obtained using the integral method and the results are compared to an analytical solution. The effects of the ratio of diffusion coefficients and of the initial equivalence ratio on flame position and fuel consumption are analysed, for different approximate mixture profiles.*

Keywords: *unsteady flames, diffusion flames, integral method, fuel consumption, flame position*

1. INTRODUCTION

Turbulent diffusion flames appear in several combustion devices, such as burners and flame holders. In many cases turbulent flames can be studied locally considering the burning of small transient laminar diffusion flames, called flamelets.

Analytical and numerical solutions for unsteady diffusion flames are usually modeled by adopting several simplifying assumptions. Constant density, constant specific heat and constant diffusion coefficients are common assumptions (Liñán and Williams, 1993; Thevenin and Candel, 1994; Marble, 1983).

Since there is mostly fuel on one side of the flame and oxidizer on the other side, the governing diffusion coefficients on the two sides of a diffusion flame can be vastly different. Consequently, the flame structure can be significantly modified. Fuel and oxidizer reach the flame position at different velocities and the temperature and mixture fraction profiles can be strongly affected.

The objective of this work is to analyse the effects of different diffusion coefficients on the structure of laminar diffusion flames, considering the burning of a single unsteady plane diffusion flame separating fuel and oxidizer which are in two semi-infinite regions.

An integral method using power profiles is adopted to obtain approximate solutions for the mixture fields, flame position and fuel consumption rates and the results are compared to the analytical solution obtained previously by Costa (2001).

The solutions can be used as basic models in the analysis of flamelets and to give insight into fundamental aspects of diffusive burning with more complex geometries.

2. MATHEMATICAL FORMULATION

2.1. Unsteady diffusion flames

The assumptions for this analysis are constant binary diffusion coefficients for the fuel side (D_1) and the oxidant side (D_2); constant and equal densities for both fuel and oxidizer; unity Lewis numbers, i.e., $\lambda_1/C_{P,1}=\rho D_1$ and $\lambda_2/C_{P,2}=\rho D_2$; the same initial temperatures, T_0, for both fuel and oxidant; fast chemistry and a single step reaction with s kg of oxidant reacting with 1 kg of fuel; no thermal diffusion; instantaneous ignition at all points of the fuel-oxidant interface; mass fluxes of fuel and oxidizer at the flame position are considered in stoichiometric proportion; fuel is in the negative half-space with initial mass fraction $Y_{F,0}$ while oxidant is in the positive half-space with initial mass fraction $Y_{O,0}$; the flame is planar, horizontal and uniform.

Defining a Schvab-Zeldovich variable (Williams, 1985) eliminates the reaction terms in the reaction-diffusion equations:

$$\beta = \frac{1+\phi\dfrac{Y_F}{Y_{F,0}}-\dfrac{Y_O}{Y_{O,0}}}{1+\phi} = 1 - \frac{\phi}{(1+s)}\frac{Y_P}{Y_{F,0}} - \frac{Y_O}{Y_{O,0}} = \frac{Y_F}{Y_{F,0}} + \frac{C_p(T-T_0)}{Y_{F,0}Q} \tag{1}$$

where $\phi = sY_{F,0}/Y_{O,0}$ is the initial equivalence ratio of the reactants. In the fuel side, $Y_{O,0} = 0$ and $\beta \equiv \beta_1$, and in the oxidizer side, $Y_{F,0} = 0$ and $\beta \equiv \beta_2$. Therefore, the governing equations for the mixture fractions in the fuel and oxidizer sides become, respectively:

$$\beta_{1,t} = D_1 \beta_{1,xx}, \quad x < x_f \tag{2}$$

$$\beta_{2,t} = D_2 \beta_{2,xx}, \quad x > x_f \tag{3}$$

where t is time, x is position and $x_f = x_f(t)$ is flame position.

The boundary and initial conditions for the problem are

$$x_f(0) = 0, \tag{4}$$

$$\beta_1(x < 0, t = 0) = 1, \quad \beta_2(x > 0, t = 0) = 0, \tag{5}$$

$$\beta_1(x \to -\infty, t) = 1, \quad \beta_2(x \to \infty, t) = 0. \tag{6}$$

The conditions at the flame position are

$$\beta_1(x_f, t) = \beta_2(x_f, t) = \beta_f \tag{7}$$

$$D_1 \beta_{1x}(x_f) = D_2 \beta_{2x}(x_f) \tag{8}$$

where $\beta_f = 1/(1+\phi)$ is a constant which depends on the stoichiometry.

2.2. Integral Solutions

Linear and power profiles satisfying the boundary and interface conditions are considered in order to obtain an integral solution:

$$\beta_1 = 1 + (\beta_f - 1)\left(\frac{x - \delta_1}{x_f - \delta_1}\right)^n, \quad \delta_1 < x < x_f \tag{9}$$

$$\beta_2 = \beta_f \left(\frac{\delta_2 - x}{\delta_2 - x_f}\right)^n, \quad x_f < x < \delta_2 \tag{10}$$

where $x_f - \delta_1$ is the fuel diffusion layer thickness, $\delta_2 - x_f$ is the oxidizer diffusion layer thickness, and $n = 1, 2, \ldots$ is the order of the power profile.

Figure 1 shows a scheme of the profiles considered. It can be seen that δ_1 and δ_2 are positions where the fuel mixture fraction and the oxidizer mass fraction are not affected by the flame presence. Note that $\beta_1(\delta_1) = 1$ and $\beta_2(\delta_2) = 0$, and for $n > 1$, $\partial^m \beta_1/\partial x^m(\delta_1) = 0$ and $\partial^m \beta_2/\partial x^m(\delta_2) = 0$, $m = 1, \ldots, n-1$.

Integrating Eqs. (2) and (3) along the diffusion layers, yields, respectively:

$$\frac{d}{dt} \int_{\delta_1}^{x_f} \beta_1 dx - \beta_f \frac{dx_f}{dt} + \frac{d\delta_1}{dt} = D_1 \beta_{1,x}(x_f) \tag{11}$$

$$\frac{d}{dt}\int_{x_f}^{\delta_2}\beta_2 dx + \beta_f \frac{dx_f}{dt} = -D_2\beta_{2,x}(x_f)$$ (12)
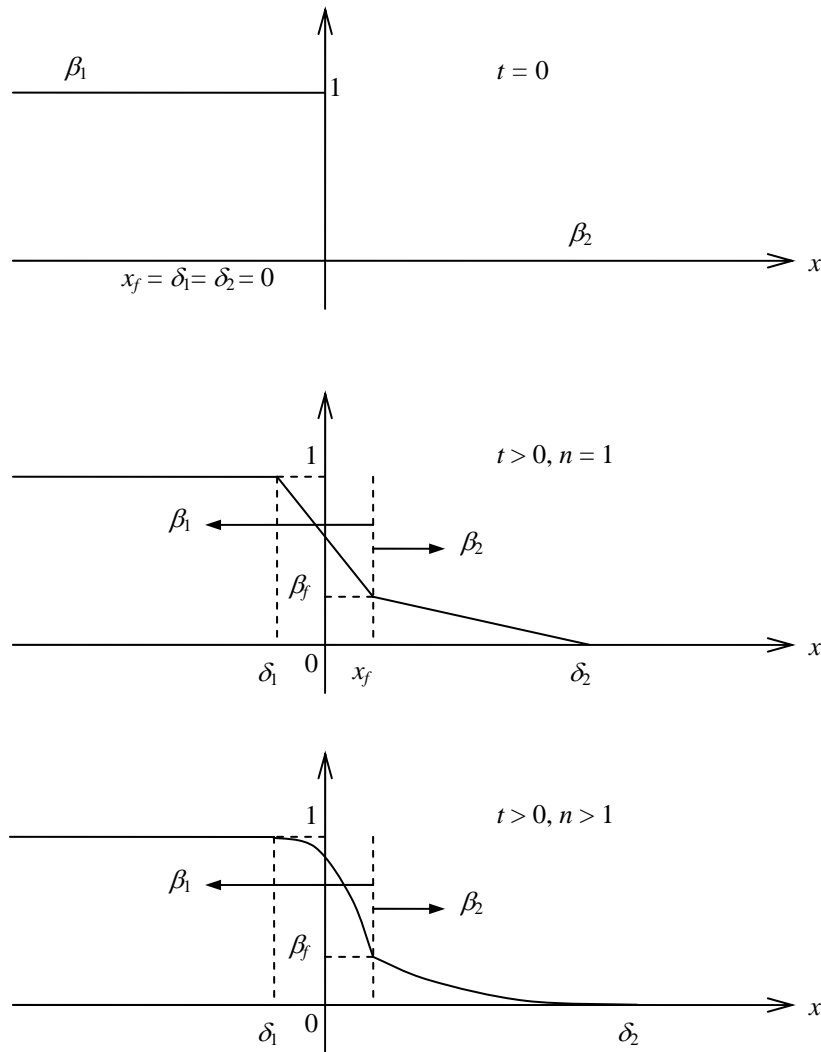

Figure 1 – Approximate power profiles used in the integral method.

Substituting Eqs. (9) and (10) into Eqs. (11) and (12), yields, respectively:

$$\left(1+\frac{\beta_f-1}{n+1}\right)\frac{d\left(x_f-\delta_1\right)}{dt} - \beta_f \frac{dx_f}{dt} + \frac{d\delta_1}{dt} = \alpha_1\beta_{1,x}(x_f)$$ (13)

$$\frac{\beta_f}{n+1}\frac{d\left(\delta_2-x_f\right)}{dt} + \beta_f \frac{dx_f}{dt} = -\alpha_2\beta_{2,x}(x_f)$$ (14)

Substituting now the given profiles at the interface position, yields:

$$\beta_{1x}(x_f) = n\frac{\beta_f-1}{x_f-\delta_1}$$ (15)

$$\beta_{2x}(x_f) = -n\frac{\beta_f}{\delta_2 - x_f} \tag{16}$$

Replacing Eqs. (15) and (16) into Eqs. (13) and (14), respectively, and rearranging, gives:

$$n\frac{dx_f}{dt} + \frac{d\delta_1}{dt} = -\frac{n(n+1)D_1}{x_f - \delta_1} \tag{17}$$

$$n\frac{dx_f}{dt} + \frac{d\delta_2}{dt} = \frac{n(n+1)D_2}{\delta_2 - x_f} \tag{18}$$

Substituting Eqs. (15) and (16) into Eq. (8), gives:

$$\delta_2 - x_f = \frac{\alpha}{\phi}\left(x_f - \delta_1\right) \tag{19a}$$

where $\alpha = D_2/D_1$. Consequently, the ratio of the diffusion layers' thicknesses is given by

$$\frac{x_f - \delta_1}{\delta_2 - x_f} = \frac{\phi}{\alpha} \tag{19b}$$

indicating that for $\alpha = 1$, the flames with $\phi > 1$ have fuel layer thickness larger than the oxidizer layer thickness, whereas flames with $\phi < 1$ have oxidizer layer thickness larger than the fuel layer thickness. If $\phi = 1$, the flames with $\alpha > 1$ have fuel layer thickness smaller than the oxidizer layer thickness, whereas flames with $\alpha < 1$ have oxidizer layer thickness smaller than the fuel layer thickness.

Now, substituting Eq. (19a) into Eq. (18) and combining with Eq. (17), yields

$$\frac{dx_f}{dt} = c\frac{d\delta_1}{dt} \tag{20}$$

where

$$c = \frac{(\alpha/\phi) - \phi}{(\alpha/\phi) + n(1+\phi) + 1} \tag{21}$$

It can be noted that $|c| < 1$, since $n \geq 1$. If $\phi = 1$, $c = (\alpha - 1)/(\alpha + 1 + 2n)$, and if $\alpha = 1$, $c = (1 - \phi)/(1 + n\phi)$. Now, integrating Eq. (20) from 0 to t, yields:

$$x_f = c\delta_1 \tag{22}$$

Therefore, x_f and δ_1 have the same sign if $\alpha > \phi^2$ and the flame remains at the origin, $x_f = 0$, when $\alpha = \phi^2$. Substituting Eq. (22) into Eqs. (17) and (19), and integrating, yields, respectively:

$$\delta_1 = -\kappa\sqrt{4D_1 t} \tag{23}$$

$$\delta_2 = -\left(c + (c-1)(\alpha/\phi)\right)\kappa\sqrt{4D_1 t} \tag{24}$$

where

$$\kappa = \left(\frac{n(n+1)}{2(1-c)(1+nc)} \right)^{1/2} \tag{25}$$

and, consequently,

$$x_f = -c\kappa\sqrt{4D_1 t} \tag{26}$$

The fuel and oxidizer diffusion layer thicknesses are, respectively,

$$x_f - \delta_1 = \kappa(1-c)\sqrt{4D_1 t} \tag{27}$$

$$\delta_2 - x_f = (c-1)\kappa\left(\alpha/\phi\right)\sqrt{4D_1 t} \tag{28}$$

It is seen in Eqs. (26-28) that the flame position and the diffusion layer thicknesses vary with $t^{1/2}$. Equation (26) can be rewritten in terms of the oxidizer diffusion coefficient:

$$x_f = \gamma_a \sqrt{4D_2 t} \tag{29}$$

where $\gamma_a = \kappa c \alpha^{-1/2}$ is an approximate coefficient for the non-dimensional flame position

2.3. Fuel consumption rate

The fuel consumption rate per unit area is given by

$$\dot{m}_F'' = -\rho D_1 \frac{\partial Y_F}{\partial x}\bigg|_{x=x_f} \tag{30}$$

where

$$\frac{\partial Y_F}{\partial x} = \frac{Y_{F,0}\left(1+\phi\right)}{\phi}\frac{\partial \beta_1}{\partial x} = n\frac{Y_{F,0}\left(1+\phi\right)}{\phi}\left(\frac{\beta_f -1}{x_f - \delta_1} \right)\left(\frac{x-\delta_1}{x_f - \delta_1} \right)^{n-1}$$

Therefore,

$$\dot{m}_{F,a}'' = \frac{n\rho D_1 Y_{F,0}}{x_f - \delta_1} \tag{31}$$

and, since $x_f - \delta_1 = \kappa\left(1-c\right)\sqrt{4D_1 t}$, then

$$\dot{m}_{F,a}'' = \frac{n\rho D_1 Y_{F,0}}{\kappa\left(1-c\right)\sqrt{4D_1 t}} \tag{32}$$

For $D_2 = D_1$, it follows that

$$c-1 = \frac{\left(1/\phi\right)-\phi}{1+n(1+\phi)+\left(1/\phi\right)} - 1 = -\frac{n+1}{n+\left(1/\phi\right)}$$

yielding:

$$\dot{m}''_{F,a}\big|_{D_2=D_1} = -\frac{n\left(n+(1/\phi)\right)}{(n+1)\kappa}\frac{\rho D_1 Y_{F,0}}{\sqrt{4D_1 t}}$$
(33)

Consequently, the ratio of the fuel consumption rate of a fuel burning with an oxidizer with a different diffusion coefficient and the fuel consumption rate of a fuel burning with an oxidizer having the same diffusion coefficient is given by

$$r_{a,D_2\neq D_1} = \frac{\dot{m}''_{F,a}\big|_{D_2\neq D_1}}{\dot{m}''_{F,a}\big|_{D_2=D_1}} = \frac{n+1}{(1-c)\left(n+(1/\phi)\right)}$$
(34)

which simplifies to $r_{a,D_2\neq D_1} = 1/(1-c)$, when $\phi=1$.

2.4. Comparison with the exact solution

Equations (1-8) represent a Stefan type problem, as described by Crank (1956, 1984) and Carslaw and Jaeger (1959). An analytical solution was obtained by Costa (1995) who found expressions for the mixture fraction profiles:

$$\beta_1 = 1 - \left(\frac{\phi}{1+\phi}\right)\left[\frac{1+erf\left(x/\sqrt{4D_1 t}\right)}{1+erf\left(\gamma\sqrt{\alpha}\right)}\right]$$
(35)

$$\beta_2 = \frac{1}{1+\phi}\left[\frac{1-erf\left(x/\sqrt{4D_2 t}\right)}{1-erf\,\gamma}\right]$$
(36)

with the flame position given by

$$x_f = \gamma\sqrt{4D_2 t}$$
(37)

where γ is a flame position coefficient, calculated from the relation

$$\frac{\sqrt{\alpha}}{\phi}\frac{\exp\left(\gamma^2\right)}{\exp\left(\alpha\gamma^2\right)} = \frac{1-erf\left(\gamma\right)}{1+erf\left(\gamma\sqrt{\alpha}\right)}$$
(38)

In Eq. (38), if the flame is stationary, i.e., $\gamma=0$, then $\alpha=\phi^2$, the same result found with the approximate solution. The analytical mass fraction gradient is given by

$$\frac{\partial Y_F}{\partial x} = -\frac{Y_{F,0}\exp\left(-x^2/4D_1 t\right)}{\left(1+erf\left(\gamma\sqrt{\alpha}\right)\right)\sqrt{\pi D_1 t}}$$
(39)

and, consequently, the exact fuel mass consumption rate is

$$\dot{m}''_{F,exact} = \frac{\rho D_1 Y_{F,0}\exp\left(-\gamma^2\alpha\right)}{\left(1+erf\left(\gamma\sqrt{\alpha}\right)\right)\sqrt{\pi D_1 t}}$$
(40)

The ratio of the approximate consumption rate to the exact fuel consumption rate is

$$r = \frac{\dot{m}''_{F,a}}{\dot{m}''_{F,exact}} = \frac{n}{\kappa(c-1)} \frac{1 + erf\left(\gamma\sqrt{\alpha}\right)}{\exp\left(-\gamma^2\alpha\right)} \qquad (41)$$

3. RESULTS AND DISCUSSION

Figure 2 compares the approximate non-dimensional position flame coefficient, γ', using 1st, 2nd and 7th order profiles. It can be verified that profiles higher than 7th order do not show significant differences from the 7th order profiles within the range considered. It is seen that γ decreases with decreasing ϕ and increasing α, however its absolute value can increase with α, for $\phi = 0.5$ and 1.0.

Figure 3 shows the analytical flame position coefficient and the approximate flame position coefficient using 7th order profiles. It is verified that the integral solution is relatively closer to the exact solution for lower γ, i.e., for flames with low velocity. The approximate coefficients have the same order of magnitude of the analytical coefficient in the range considered.

Figures 4 and 5 show the fuel consumption ratio r versus α and ϕ, for a 7th order and a 1st order profile, respectively. It can be seen that 1st order profiles gives the best approximation in terms of fuel mass consumption rates, since r is closer to unity in most cases.
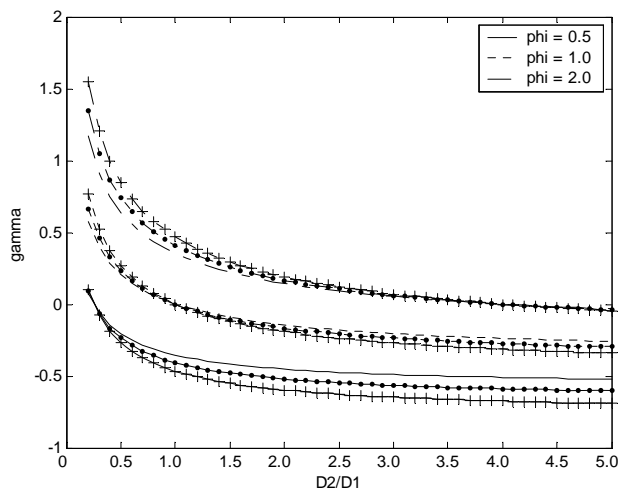

Figure 2 – Non-dimensional flame position coefficient versus ratio of diffusion coefficients for several initial equivalence ratios. (1st order - no symbols; 2nd order: dotted; 7th order: +).
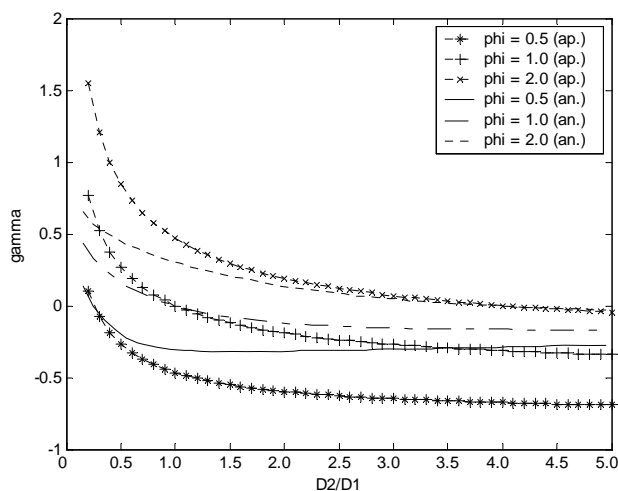

Figure 3 – Comparison of analytical flame position coefficients, γ, and 7th order approximate flame position coefficients, γ_a.
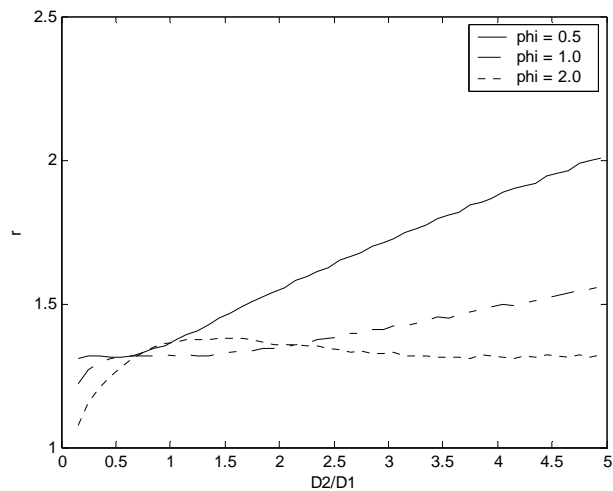
Figure 4 – Ratio of approximate and exact fuel consumption rates, r, versus diffusivity ratio, $\alpha = D_2/D_1$, and initial equivalence ratio, ϕ, for a 7th order profile.
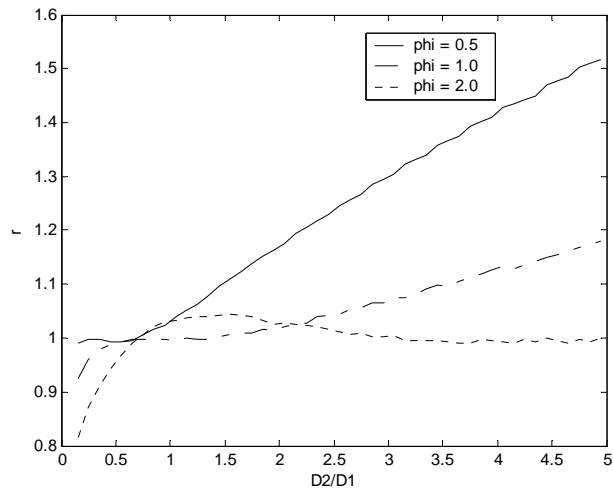

Figure 5 – Ratio of approximate and exact fuel consumption rates, r, versus diffusivity ratio, $\alpha = D_2/D_1$, and initial equivalence ratio, ϕ, for a 1st order profile.

4. CONCLUSIONS

An integral solution describing the propagation of a single unsteady plane diffusion plane separating two semi-infinite regions has been presented and compared to the analytical solution. The results indicate that the flame position coefficients from the approximate solutions have the same order of magnitude of the exact solution coefficients. Low velocity flames yield the best approximate results. The fuel consumption rates obtained from lower order profiles were closer to the analytical consumption rates than those obtained from higher order profiles. The present method can be easily applied to other geometries.

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