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# Bounds for the speed of combustion flames: The effect of mass diffusion

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**Abstract**

In this paper we analyze the speed of gas flames in a combustion premixed model that consists of two species (fuel and non-fuel). The main novelty with respect to recently published papers is that here we take into account the effect of the diffusion velocities in the energy equation. This means that the speed of the traveling wave obtained by numerically solving the combustion model (i.e., a system of two coupled one-dimensional partial differential equations) is a function of the Lewis number.

New bounds for the propagation speed of the combustion flame are derived here by performing a mathematical procedure that reduces the full combustion model into a single reaction-diffusion equation of a single variable. The new expressions derived here predict bounds that agree well with the flame speeds obtained from simulations of the full combustion model.

We finally analyze the case that includes the effect of radiative losses. Now, pulses rather than fronts propagate, whose speeds are also correctly predicted by the new expressions derived here.


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## 1. Introduction

Reaction-diffusion (RD) fronts arise in many systems, e.g., bacteria growth [1], migration in population dynamics [2], nuclear burning in supernova simulations [3], predator–prey models [4], epidemics [5], biological invasions [6], combustion processes [7], etc. Actually, combustion is a very complex process since it involves exothermic chemical reactions and transfer of mass, momentum and heat [8,9]. A lot of work has been devoted to obtain experimental data as well as numerical simulations through very detailed models on the propagation speed of flames in a large variety of combustion systems (e.g., turbulent flows [10,11], several flame types [12,13], etc.).

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Nevertheless, simplified combustion models have also been analyzed with the aim of providing a better understanding on the behavior of the system [7,14,15]. More specifically, the thermal propagation of flames in simple cases has been modelled with one-dimensional RD equations (see, e.g., Ref. [7]), although analytical values for its propagation speed can be only obtained once very restrictive assumptions are applied [8,16]. This is the reason why many authors have derived expressions for defining both lower and upper bounds for the speed of flames under more general conditions (see, e.g., Refs. [7,15]).

The purpose of this paper is to generalize the bounds for the speed of premixed combustion flames obtained by Fort et al. [15] by including the effect of mass diffusion (neglected in Ref. [15]), since this effect is known to substantially reduce the propagation speed. The contribution to temperature change rate due to the diffusion of species with different diffusion coefficients and heat capacities is included as a term within the energy equation, which added to that arising from Fourier's law of conduction is known to yield the total diffusive heat flux [8,14,17]. Although the effect of not neglecting mass diffusion has received numerous attention in combustion (e.g., Ref. [18]), its application to simplified RD models has not yet been carried out. Therefore, it is the first time that lower and upper bounds for the propagation speed of the flame are derived including the effect of mass diffusion.

The structure of the paper is as follows. First we describe the mathematical model of the premixed flame in Section 2. It follows Warnatz et al. [8] and it consists of two coupled partial differential equations (temperature and density of fuel). This is referred to as the full model, from which we obtain the numerical simulations by applying a standard finite-difference scheme in time and space [19]. Second, we derive the new expressions for the bounds for the speed of the flame in Section 3. These bounds are compared with the results obtained from the simulations of the full model (see Section 2). There is reasonably good agreement between the bounds and the simulated values, which reveals the interest of the present study. Note that, in order to obtain a one-dimensional RD equation suitable for deriving both lower and upper bounds for the propagation speed of the flame, we generalize the mathematical procedure by Fort et al. [15] for reducing the full model into a single RD equation of a single variable (temperature). We stress that whereas the expressions for the bounds follow from the reduced model, the simulated values follow from the full model. Third, we include radiative losses into the combustion model in Section 4. This term leads to pulses rather than fronts since the radiative energy losses extinguishes the flame. In this case, the procedure carried out in Section 3 for deriving the bounds for the propagation speed cannot be applied. However, the upper bound found in Section 3 still provides a reasonable limit for the flame speed. Finally, Section 5 is devoted to concluding remarks.

## 2. One-dimensional combustion model of a laminar premixed flame

In general, combustion flames may be divided into premixed and non-premixed ones [8]. The chemistry formulation is easier in premixed flames since both the fuel and the oxidizer are mixed before the burning process takes place. In addition, it has been observed that laminar premixed flames may produce fronts that propagate with a given speed [8,9]. Here we use a one-dimensional combustion model of a premixed laminar gas flame based on Warnatz et al. [8]. It consists of two species only: fuel $F$ and non-fuel (i.e., inert gases and oxidizers) $NF$. Note that we neglect external forces, both Duffour and Soret effects, and also convection (this is reasonable in microgravity and free-fall experiments). We assume constant pressure, local thermal equilibrium and a radially-symmetric flame. Under such assumptions, Warnatz et al. [8] show that the conservation equations for the species $i = F, NF$ in radial space coordinates read,

$$\frac{\partial \rho_i}{\partial t} + \frac{\partial (\rho_i v_i)}{\partial r} = r_i, \tag{1}$$

where $\rho_i$ is the density of species $i$ ($=F, NF$), $r_i$ is the source term (chemical consumption or generation of species $i$), and $v_i$ is the diffusion velocity of species $i$ which satisfies,

$$\rho_F v_F = -\rho_{NF} v_{NF}, \tag{2}$$

since the mean mass velocity is zero (i.e., convection is neglected, as explained above). From the evolution equation for the total density, this last assumption also implies a constant value for the total density $\rho$ (non-compressible mixture). Note that the total density $\rho$ may be obtained as $\rho = \rho_F + \rho_{NF}$.

In addition to Eq. (1), the equation for the conservation of energy reads [8],

$$\rho c_p \frac{\partial T}{\partial t} = \frac{\partial}{\partial r}\left(\lambda \frac{\partial T}{\partial r}\right) - \sum_i c_{p,i}\rho_i v_i \frac{\partial T}{\partial r} + q', \tag{3}$$

where $T$ is the temperature, $c_p$ is the specific heat of the mixture whose compounds have specific heats $c_{p,i}$ ($\rho c_p = \rho_F c_{p,F} + \rho_{NF} c_{p,NF}$), $\lambda$ is the thermal conductivity, and $q'$ represents the source term. In Eq. (3), the rate of temperature change does not only depend on the conductive term (first term on the r.h.s. in (3) plus the reaction (combustion) term (last term in (3)) but also on the diffusion of species with different heat capacities (second term on the r.h.s. in (3)).

By substituting Eq. (2) into Eq. (3), we obtain,

$$\rho c_p \frac{\partial T}{\partial t} = \frac{\partial}{\partial r}\left(\lambda \frac{\partial T}{\partial r}\right) - \left(c_{p,F} - c_{p,P}\right)\rho_F v_F \frac{\partial T}{\partial r} + q'. \tag{4}$$

Finally, we apply Fick's law for evaluating the mass flux $\rho_F v_F$ [8],

$$\rho_F v_F = -D_F \frac{\partial \rho_F}{\partial r}, \tag{5}$$

where $D_F$ is the diffusion coefficient of the fuel. The substitution of Eq. (5) into Eq. (4) leads to,

$$\rho c_p \frac{\partial T}{\partial t} = \frac{\partial}{\partial r}\left(\lambda \frac{\partial T}{\partial r}\right) + \left(c_{p,F} - c_{p,P}\right) D_F \frac{\partial \rho_F}{\partial r}\frac{\partial T}{\partial r} + QA\rho_F\left(\mathrm{e}^{-\frac{E_a}{RT}} - \mathrm{e}^{-\frac{E_a}{RT_0}}\right), \tag{6}$$

where the expression of the source term $q'$ derived in Ref. [15] has been made use of, which is an Arrhenius function of the fuel density and mixture temperature. The second term on the r.h.s. in Eq. (6) is the contribution to the internal energy change rate due to the effects of diffusion. Note that, as already pointed out by de Groot and Mazur [17], this term vanishes in a mixture of two species with the same specific heats. In the source term $q'$, $Q$ is the heat produced by the combustion reaction per unit mass of fuel, $R$ is the universal gas constant, $E_a$ is the activation energy per mole and $A$ is the pre-exponential factor. The source term in Eq. (6) is an approximation of the more physically realistic expression $QA\rho_F\mathrm{e}^{-\frac{E_a}{RT}} - QA\rho_0\mathrm{e}^{-\frac{E_a}{RT_0}}$, where the first term (i.e., $QA\rho_F\mathrm{e}^{-\frac{E_a}{RT}}$) corresponds to the classical Arrhenius function for expressing the heat per unit time and volume which has been released from the combustion process at a given temperature $T$, and the second term (i.e., $QA\rho_0\mathrm{e}^{-\frac{E_a}{RT_0}}$) corresponds to the usual so-called 'cold boundary layer' heat loss term (i.e., a reaction cut-off) in order to ensure steadiness if all the points of the system are at room temperature $T = T_0$ (i.e., $\partial T/\partial t = 0$ at $T = T_0$ [15]). Since at high temperatures $\rho_0\mathrm{e}^{-\frac{E_a}{RT_0}} \ll \rho_F\mathrm{e}^{-\frac{E_a}{RT}}$ and $\rho_F\mathrm{e}^{-\frac{E_a}{RT_0}} \ll \rho_F\mathrm{e}^{-\frac{E_a}{RT}}$ we approximate the source term $QA\rho_F\mathrm{e}^{-\frac{E_a}{RT}} - QA\rho_0\mathrm{e}^{-\frac{E_a}{RT_0}} \simeq QA\rho_F(\mathrm{e}^{-\frac{E_a}{RT}} - \mathrm{e}^{-\frac{E_a}{RT_0}})$. The validity of this approximation has already been checked numerically in Ref.[15]. This requirement that the initial state is a steady one will be needed to apply the variational method for obtaining upper and lower bounds (Section 3).

In addition to Eq. (6), the conservation equation for the fuel (mass species $i = F$ in Eq. (1)) may be expressed in terms of mass diffusion, leading to,

$$\frac{\partial \rho_F}{\partial t} = \frac{\partial}{\partial r}\left(D_F \frac{\partial \rho_F}{\partial r}\right) - A\rho_F\left(\mathrm{e}^{-\frac{E_a}{RT}} - \mathrm{e}^{-\frac{E_a}{RT_0}}\right). \tag{7}$$

According to the last term in Eq. (6), the local temperature will increase, but, according to (7), the fuel will eventually become locally exhausted. Once the fuel has been extinguished, the temperature does not decrease since here we do not take radiative losses into account (this will be done in Section 4). Therefore, the solution obtained has the form of a front that propagates with a constant speed. We point out that equations (6) and (7) revert to the expressions analyzed by Fort et al. [15] once the mass diffusion coefficient $D_F$ is zero, as they should.

For convenience, we rewrite Eqs. (6) and (7) in the dimensionless form by defining the following variables and parameters

$$\theta \equiv T\frac{R}{E_a}, \tag{8}$$

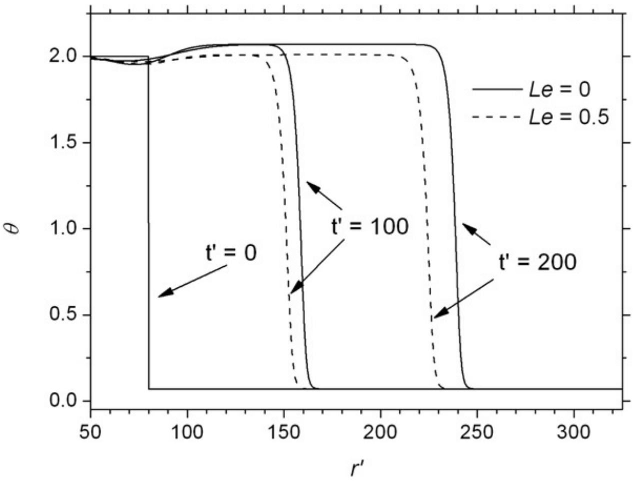


Fig. 1. Examples of dimensionless temperature $\theta$ profiles obtained by numerically solving the full model (i.e., Eqs. (15) and (16)) for $Le = 0$ (solid lines) and $Le = 0.5$ (dashed lines). The solutions are fronts since no radiation losses are taken into account (in contrast to Fig. 4). Note that the maximum temperature achieved in the front decreases as $Le$ increases. However, this variation is lower than 5% for $Le \leqslant 0.8$, as it is shown in Fig. 2. Here we have used $C = 0.5$, $\Delta c_p/c_p = 0.5$ and $\theta_0 = 0.07$ (see Ref. [15]).

$$t' \equiv t\frac{RQA}{c_p E_a}, \tag{9}$$

$$r' \equiv r\sqrt{\frac{RQA\rho}{\lambda E_a}}, \tag{10}$$

$$\rho' \equiv \frac{\rho_F}{\rho}, \tag{11}$$

$$C \equiv \frac{c_p E_a}{RQ}, \tag{12}$$

$$\Delta c_p \equiv c_{p,F} - c_{p,NF}, \tag{13}$$

$$Le \equiv \frac{\rho D_F c_p}{\lambda}, \tag{14}$$

from which (6) and (7) become

$$\frac{\partial\theta}{\partial t'} = \frac{\partial^2\theta}{\partial r'^2} + Le\frac{\Delta c_p}{c_p}\frac{\partial\rho'}{\partial r'}\frac{\partial\theta}{\partial r'} + \rho'\left(\mathrm{e}^{-\frac{1}{\theta}} - \mathrm{e}^{-\frac{1}{\theta_0}}\right), \tag{15}$$

$$\frac{\partial\rho'}{\partial t'} = Le\frac{\partial^2\rho'}{\partial r'^2} - C\rho'\left(\mathrm{e}^{-\frac{1}{\theta}} - \mathrm{e}^{-\frac{1}{\theta_0}}\right), \tag{16}$$

where we have assumed constant values for the thermal conductivity $\lambda$ and the mass diffusivity of fuel $D_F$.

Note that $\Delta c_p$ in Eq. (13) is a positive value since for a typical gaseous fuel (such as propane or $n$-butane) $c_{p,F} \approx 1.5$ kJ K$^{-1}$ kg$^{-1}$ whereas for the non-fuel species (e.g., air) $c_{p,NF} \approx 1$ kJ K$^{-1}$ kg$^{-1}$. $Le$ in Eq. (14) stands for the Lewis number, i.e. the dimensionless ratio of mass diffusivity to heat conductivity. This number has a great relevance in the combustion processes where diffusion is not neglected (see, e.g., [13,18]). Typical values of $Le$ lie between 0 and 1. In the limit case of $Le = 0$, Eqs. (15) and (16) lead to those obtained by Fort et al. [15], as they should, since they did not take diffusion into account. The effect of including diffusion reduces the speed of both temperature and fuel density fronts. This effect is seen in Fig. 1, where the numerical solution to Eqs. (15) and (16) is shown for $Le = 0$ and $Le = 1$ (for $C = 0.5$ and $\theta_0 = 0.07$). Numerical integrations use an initial step function for both temperature and density of fuel with $T(r, t = 0) = T_0$ for those values of $r$ such that $\rho_F(r, t = 0) = \rho_0$. The numerical procedure uses a standard finite-difference scheme in both time and space (see, e.g., [19]).

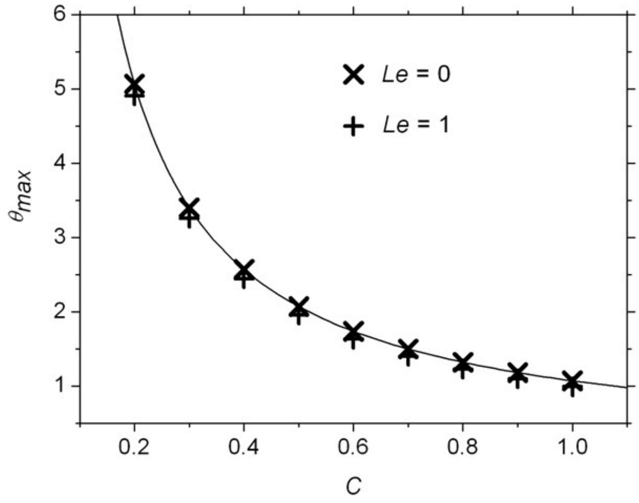


Fig. 2. Theoretical values (curves) for $\theta_{\max}$ as a function of the fuel parameter $C$ in comparison with observed ones from numerical simulations of the full model (i.e., Eqs. (15) and (16)) for two different values of Lewis number $Le$. Here we have used $\Delta c_p/c_p = 0.5$ and $\theta_0 = 0.07$.

## 3. Bounds for the propagation speed of fronts

In this section we apply the method of calculus of variations for obtaining the expressions for both upper and lower bounds for the propagation speed of the front. In essence, this method is based on the method developed by Benguria and Depassier [21] (here generalized to include the mass diffusion effect), which may be applied to systems described by a single RD equation. Therefore, we shall first reduce the full model (Eqs. (15) and (16)) into a simplified one, that will consist of a single RD equation of a single variable (temperature). We carry out this reduction (i.e., from Eqs. (15) and (16) to a single one) with the only purpose of deriving upper and lower bounds for the speed of the combustion flame. Numerical simulations will follow from the full model described by Eqs. (15) and (16).

### *3.1. RD combustion model of a single variable*

We get rid of $\rho'$ in Eq. (15) by using a simple relationship between $\rho'$ and $\theta$ that follows from the procedure employed in Fort et al. [15]. Thus, we first look for an expression for the maximum temperature $\theta_{\max}$ reached in the front. For doing so, Eqs. (15) and (16) are integrated from $t' = 0$ (before the flame front arrives at the point considered) to $t' = \infty$ (after the flame front has passed) with the following boundary conditions,

$$\begin{aligned} &\theta(t' = \infty) = \theta_{\max} \\ &\theta(t' = 0) = \theta_0 \\ &\rho'(t' = \infty) = 0 \\ &\rho'(t' = 0) = 1 \end{aligned} \tag{17}$$

under the assumption that the thermal and mass gradients are non-zero only in a narrow region (i.e., where the flame front arises). This implies that the term for the total diffusive heat flux in Eq. (15) and the term for the mass diffusion in Eq. (16) are negligible once we integrate Eqs. (15) and (16) over time from 0 to $\infty$. Then, the resulting equation obtained by substituting Eq. (16) into (15) and by integrating over time leads to

$$\theta_{\max} = \theta_0 + \frac{1}{C}, \tag{18}$$

once we apply the boundary conditions (17).

The validity of Eq. (18) is shown in Fig. 2 where we compare the maximum temperature obtained from Eq. (18) with that reached in the front by numerically solving Eqs. (15) and (16) as a function of $C$ and for two different values of $Le$ (= 0 and 1). The agreement is excellent not only in the non-diffusive case ($Le = 0$) but also for high values of $Le$ number ($Le = 1$). We stress that (18) is a key point in the derivation of both upper and lower bounds for the propagation speed of the flame, since it will allow us to define a new dimensionless variable whose range of values will lie between 0 and 1. This is essential for a correct application of the methods detailed below. As already pointed out by Fort et al. [15], Eq. (18) written in terms of the original variable $T$ reads,

$$T_{\max} = T_0 + \frac{Q}{c_p} \tag{19}$$

which is a special case of the Zeldovich equation for the conservation of energy [16]

$$\rho_0 c_p (T - T_0) = Q(\rho_0 - \rho_F), \tag{20}$$

or, in terms of the variables $\theta$ and $\rho'$,

$$\theta - \theta_0 = \frac{1 - \rho'}{C}, \tag{21}$$

from which (19) follows in the limit where $t$ goes to infinite (so $T \to T_{\max}$ and $\rho_F \to 0$).

By means of Eq. (21), we can rewrite Eq. (15) getting rid of the field $\rho'$,

$$\frac{\partial \theta}{\partial t'} = \frac{\partial^2 \theta}{\partial r'^2} - C Le \frac{\Delta c_p}{c_p} \left( \frac{\partial \theta}{\partial r'} \right)^2 + [1 - C(\theta - \theta_0)] \left( e^{-\frac{1}{\theta}} - e^{-\frac{1}{\theta_0}} \right). \tag{22}$$

Eq. (22) is a RD equation for a single variable $\theta$, no longer coupled to the density $\rho'$. Eq. (21) or, equivalently, the Zeldovich equation for the conservation of energy (20) is the key equation for reducing the set of two coupled equations (15) and (16) into a single one (22). For the values of the parameters $C$ and $\theta_0$ used here, Eq. (21) is a reasonable equation. In addition, the good agreement between the values for the bounds found in this section and the speed of the flame simulated from the full model (previous section) confirms the validity of equation (22) for providing estimates for the propagation speed of the premixed flame in our simple combustion model. This was also confirmed by Fort et al. [15] for the particular case of $Le = 0$. Moreover, other authors have used single RD models of a single variable for analyzing the speed of the flame in combustion processes (see, e.g., Ref. [3]). However, we stress, again, that (22) is used here for deriving the bounds only. Numerical simulations follow from the full coupled model (15) and (16).

For applying the techniques needed for obtaining upper and lower bounds for the propagation speed of the front, it is convenient to express equation (22) in terms of a new dimensionless variable,

$$\theta' \equiv \frac{\theta - \theta_0}{\theta_{\max} - \theta_0}, \tag{23}$$

whose value varies within the interval $0 < \theta' < 1$, with extremes $\theta' = 0$ (room temperature $T = T_0$) and $\theta' = 1$ (maximum flame temperature $T = T_{\max}$). Then, by substituting Eq. (23) into Eq. (22), we obtain,

$$\frac{\partial \theta'}{\partial t'} = \frac{\partial^2 \theta'}{\partial r'^2} - B \left( \frac{\partial \theta'}{\partial r'} \right)^2 + f(\theta'), \tag{24}$$

where,

$$B \equiv Le \frac{\Delta c_p}{c_p}, \tag{25}$$

is a positive value and,

$$f(\theta') = C(1 - \theta') \left( e^{-\frac{1}{\theta_0 + (\theta_{\max} - \theta_0)\theta'}} - e^{-\frac{1}{\theta_0}} \right). \tag{26}$$

Note that the extremes of the new dimensionless variable $\theta' = 0$ and $\theta' = 1$ correspond to steady states $f(0) = 0$ and $f(1) = 0$ with $f(\theta') > 0$.

### 3.2. Lower bound

As shown in Fig. 1, the solution of Eq. (24) consists of traveling fronts $\theta'(r' - vt')$, where $v$ is its speed. Although many authors have analyzed the bounds for the propagation speed of fronts obtained in generalized RD equations [21, 22], there are no results for the combustion processes modelled by Eq. (24). Therefore, here we need to develop the calculation of these bounds. The method employed is based on the variational calculations proposed by Benguria et al. [7], who express the partial derivatives found in Eq. (24) in terms of the variable $z = r' - vt'$, from which we obtain,

$$\frac{\partial^2\theta'}{\partial z^2} + v\frac{\partial\theta'}{\partial z} - B\left(\frac{\partial\theta'}{\partial z}\right)^2 + f(\theta') = 0. \tag{27}$$

Note that Benguria et al. [7] analyze Eq. (27) for the particular case of $B = 0$.

We work in the phase space by defining,

$$p(\theta') = -\frac{\partial\theta'}{\partial z}, \tag{28}$$

where $p(0) = p(1) = 0$ and $p(\theta') > 0$ in (0, 1).

In the phase space, Eq. (27) reads

$$p\frac{\mathrm{d}p}{\mathrm{d}\theta'} - vp - Bp^2 + f(\theta') = 0. \tag{29}$$

Then, and following Ref. [22], we define $g(\theta')$ as an arbitrary positive function. Next, we multiply Eq. (29) by $g/p$ and integrate over $\theta'$ in the entire domain,

$$v\int_0^1 g\mathrm{d}\theta' = \int_0^1 \mathrm{d}\theta'\left(\frac{fg}{p} - Bgp + g\frac{\mathrm{d}p}{\mathrm{d}\theta'}\right), \tag{30}$$

which by integrating by parts the last term on the r.h.s. leads to,

$$v\int_0^1 g\mathrm{d}\theta' = \int_0^1 \mathrm{d}\theta'\left[\frac{fg}{p} + p\left(h - Bg\right)\right], \tag{31}$$

where,

$$h = -\frac{\mathrm{d}g}{\mathrm{d}\theta'}. \tag{32}$$

By choosing $g(\theta')$ such that,

$$h - Bg > 0, \tag{33}$$

and since $p$ and $f$ are positive, the following inequality holds,

$$\frac{fg}{p} + p\left(-\frac{\mathrm{d}g}{\mathrm{d}\theta'} - Bg\right) \geqslant 2\sqrt{fg\left(h - Bg\right)}, \tag{34}$$

which introduced into Eq. (31) leads to the lower bound for the propagation speed of the front,

$$v \geqslant \frac{2\int_0^1 \mathrm{d}\theta'\sqrt{fg\left(h - Bg\right)}}{\int_0^1 g\mathrm{d}\theta'}. \tag{35}$$

In order to provide a lower bound for $v$, we use the following trial function that satisfies Eq. (33) within the range of values for $B$ assumed in the present work ($0 \leqslant B \leqslant 0.5$; since $0 \leqslant Le \leqslant 1$ and $\Delta c_p/c_p = 0.5$),

$$g = \left(1 - \theta'\right)^n, \tag{36}$$

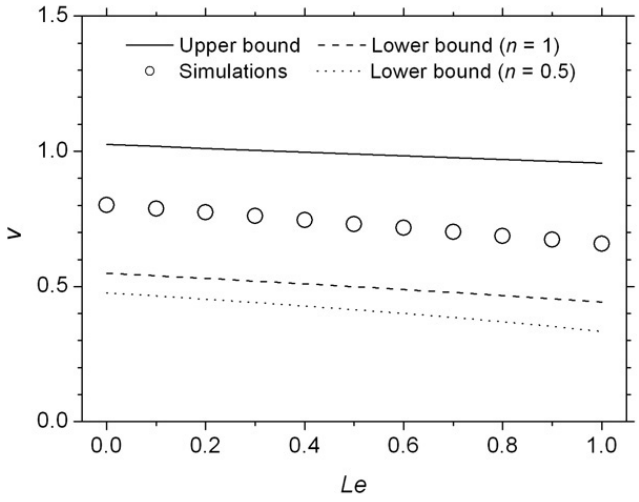


Fig. 3. Upper bound (solid line) and lower bounds ($n = 1$; dashed line; $n = 0.5$; dotted line) obtained with the new expressions derived in the present paper in comparison with the exact value of $v$ (squares) obtained from simulations of the full model Eqs. (15) and (16), as a function of *Le* number. Here we do not take energy losses into account and we have used $C = 0.5$ and $\Delta c_p/c_p = 0.5$.

with $0.5 \leqslant n \leqslant 1$. Then, substituting Eq. (36) into Eq. (35), we obtain,

$$v \geqslant 2(n+1)\int_0^1 \mathrm{d}\theta' \sqrt{f\left[n\left(1-\theta'\right)^{2n-1} - B\left(1-\theta'\right)^{2n}\right]}. \tag{37}$$

We integrate Eq. (37) numerically in order to obtain a lower bound and the results for $n = 0.5$ and $n = 1$ are shown in Fig. 3, where the predicted speed obtained by the numerical simulation of Eqs. (15) and (16) is also depicted. The bounds found here for $n = 1$ agree well with the numerical results, which confirms the validity of equation (37) for our combustion model that includes diffusion. Note that the trial function used here (36) differs from those applied by other authors [7] since the requirement (33) must be fulfilled. Also note that, since here $B \neq 0$ (more precisely: $0 \leqslant B \leqslant 0.5$), Eq. (37) is a generalization of the analysis carried out by Benguria et al. [7].

### 3.3. Upper bound

The variational principle applied above provides lower bounds once we suitably choose the trial function $g$. Here we derive the upper bounds. Following Benguria et al. [22] in the analysis of RD equations for non-combustion processes with $B = 0$, we consider a set of trial functions $\hat{g}$ such that,

$$\frac{f\,\hat{g}}{p} = p\left(-\frac{d\,\hat{g}}{\mathrm{d}\theta'} - B\,\hat{g}\right). \tag{38}$$

This implies that the equality in Eq. (34) holds. In this case, and by using Eq. (29), we find that,

$$\frac{1}{\hat{g}}\frac{d\,\hat{g}}{\mathrm{d}\theta'} - \frac{1}{p}\frac{\mathrm{d}p}{\mathrm{d}\theta'} = -\frac{v}{p} - 2B, \tag{39}$$

which can be integrated to obtain,

$$\frac{\hat{g}\,(\theta')}{p(\theta')} = \frac{\hat{g}\,(\theta'_0)}{p(\theta'_0)}\exp\left[-\int_{\theta'_0}^{\theta'}\left(\frac{v}{p(u)} + 2B\right)du\right], \tag{40}$$

with $0 < \theta'_0 < 1$. For the existence of the set $S$ of admissible trial functions $\hat{g}$, we require the convergence of the integrals in Eq. (40), which has been proved by Benguria et al. in a generalized RD equation with $B = 0$ [22].

However, and since $B > 0$, this new term does not compromise the convergence of Eq. (40). In addition, it is easily seen that $\hat{g}$ in Eq. (40) satisfies the requirement of equation (33). By following a similar procedure to that applied in the lower bound case (i.e., multiply Eq. (39) by $gp$ and integrate over $\theta$), Eq. (39) leads to

$$v = \frac{2\int_0^1 \mathrm{d}\theta' \sqrt{fg\,(h - Bg)}}{\int_0^1 g\mathrm{d}\theta'}, \tag{41}$$

for $g \in S$ (i.e., for values of the trial function $g$ that satisfy Eq. (38)). Note that in Eq. (41) we have already used the condition expressed in (38).

We define the velocity $v_*$ as the supremum of the velocities $v$ obtained from Eq. (41) over all $g \in S$,

$$v_* = \sup_g \frac{2\int_0^1 \mathrm{d}\theta' \sqrt{fg\,(h - Bg)}}{\int_0^1 g\mathrm{d}\theta'}. \tag{42}$$

Then, the upper bound for the propagation speed $v_*$ follows from considering that (similarly to (34)),

$$\frac{fg}{\alpha\theta'} + \alpha\theta' \left(-\frac{\mathrm{d}g}{\mathrm{d}\theta'} - Bg\right) \geqslant 2\sqrt{fg\,(h - Bg)}, \tag{43}$$

$\alpha$ being a positive constant. Using this into Eq. (42), leads to

$$v_* \leqslant \sup_g \frac{\int_0^1 \mathrm{d}\theta' \left[\frac{fg}{\alpha\theta'} + \alpha\theta' \left(-\frac{\mathrm{d}g}{\mathrm{d}\theta'} - Bg\right)\right]}{\int_0^1 g\mathrm{d}\theta'}. \tag{44}$$

Since $g(0) = g(1) = 0$, the integration by parts of the term $\alpha\theta'\mathrm{d}g/\mathrm{d}\theta'$ in Eq. (44) leads to,

$$v_* \leqslant \sup_g \frac{\int_0^1 g \left(\frac{f}{\alpha\theta'} + \alpha - \alpha B\theta'\right) \mathrm{d}\theta'}{\int_0^1 g\mathrm{d}\theta'}. \tag{45}$$

Therefore, and since $\alpha - \alpha B\theta' > 0$ for all positive values of $\theta'$, we obtain from Eq. (45),

$$v_* \leqslant \sup \left(\frac{f}{\alpha\theta'} + \alpha - \alpha B\theta'\right), \tag{46}$$

where $\theta' \in [0, 1]$.

By choosing the constant $\alpha$ such as,

$$\alpha = \sup \sqrt{\frac{f}{\theta'}}, \tag{47}$$

Eq. (46) reads,

$$v_* \leqslant \sup \left[\frac{f}{\theta'\left(\sup\sqrt{\frac{f}{\theta'}}\right)} - \left(\sup\sqrt{\frac{f}{\theta'}}\right) B\theta'\right] + \sup\sqrt{\frac{f}{\theta'}}, \tag{48}$$

where $\theta' \in [0, 1]$. This result reduces to the Aronson and Weinberger upper bound for the propagation speed of fronts in classical RD equations in the case of $B = 0$ (no diffusion), namely $v_* \leqslant \sup 2\sqrt{\frac{f}{\theta'}}$ (see [23]). Note that Eq. (48) differs from the upper bound found by Benguria et al. [7] in the analysis of combustion fronts since here we have generalized the reaction-diffusion equation used in Ref. [7] by including the mass diffusion contribution (i.e., here we use $B \neq 0$ in contrast with the $B = 0$ case analyzed by Ref. [7]).

We have solved Eq. (48) numerically for different values of $Le$. The results are also shown in Fig. 3. The upper bounds found here agree well with the front speed obtained by the numerical simulation of the full combustion model.

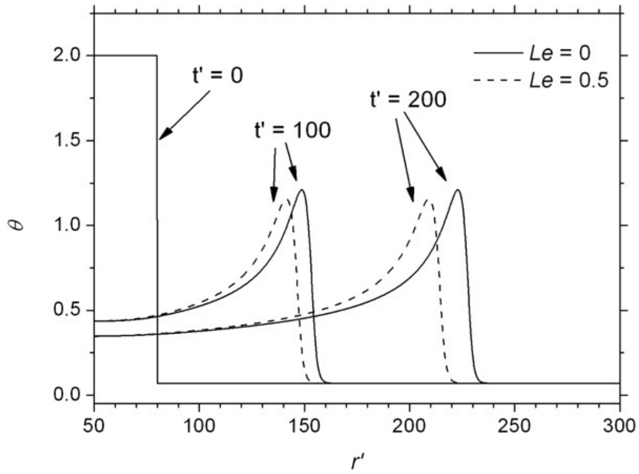


Fig. 4. Temperature profiles as in Fig. 1 except for using Eqs. (50) and (51), which take into account radiative energy losses. Note that, here the solutions are pulses instead of fronts. We have used $C = 0.5$, $\Delta c_p/c_p = 0.5$, $\theta_0 = 0.07$ and $\varepsilon = 0.04$ (see Ref. [15]).

This indicates the validity of the above expression for predicting the maximum value of the speed that may reach a front in a system that satisfies the constraints detailed in Section 2. Therefore, we have obtained upper bounds for the speed of fronts valid for arbitrary values of the Lewis number $Le$.

## 4. Bounds for the propagation speed of pulses (radiative losses)

In the preceding section, we have neglected the energy losses due to radiation. Although not totally realistic, this assumption has been taken into account by several authors [7,20–22] in the investigation of the front speed problem. A further step towards a more realistic approach of the combustion process involves the introduction of radiative losses. In essence, this effect includes a new term in Eq. (6), which now generalizes into

$$\rho c_p \frac{\partial T}{\partial t} = \frac{\partial}{\partial r}\left(\lambda \frac{\partial T}{\partial r}\right) + \left(c_{p,F} - c_{p,P}\right) D_F \frac{\partial \rho_F}{\partial r}\frac{\partial T}{\partial r} + QA\rho_F\left(\mathrm{e}^{-\frac{E_a}{RT}} - \mathrm{e}^{-\frac{E_a}{RT_0}}\right) - 4a\sigma\left(T^4 - T_0^4\right), \tag{49}$$

where $a$ is the absorption coefficient and $\sigma$ is the Stefan–Boltzmann constant (see, e.g., Ref. [15]). By applying the dimensionless variables and parameters introduced in Section 2, (with $\lambda$ and $D_F$ constants) we finally obtain the set of two equations that drive the evolution of the premixed laminar flame in radial space coordinates and with radiative losses,

$$\frac{\partial \theta}{\partial t'} = \frac{\partial^2 \theta}{\partial r'^2} + Le\frac{\Delta c_p}{c_p}\frac{\partial \rho'}{\partial r'}\frac{\partial \theta}{\partial r'} + \rho'\left(\mathrm{e}^{-\frac{1}{\theta}} - \mathrm{e}^{-\frac{1}{\theta_0}}\right) - \varepsilon\left(\theta^4 - \theta_0^4\right), \tag{50}$$

$$\frac{\partial \rho'}{\partial t'} = Le\frac{\partial^2 \rho'}{\partial r'^2} - C\rho'\left(\mathrm{e}^{-\frac{1}{\theta}} - \mathrm{e}^{-\frac{1}{\theta_0}}\right), \tag{51}$$

where we have defined the dimensionless emissivity,

$$\varepsilon \equiv \frac{4a\sigma}{QA\rho}\left(\frac{E_a}{R}\right)^4. \tag{52}$$

Eqs. (50) and (51) become (15) and (16) for a system with negligible radiative losses. Eqs. (50) and (51) are, indeed, the equations numerically solved in order to obtain the propagation speed of the flame. Fig. 4 shows the evolution of the flame obtained for $Le = 0$ and $Le = 1$ with $\Delta c_p/c_p = 0.5$ (using the same values for $\theta_0 = 0.07$, $C = 0.5$ and $\varepsilon = 0.04$, as in Ref. [15]). Note that, now, it is a pulse (Fig. 4) rather than a front (Fig. 1) what propagates (since the heat losses by radiation extinguishes the flame).

It is clear that one of the conditions needed in Section 3 for obtaining both lower and upper bounds (i.e., $\partial\theta/\partial z < 0$, see Eq. (28) and the text below it) will not be accomplished here. Thus, none of the methods applied above are valid for predicting the bounds of the propagation speed of the pulses that arise from Eqs. (50) and (51). Nevertheless, and

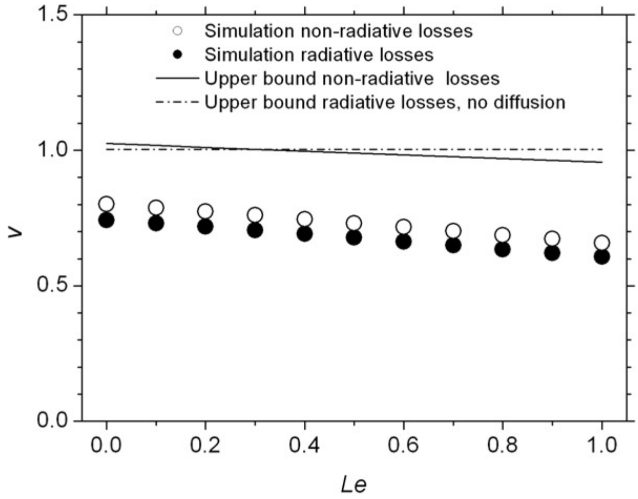


Fig. 5. Comparison between the upper bound (solid line) depicted in Fig. 3 and the exact value of $v$ for a system without radiative losses (open circles, as in Fig. 3) and with radiative losses (closed circles). We also show the upper bound obtained by Fort et al. [15] (dash–dot line), who take radiative losses into account but ignore diffusion effects. Note that pulses are slower than fronts since they have a lower flame energy available due to radiative energy losses.

since radiative losses will always decrease the speed of the flame, we may use the same upper bound found in Eq. (48) as a valid one. The results are shown in Fig. 5, where we also depict the speed of the fronts found in Section 3 (see Fig. 3). Also in Fig. 5, we show the upper bound obtained by Fort et al. [15], which includes radiative losses but ignores the diffusion process (i.e., with $Le = 0$ in equations (50) and (51)). Fig. 5 confirms that the expression for the upper bounds found in Section 3 for non-radiative processes is a valid one. Also, it predicts the correct order of magnitude of the flame speed, and it provides better bounds at high values of $Le$ than the upper bound obtained by including radiative processes in a non-diffusive system.

## 5. Concluding remarks

Experiments carried out by several authors have found that diffusion of species with different specific heats and diffusion coefficients lead to temperature evolution patterns that modify the propagation speed of the flame [11, 18]. This effect, however, has not been taken into account in former analytical studies of combustion through one-dimensional RD equations (see, e.g., Refs. [15,21]). Therefore, here we extend a previous work carried out in Ref. [15] by including diffusion in a simple combustion model of a premixed laminar flame in a gaseous fuel. This full model consists of two coupled partial differential equations (temperature and density of fuel). The effect of mass diffusion adds a new term in the evolution equations that depends on the Lewis number $Le$, which is a fundamental parameter in the study of combustion processes. It is a dimensionless ratio between the mass diffusion coefficient and the heat conductivity. For $Le = 0$, all of the results found here revert to previously published ones, as they should.

First, we have analyzed the system without taking radiative losses into account (Section 3). With the aim of obtaining the new expressions for the bounds of the flame speed, the set of two evolution equations of the full model (temperature and density of fuel) is reduced to a single one-dimensional RD equation (temperature) by following the procedure found in Ref. [15]. Then, by generalizing the variational method developed by Benguria and Depassier [21], we derive lower and upper bounds for the propagation speed of flames as a function of the Lewis number. For $Le = 0$ the upper bound reverts to the classical expression obtained by Aronson and Weinberger [23], whereas the lower bound corresponds to the expression obtained by Benguria and Depassier [20]. We point out that the propagation speed computed from the numerical simulations of the full combustion model is well predicted by both upper and lower bounds, giving the same order of magnitude. Since in simple combustion models with no diffusion some bounds may differ in orders of magnitude (e.g., the Kolmogorov–Petrovski–Piskunov method [15,16]), the good agreement shown here proves the usefulness of the new expressions for the bounds deduced here.

Second, we have included radiative losses in the full combustion model employed here (Section 4). This contribution leads to pulses rather than fronts, since heat losses extinguish the flame [15]. They also reduce the propagation speed. Unfortunately, the existence of pulses invalidates the application of the variational method employed in Section 3 since the temperature gradient changes its sign. Nevertheless, the expression for the upper bounds obtained in Section 3 may still be used and the results are compared with the upper bound proposed in Ref. [15] for the case of neglecting diffusion ($Le = 0$). For reasonable values of the emissivity parameter (see Ref. [15]), the results show how the upper bounds found for fronts in Section 3 may be also applied to pulses without substantially increasing the difference between actual values and predicted bounds.

It is important to stress that the diffusion terms considered here may substantially influence the speed of the flame. Indeed, the numerical simulations carried out here for the full model (two coupled partial differential equations) show a decrease in the propagation speed of fronts and pulses of the order of 18% for $Le = 1$ in comparison with the case with $Le = 0$. This shows the relevance of the expressions for the bounds reported here, that may be used as a first approximation in the analyses for the propagation speed of flames in more complex combustion models.

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