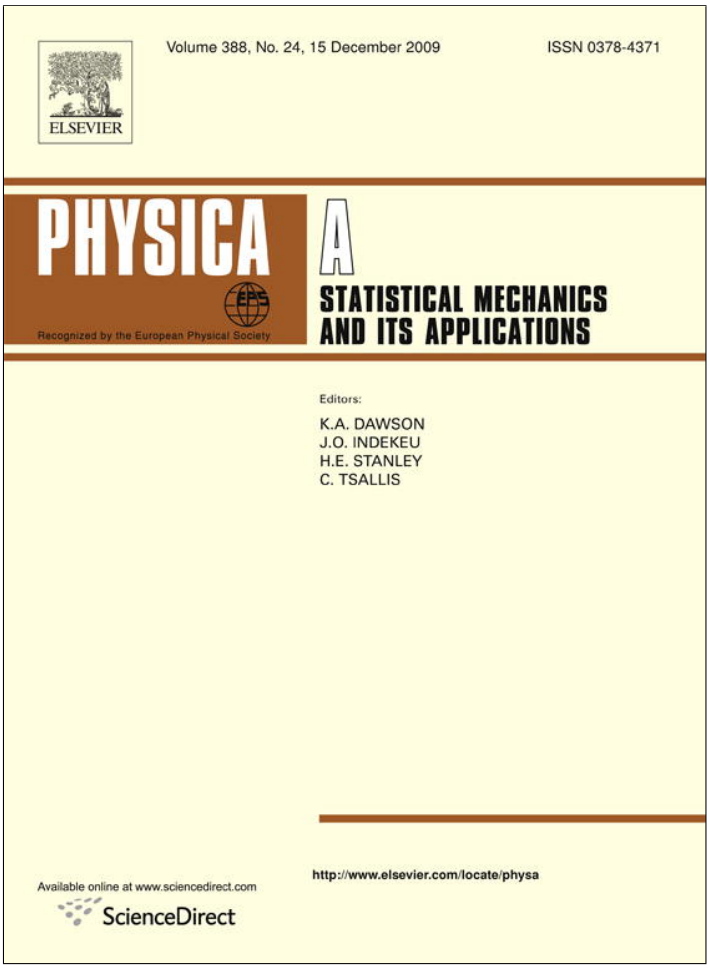

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Generalized analytical expressions for the burning velocity in a combustion model with non-constant transport coefficients and several specific heats

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ABSTRACT

We derive new expressions to estimate the burning velocity of a laminar gas flame in a simplified combustion model based on a one-step single reaction with transport coefficients (mass and heat) depending on temperature, and species with different specific heats. These new expressions generalize the bounds and approximations previously derived by Williams, von Karman, Zeldovich and Frank–Kamenetskii, Benguria and Depassier, and the matching asymptotic expansion method in a two zone model. The comparison of the flame speed predicted by these new analytical expressions with that numerically simulated by the full combustion model for a large variety of cases allows us to determine their range of validity. The upper bound based on the Benguria and Depassier method provides very good approximations for the actual propagation speed of combustion flames, being substantially better than the asymptotic method used in the recent papers.

1. Introduction

In laminar flame theory, the combustion of premixed gases with no energy losses develops a flame front that propagates at a constant speed [1,2]. Classical analyses carried out by several investigators (e.g., Refs. [3–5]) have provided well-known analytical expressions for predicting this laminar burning velocity on simplified combustion models. Although currently thought of having limited interest, some of these methods are still in use when investigating the essence of realistic combustion processes. A very recent example may be the analysis of the propagation of laminar premixed flames with a reversible reaction term [6]. Analytical approaches are also useful, as a first step, to test numerical codes before introducing more complicated effects (e.g., heat losses) that make analytical estimations of the flame speed impossible.

Most well-known analytical expressions usually adopt a simplified one-dimensional (1D) model of a unimolecular binary mixture with a single-step reaction, with background flow at rest and with constant transport coefficients and specific heats. Some attempts to generalize these expressions to more realistic conditions have been carried out, although focusing in one particular methodology applied to solve a specific combustion problem (see, e.g., Refs. [7–10]). In contrast, the purpose of the present paper is to discuss the validity of a wide range of methodologies for estimating the burning velocity in a 1D combustion model that takes account of (1) the temperature dependence of mass and heat diffusivities and (2) the differences of specific heats between reactants and products. In addition, our model takes into consideration the very realistic case of including a non-zero flow velocity across the flame front due to density variations (see, e.g., Ref. [11]). Note that this effect has not been included in the recent studies focused on derived analytical expressions for the wavefront speed of combustion flames [1,2,5,8,9].

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For doing so, we have generalized the expressions of (1) the burning-rate eigenvalue method [4], (2) the von Kármán [4] and (3) the Zeldovich and Frank–Kamenetskii [3] approximations, (4) the matching asymptotic expansion method based on a two zone model [12], (5) the Kolmogorov–Petrovski–Piskunov approximation [13], and the rigorous (6) lower and (7) upper bounds based on the variational principle developed by Benguria and Depassier [5,14,15]. We believe that this is the first comparison of all of those methods that takes into consideration the temperature dependence of transport coefficients and gases with different specific heats. Estimates for the burning velocity are compared with the value obtained by simulating the full combustion model, here numerically solved using a finite difference method with a Crank–Nicholson scheme [16]. We have found that the new analytical expression for the upper bound provides the best approximation to the flame speed, being substantially better than the matching asymptotic expansion method recently adopted in different studies (see Refs. [7,6,17]).

The structure of the paper is as follows. We first formulate the combustion model in Section 2, where it is integrated numerically. Section 3 focuses on the new analytical expressions for estimating the burning velocity. Their detailed derivations are given in Appendix A–E. Section 4 makes a comparison between the flame speed obtained from numerical simulations (Section 2) and that deduced from the wide variety of analytical methods here analyzed (Section 3). Finally, the main conclusions extracted from the present paper are found in Section 5.

2. Combustion model

2.1. 1D model of a premixed flame

We analyze a 1D system consisting of an ideal gas that contains a binary mixture in which the unimolecular reaction $R \rightarrow P$ takes place, where R stands for reactants and P for products. This process occurs at constant pressure and, as explained in Section 1, no energy losses are assumed. Further assumptions are null mean mass velocity (i.e., background flow at rest) except in the flame front where density variations lead to non-zero values for the flow velocity, system in local thermodynamic equilibrium and negligible external forces. The model equations for this reacting ideal-gas mixture reduce to the following three conservation equations [4,18].

The conservation of total mass, reads

$$\frac{\partial \rho}{\partial t} + \frac{\partial (\rho v)}{\partial z} = 0, \tag{1}$$

where ρ is the total density, v is the flow velocity, z the spatial coordinate and t the time.

The conservation of species $i = R$ (fuel), P (products), with Y_i the mass fraction of species i ($Y_P + Y_R = 1$)

$$\rho \frac{\partial Y_i}{\partial t} + \rho v \frac{\partial Y_i}{\partial z} + \frac{\partial j_i}{\partial z} = w_i, \tag{2}$$

where j_i and w_i are the mass diffusion flux and the reaction rate of species i, respectively. In this binary mixture, $j_R + j_P = 0$ and $w_R + w_P = 0$ (see, e.g., Ref. [18]).

Finally, the conservation equation for the enthalpy h of the mixture reads

$$\rho \sum_i Y_i \frac{\partial h_i}{\partial t} + \rho v \sum_i Y_i \frac{\partial h_i}{\partial z} + \sum_i h_i w_i + \sum_i j_i \frac{\partial h_i}{\partial z} + \frac{\partial j_q}{\partial z} = 0, \tag{3}$$

where j_q is the heat flux and $h_i = h_{i0} + c_{p,i}(T - T_0)$ correspond to the enthalpy of species i ($h = Y_P h_P + Y_R h_R$), with T the absolute temperature, h_{i0} the enthalpy at the room absolute temperature T_0 and $c_{p,i}$ the specific heat of species i (assumed constant).

Heat j_q and mass j_i fluxes follow from Fourier's and Fick's law, neglecting both Soret and Duffour effects [18,19],

$$j_q = -\lambda \frac{\partial T}{\partial z}, \qquad j_i = -\rho D_M \frac{\partial Y_i}{\partial z} \tag{4}$$

where λ is the heat conductivity and D_M is the mass diffusion coefficient, which, in a binary mixture, is the same for both species because $Y_P = 1 - Y_R$ and $j_P = -j_R$ [18]. Following Ref. [3], we assume a power law dependence of both heat and mass transport coefficients on temperature as follows,

$$\frac{\lambda}{c_p \rho} = D_H = D_{H0} \left(\frac{T}{T_0}\right)^n; \qquad D_M = D_{M0} \left(\frac{T}{T_0}\right)^n \tag{5}$$

where D_H is the heat diffusivity and c_p is the specific heat of the mixture ($c_p = Y_P c_{p,P} + Y_R c_{p,R}$). D_{H0} and D_{M0} are the heat and mass diffusivities at the room temperature T_0. Note that, following Ref. [3], D_H and D_M have the same temperature dependence, so the ratio D_M/D_H becomes constant, being defined as the Lewis number Le. Classical reviews on combustion theory for premixed laminar flames usually adopt $Le = 1$ and values of the power law exponent n in Eq. (5) ranging from $n = 1$ to 2 [3,4].

Finally, the reaction rate in Eq. (2) is determined by [1]

$$w_P = A\rho (1 - Y_P) \left(e^{-\frac{E_a}{RT}} - e^{-\frac{E_a}{RT_0}} \right) \tag{6}$$

where A is the pre-exponential factor, E_a is the activation energy per mole and R is the universal gas constant. Note that Eq. (6) is an Arrhenius type reaction rate with the $e^{-\frac{E_a}{RT_0}}$ term added on the r.h.s. This extra term has been very recently used in the study of premixed flames [1,8,9], since it leads to equilibrium states if both $T = T_0$ and $Y_P = 0$ everywhere (i.e., at the initial state; this condition is very reasonable and is, in fact, required when we apply the variational method in Section 3). This last term in Eq. (6) is sometimes referred to as a cold-boundary term. We would like to stress that we have performed several tests by numerically solving the above combustion model without using the $e^{-\frac{E_a}{RT_0}}$ term and the results for the flame speed match those obtained with the $e^{-\frac{E_a}{RT_0}}$ term. This is because $e^{-\frac{E_a}{RT_0}} \ll e^{-\frac{E_a}{RT}}$ at high temperatures.

For convenience, we shall work in terms of dimensionless variables related to temperature T, mass fraction of products Y_P, flow velocity v, spatial coordinate z and time t. Thus, we define the dimensionless temperature $\theta = (T - T_0)/(T_\infty - T_0)$, where T_∞ is the maximum temperature achieved in the flame front, and the dimensionless mass fraction of products $Y = (Y_P - Y_{P0})/(Y_{P\infty} - Y_{P0})$, where $Y_{P\infty}$ (=1) and Y_{P0} (=0) correspond to the maximum and to the initial mass fraction of products respectively. Dimensionless time $t' = t\alpha^2 A/\beta$ and space $z' = z\sqrt{\alpha^2 A/(\beta D_{H0})}$ make use of the dimensionless heat-release coefficient $\alpha = (T_\infty - T_0)/T_\infty$ and the Zeldovich number $\beta = \alpha E_a/(RT_\infty)$ and allow us to define the dimensionless flow velocity $v' = v\sqrt{\beta/(\alpha^2 A D_{H0})}$.

By using these dimensionless variables and parameters, and with the ideal-gas law for determining the temperature dependence of ρ on temperature T assuming a process at constant pressure, Eq. (1) reads

$$\frac{\partial(1/\theta)}{\partial t'} + \frac{\partial\left(v'/\theta\right)}{\partial z'} = 0, \tag{7}$$

Eq. (2) for $i = P$ is

$$\frac{\partial Y}{\partial t'} + v'\frac{\partial Y}{\partial z'} = \frac{\varphi}{Le}\frac{\partial}{\partial z'}\left[\varphi^{n-1}\frac{\partial Y}{\partial z'}\right] + F, \tag{8}$$

and Eq. (3) leads to

$$\frac{\partial \theta}{\partial t'} + v'\frac{\partial \theta}{\partial z'} = \varphi\frac{\partial}{\partial z'}\left[\varphi^{n-1}\frac{\partial \theta}{\partial z'}\right] - \frac{\Delta c_p}{c_p}\frac{\varphi^n}{Le}\frac{\partial \theta}{\partial z'}\frac{\partial Y}{\partial z'} + f, \tag{9}$$

where $\Delta c_p = c_{p,R} - c_{p,P}$ and the functions φ, f and F are

$$\varphi = \left(1 + \tfrac{\alpha}{1-\alpha}\theta\right), \tag{10}$$

$$F = \tfrac{\beta}{\alpha^2}(1 - Y)\left[e^{-\frac{\beta}{\alpha(\alpha\theta+1-\alpha)}} - e^{-\frac{\beta}{\alpha(1-\alpha)}}\right], \tag{11}$$

$$f = \left(1 + \tfrac{\Delta c_p}{c_p}\theta\right)F. \tag{12}$$

The set of three PDEs with three variables (θ, Y and v') defined by Eqs. (7)–(9) becomes our full combustion model. For $\Delta c_p = 0$ and $Le = 1$, Eqs. (8) and (9) reduce to a single one for $\theta = Y$. This simplified combustion model involves only two variables ($\theta = Y$ and v') and two equations (7), (8)–(9). Indeed, the assumption $\theta = Y$, which is based on the Zeldovich energy conservation equation, has been usually applied by other authors in the study of the flame front speed in simple 1D combustion models (see, e.g., Refs. [1,8,9]). The full combustion model, however, is here used for a better comparison between numerical simulations and generalized analytical expressions since values of $\Delta c_p \neq 0$ and $Le \neq 1$ may be used and, then, the assumption $\theta = Y$ breaks down. Nevertheless, at the end of Section 4 we investigate the differences in the burning velocities obtained between the full and the simplified model when the latter one is extended to analyze cases with $\Delta c_p \neq 0$.

2.2. Numerical simulations

Eq. (8)–(9) are numerically integrated by using the finite difference method where the value for the dimensionless flow velocity v' is obtained by solving Eq. (7). In order to provide both robustness and accuracy, the Crank–Nicholson scheme has been implemented [16]. We have performed several simulations by varying the values of the Zeldovich number β (equivalent to varying the activation energy E_a), the power law coefficient n and the difference between specific heats of reactants and products Δc_p. A constant value of the dimensionless parameter α (=0.85) has been chosen, corresponding to a room temperature $T_0 = 300$ K and to a flame temperature $T_\infty = 2000$ K. For simplicity, a constant value for the specific heat c_p (=1 kJ K^{-1} kg^{-1}) has been assumed in the numerical integrations that involve cases with $\Delta c_p \neq 0$. We point out that the maximum value of Δc_p used corresponds to $\Delta c_p = 0.5$ kJ K^{-1} kg^{-1}, which sets a realistic range for methane–air mixtures.

The numerical integration uses an initial step-like profile, with both $\theta = 1$ and $Y = 1$ at $t' = 0$ within a region around $z' = 0$ (ignition zone), and zero elsewhere. For $t' > 0$, Eq. (7)–(9) may develop a front that propagates at a constant speed. As an example of this type of solution, Fig. 1 shows the leftwards propagation of both Y and θ profiles at $t' = 0$, 100, 200, 300 and

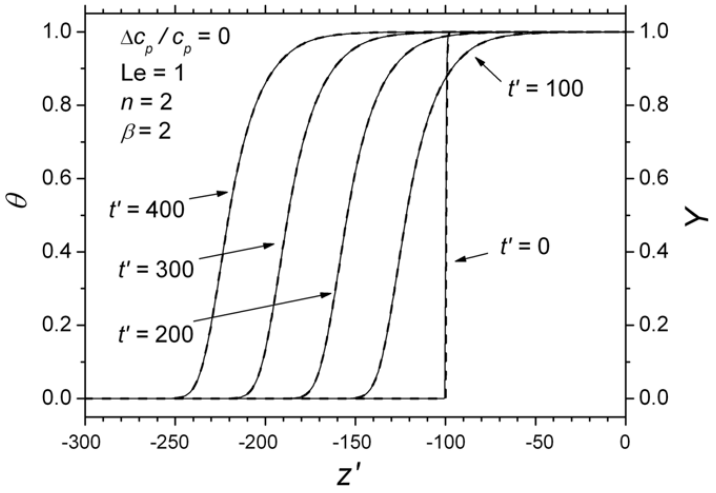

Fig. 1. Profiles of the dimensionless temperature θ (solid lines) and dimensionless mass fraction of products Y (dashed lines) obtained at five different dimensionless time t' by numerically solving Eqs. (7)–(9) for $Le = 1$, $\Delta c_p/c_p = 0$, $n = 2$, $\beta = 2$. Note the initial step-like condition at $t' = 0$ and that both profiles almost perfectly match.

400 for a combustion model with $Le = 1$, $\Delta c_p/c_p = 0$, $n = 2$ and $\beta = 2$. Note that, from Eq. (5), the condition $n = 2$ is equivalent to a linear dependence of the heat conductivity λ on temperature T (as in Ref. [4]). In addition the condition $\beta = 2$, with the values of T_0 and T_∞ assumed above, corresponds to a value for the activation energy $E_a \approx 30$ kJ/mol, which is reasonable for these types of problems [18]. Nevertheless, the sensitivity of the methods here employed to changes in the activation energy, and hence, in β is investigated in Sec. III. Profiles of dimensionless temperature θ match almost perfectly those for Y shown in Fig. 1. The dimensionless burning velocity c' corresponds to the propagation speed of the front shown in Fig. 1. This value is obtained by a linear fit of the distance corresponding to the front position with $Y = 0.5$ with respect of time.

3. Methods to estimate the burning velocity

Here we give generalized expressions for estimating the dimensionless flame speed c'. We have obtained them by extending several approaches by including the power law dependence of transport coefficients on temperature, as well as the possibility of species with different specific heats. The mathematical derivations of these new expressions are detailed in the corresponding appendices.

3.1. Williams approximation

Several approximations to the burning velocity make use of a parameter called the burning-rate eigenvalue Λ deduced from both the energy conservation equation and the conservation equations of species (see Appendix A). In one of these approximations, Williams [4] works in the phase space for the $\Delta c_p = 0$, $Le = 1$ and constant transport coefficients case, finally deriving both upper and lower bounds for the burning-rate eigenvalue and, hence, for the front flame speed. We have extended this method for the more general case $n \neq 0$ and $\Delta c_p \neq 0$ from which the dimensionless burning velocity c'_W reads (see Appendix A)

$$c'_W = \sqrt{\frac{\int_0^1 \mathrm{d}\theta \frac{F\varphi^{n-2}}{\theta}\left(1+\frac{\Delta c_p}{c_p}\theta\right)}{\left[1+\frac{1}{2}\frac{\Delta c_p}{c_p}\left(1+\frac{1}{Le}\right)\right]}}, \tag{13}$$

where φ and F are given by Eqs. (10) and (11), respectively.

The numerator in Eq. (13) can be easily obtained through numerical integration. Note that, as discussed in the Appendix A, Eq. (13) shall be viewed as an approximation to c' but not as a bound.

3.2. von Kármán approximation

The burning-rate eigenvalue Λ is also evaluated by von Kármán by assuming a given dependence of θ on Y in the vicinity of the hot boundary (i.e., the zone with no reactants) [4]. The dimensionless burning velocity c'_K, extended to include $n \neq 0$ and $\Delta c_p \neq 0$ becomes (see Appendix B)

$$c'_K = \sqrt{2\left(1+\frac{\Delta c_p}{c_p}\right)^{-1}\int_0^1 \mathrm{d}\theta F\varphi^{n-2}}, \tag{14}$$

where φ and F are again given by Eqs. (10) and (11), respectively.

3.3. Asymptotic analysis with a two zone model

In this method, the flame structure is divided into two zones [4,7,12]. In the convective–diffusive zone, the reaction rate is negligible, whereas in the thinner reactive–diffusive zone, which is very close to the hot boundary, both reaction and diffusion are the main processes (see Appendix C). In both zones, the variables are expanded in power-series of the Zeldovich number β and, then, substituted into the governing equations. Matching conditions between both zones allow us to determine the burning-rate eigenvalue Λ at different orders of β (see Appendix C). At first order on β, we have

$$c'_{TZ1} = \sqrt{\frac{2Le}{\beta\alpha^2\,(1-\alpha)^{n-2}}}\,\frac{\mathrm{e}^{-\frac{\beta}{2\alpha}}}{\left(1+\frac{\Delta c_p}{c_p}\right)}, \tag{15}$$

whereas at second order

$$c'_{TZ2} = c'_{TZ1}\left(1-\frac{1}{2}\frac{\Lambda_1}{\Lambda_0}\frac{1}{\beta}\right), \tag{16}$$

where

$$\frac{\Lambda_1}{\Lambda_0} = 6\alpha - 4.688 + Le\frac{2-2.688\frac{\Delta c_p}{c_p}}{\left(1+\frac{\Delta c_p}{c_p}\right)^2} + \frac{1.688\frac{\Delta c_p}{c_p}}{\left(1+\frac{\Delta c_p}{c_p}\right)} + 2\alpha\,(n-2)\,. \tag{17}$$

Note that this method is valid only for large values of β. However, as pointed out by Williams [4], Ref. [12] obtains very reasonable results for $\beta \geq 2$ in a model with constant transport coefficients and equal specific heats. In Section 4, c'_{TZ1} and c'_{TZ2} values for low β (<2) are shown for illustrative purposes only. Note that Ref. [10] provides an expression of the burning-rate eigenvalue assuming a temperature dependence of heat conductivity but for the very particular case of no mass diffusion (i.e. $Le \to \infty$) and constant specific heats.

3.4. Zeldovich and Frank–Kamenetskii approximation

Focused on the reaction zone, Zeldovich and Frank–Kamenetskii [20] derived an expression for the burning velocity which can be easily extended for our $n \neq 0$ and $\Delta c_p \neq 0$ combustion model (see Appendix D). The dimensionless burning velocity now reads

$$c'_{ZFK} = \sqrt{2\int_0^1 \mathrm{d}\theta\left(1+\frac{\Delta c_p}{c_p}\theta\right)F\varphi^{n-2}}, \tag{18}$$

where φ and F are again given by Eqs. (10) and (11), respectively.

3.5. Kolmogorov–Petrovski–Piskunov approximation

This method consists of working in a reference frame attached to the flame front (i.e., introducing the variable $s' = z' + c't'$ in Eq. (9)), and requiring a solution that dies out exponentially $s' \to \infty$. The linearization of Eq. (9), here not shown, gives the very same expression as in Ref. [1]

$$c'_{KPP} = 2\sqrt{\left(\frac{\mathrm{d}F}{\mathrm{d}\theta}\right)_{\theta=0}}, \tag{19}$$

where F is again given by Eq. (11).

3.6. Upper and lower bounds

Lower and upper bounds may be deduced by extending the variational method developed by Benguria and Depassier in the analysis of 1D convective–diffusive–reactive equations of a single variable [5,14,15]. The solution for the upper bound reads (see Appendix E)

$$c'_{UB} = \sup\left[\frac{f\varphi^{n-2}}{\mu\theta} + \mu\left(1-\frac{\Delta c_p}{c_p}\frac{\theta}{Le}\right)\right], \tag{20}$$

with μ an arbitrary positive function and f given by Eq. (12). Here we choose μ as

$$\mu = \sup\sqrt{\frac{f\varphi^{n-2}}{\theta}}, \tag{21}$$

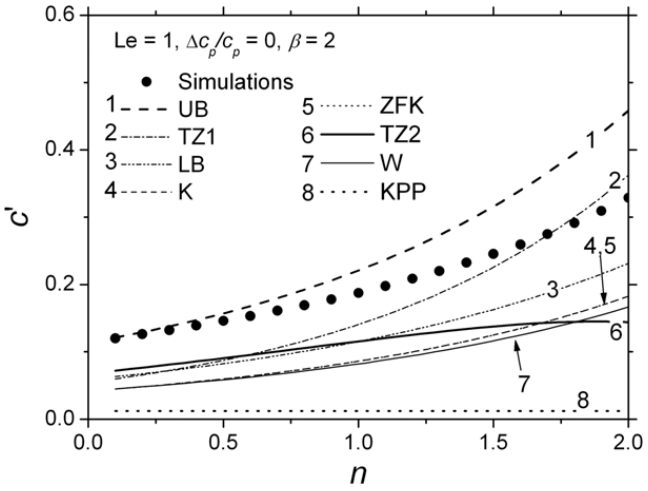

Fig. 2. Dimensionless burning velocity c' as a function of n (the exponent in the power law dependence for both mass and heat diffusivities on temperature) obtained by simulations (dots) and by the analytical expressions here generalized. W = Williams method, K = von Kármán approximation, KPP = Kolmogorov–Petrovski–Piskunov method, ZFK = Zeldovich and Frank–Kamenetskii method, TZ1 and TZ2 = first and second order expressions of the matching asymptotic expansion method, UB and LB = upper and lower bounds based on the Benguria and Depassier variational principle. Values of the parameters are $Le = 1$, $\Delta c_p/c_p = 0$, $\beta = 2$.

that substituted into Eq. (20) for the $n = 2$ (linear dependence of heat conductivity on temperature) and $\Delta c_p = 0$ case reverts to the classical upper bound derived by Aronson and Weinberger [21],

$$c'_{AW} = 2 \sup \sqrt{\frac{F}{\theta}}. \tag{22}$$

Note that instead of working with a reaction–diffusion equation, we analyze a more realistic convection–reaction–diffusion equation where density variations arising in the flame front lead to non-zero flow velocities. This implies that Eq. (20)–(21) for the $n = 0$ and $\Delta c_p = 0$ case do not revert to the Aronson and Weinberger classical result.

On the other hand, the variational principle gives us the following lower bound (see, again, Appendix E)

$$c'_{LB} = 2 \frac{\int_0^1 \mathrm{d}\theta \sqrt{g f \varphi^{n-2} \left(-\frac{\Delta c_p}{c_p} \frac{1}{Le} g - \frac{\mathrm{d}g}{\mathrm{d}\theta} \right)}}{\int_0^1 \mathrm{d}\theta g}, \tag{23}$$

where

$$g = \sqrt{1-\theta}. \tag{24}$$

4. Results

Dimensionless burning velocities predicted by the expressions shown in the preceding section are here compared with the results obtained by numerically integrating the full model Eqs. (7)–(9). We have performed several analyses by (1) varying the n-exponent for the temperature dependence of both mass and heat diffusivities, see Eq. (5), (2) using different specific heats for products and reactants, and (3) varying the value of the Zeldovich number β. All cases take $Le = 1$ into consideration since it is very reasonable in premixed laminar flames (see, e.g., Ref. [4]).

Values of the dimensionless flame speed c' as a function of n are shown in Fig. 2 for the $\beta = 2$, $Le = 1$ and $\Delta c_p/c_p = 0$ case. For the particular case of $n = 2$ (i.e., a linear dependence of heat conductivity on temperature), Fig. 1 shows the first steps on the propagation of the simulated combustion front. Note that the simulated flame front speed increases as n increases due to the enhancement of the heat flux that warms up the reactant zone and, hence, the amount of heat produced by the combustion reaction. In Fig. 2, the expression for the dimensionless front speed c'_K gives the same result than c'_{ZFK} since $\Delta c_p/c_p = 0$ in Eqs. (14) and (18). The upper bound c'_{UB} provides very reasonable estimates for the flame speed for all ranges of n analyzed. The rigorous lower bound c'_{LB} here found also appears as a reasonable approximation.This is not the case for the c'_K, c'_{ZFK} and c'_W approximations since they reach substantially smaller values than the simulated one for large n.

The method of matching asymptotic expansion applied to the two zone model at first order on the burning-rate eigenvalue ($TZ1$ in Fig. 2) overestimates the simulated flame speed at large values of n and underestimates it at low values of n. The solution at second order ($TZ2$) gives a better result (although being worst than the upper bound) at low values of n, whereas it clearly breaks down as n increases. This indicates that the asymptotic expansion method is reasonably accurate when neglecting the temperature dependence of both mass and heat transport coefficients but it fails when this effect is taken into account. Note also that, in this case, extrapolating the $n = 0$ results $TZ1$ and $TZ2$ for estimating $n \neq 0$ cases may

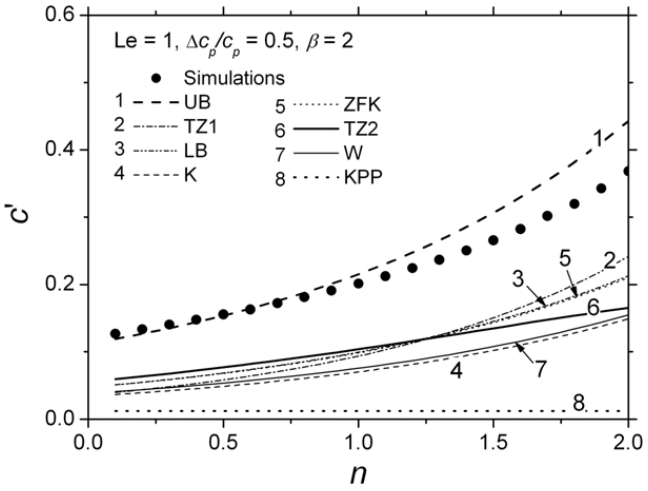

Fig. 3. As in Fig. 2 but for $\Delta c_p/c_p = 0.5$. W = Williams method, K = von Kármán approximation, KPP = Kolmogorov–Petrovski–Piskunov method, ZFK = Zeldovich and Frank–Kamenetskii method, TZ1 and TZ2 = first and second order expressions of the matching asymptotic expansion method, UB and LB = upper and lower bounds based on the Benguria and Depassier variational principle.

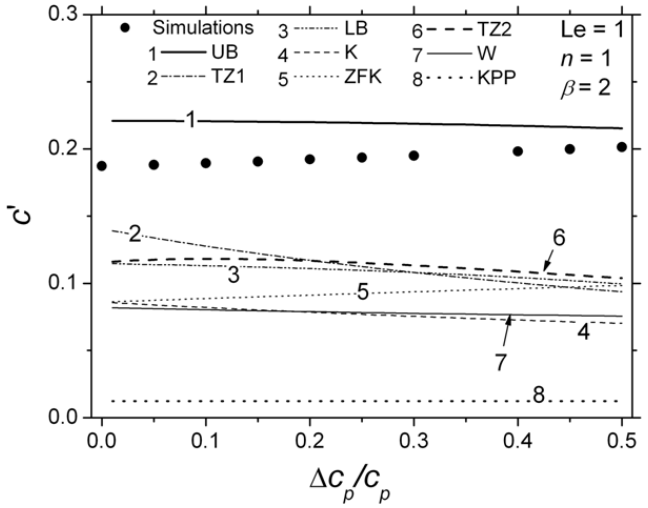

Fig. 4. Dimensionless burning velocity c' as a function of $\Delta c_p/c_p$ for the $Le = 1$, $n = 1$ and $\beta = 2$ case. W = Williams method, K = von Kármán approximation, KPP = Kolmogorov–Petrovski–Piskunov method, ZFK = Zeldovich and Frank–Kamenetskii method, TZ1 and TZ2 = first and second order expressions of the matching asymptotic expansion method, UB and LB = upper and lower bounds based on the Benguria and Depassier variational principle.

lead to significant errors, with other expressions having a higher accuracy on estimating the flame speed (e.g., the upper bound UB in Fig. 2).

Note in Fig. 2 that the burning velocity predicted from the KPP method is two orders of magnitude smaller than the simulated speed ($c'_{KPP} = 0.012$ and independent of n).

If the reactant has a higher specific heat than the product, this enhances the burning velocity as shown in Fig. 3, where dots correspond to simulated values for the $Le = 1$, $\beta = 2$ case, as in Fig. 2, but now $\Delta c_p/c_p = 0.5$ (similar to methane–air reactions). Note that c'_{UB} is also a very good estimate for the flame speed although now it is not a rigorous bound since the assumption $Y \approx \theta$ may not be completely fulfilled for the $\Delta c_p/c_p \neq 0$ case. The lower bound c'_{LB} gives a better estimate than c'_K, c'_W and, especially, c'_{KPP}. Indeed, c'_{LB}, c'_{ZFK} and c'_{TZ1} provide very similar values. In comparison with Fig. 2, the expression c'_{TZ2} derived from the matching asymptotic expansion method in the two zone model provides a better agreement with respect to the simulated burning speeds, although its accuracy is still poor as n increases.

In Fig. 4 we show the behavior of the front speed for the $Le = 1$, $\beta = 2$ and $n = 1$ case as a function of the value of $\Delta c_p/c_p$. Values for $\Delta c_p/c_p = 0$ and $\Delta c_p/c_p = 0.5$ correspond to those at $n = 1$ in Figs. 2 and 3 respectively. Fig. 4 clearly shows that the accuracy of the upper bound c'_{UB} is more satisfactory than the other methods, which gives us confidence of its use in the analysis of front speeds in convection–reaction–diffusion systems [8,9]. However, c'_{UB} velocities decrease as $\Delta c_p/c_p$ increases, which conflicts with the behavior expected intuitively.

In Fig. 4, expressions from the matching asymptotic method c'_{TZ1} and c'_{TZ2} give similar results than the lower bound c'_{LB} and the c'_{ZFK} approximation. In addition to the c'_{KPP} approach, the worst estimates correspond to the c'_W and c'_K cases.

The influence of the Zeldovich number β on the dimensionless burning velocity c' is shown in Fig. 5, where dots correspond to simulated values for the $Le = 1$, $\Delta c_p/c_p = 0.5$, and $n = 1$ case. As β increases, the heat released by the

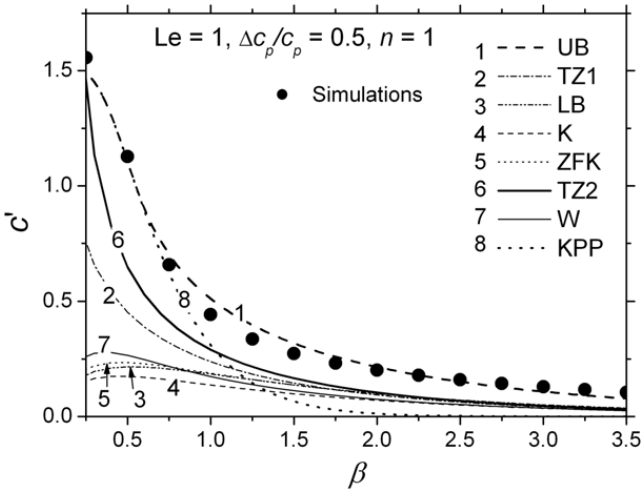

Fig. 5. Dimensionless burning velocity c' as a function of Zeldovich number β for the $Le = 1$, $n = 1$ and $\Delta c_p/c_p = 0.5$ case. W = Williams method, K = von Kármán approximation, KPP = Kolmogorov–Petrovski–Piskunov method, ZFK = Zeldovich and Frank–Kamenetskii method, TZ1 and TZ2 = first and second order expressions of the matching asymptotic expansion method, UB and LB = upper and lower bounds based on the Benguria and Depassier variational principle.

reaction term decreases and, hence, the flame velocity slows down. As expected from the methodology employed in the asymptotic analysis (see Appendix C), the c'_{TZ1} and, especially, the c'_{TZ2} expressions increase their accuracy as β increases. However, the c'_{UB} value for all β becomes a very remarkable approximation to the burning velocity. As explained above, the assumptions applied for the analytical derivation of c'_{UB} may fail at very large values of $\Delta c_p/c_p$. This is the reason why c'_{UB} is not a rigorous upper bound in Fig. 5. Indeed, analyses with different values of the Zeldovich number β for the $\Delta c_p/c_p = 0$ case do show that c'_{UB} is a rigorous upper bound in that case.

In Fig. 5, we may observe that the first order c'_{TZ1} expression is not as accurate than the second order c'_{TZ2} at $n = 1$. At very large values of β, all expressions except c'_{UB} tend to predict the same value that underestimates the simulated result. For low values of β, we have found that c'_W, c'_K, c'_{ZFK} and, even, c'_{LB} fail in comparison with simulated data.

Note in Fig. 5, that the KPP expression gives the right order of magnitude for the simulated velocity at very low values of β, since the reaction term becomes increasingly important in comparison with the diffusive term as $\beta \to 0$ and the non-linearity in the governing equations tends to disappear.

Simulations with several values of the Lewis number Le have been also performed, but they are not shown here for brevity since changes in the front speed are much smaller than those provided by n (Figs. 2 and 3) and β (Fig. 5), and the approximate analytical solutions behave similarly to Fig. 4 (with Le^{-1} instead of $\Delta c_p/c_p$).

In front propagation research, the recent works study the flame speed c' as a function of the velocity v' of the steady flow. Thus, for example, Cencini et al. [22] obtain an asymptotic behavior of $c' \sim v'/\ln v'$ in a steady cellular flow, whereas Yakhot [23] and Sivashinsky [24] propose $c' = \exp\left[d\left(v'_{rms}/c'\right)^a\right]$ in turbulent flows with $a = 2$, $d = 1$ and v'_{rms} the dimensionless root mean square field velocity. In our case, the background flow is at rest and v' arises in the flame front only, where density variations occur. Nevertheless, it is interesting to analyze the behavior of the burning velocity c' as a function of the mean-averaged value of the dimensionless flow speed in the flame front $\langle v' \rangle$. This is shown in Fig. 6 for the case analyzed in Fig. 3. Also in Fig. 6, we show the results obtained by using the simplified model (open circles).

Since here we work within the laminar regime with low flow velocities, c' does not follow the asymptotic behavior $v'/\ln v'$. Also for the full model, c' does not agree with the expression $\exp\left[\left(v'_{rms}/c'\right)^a\right]$ neither for $a = 1$ as in Ref. [22] nor for $a = 2$ as in Refs. [23,24] when substituting $v'_{rms} = \langle v' \rangle$. This is not surprising since, as we have already pointed out, we are analyzing a laminar flame with background flow at rest (v' is different than zero in the flame front only).

For the simplified model, however, a correlation coefficient equal to 0.95 is obtained for a linear regression of c' as a function of $\exp\left[v'_{rms}/c'\right]$ (as proposed in Cencini et al. [22] for steady cellular flow). Note that the simple model matches the full one for $Le = 1$ and $\Delta c_p/c_p = 0$ as it is assumed in many combustion processes. The generalization to $Le \neq 1$ and $\Delta c_p/c_p \neq 0$ leads to a break down of the $\theta = Y$ condition. In this case, the use of a single reaction–advection–diffusion equation with a single variable predicts lower values of the burning velocity. For the $n = 0.1$, $Le = 1$, $\Delta c_p/c_p = 0.5$, $\beta = 2$ case (lower-left points in Fig. 6), the simple model gives a value of the flame front speed ≈5% lower than that of the full model. For $n = 2.0$ differences reach 12%. For data shown in Fig. 5, the $n = 1$, $Le = 1$, $\Delta c_p/c_p = 0.5$ and $\beta = 3.5$ case gives a 12% burning velocity difference between the simple (lower value) and the full combustion model. This difference reduces as the β value diminishes.

5. Conclusions

The aim of the present paper is to provide a detailed comparison between the most common methods currently used for estimating the values of the dimensionless burning velocity c' in laminar flame theory. Our main novelties consist of

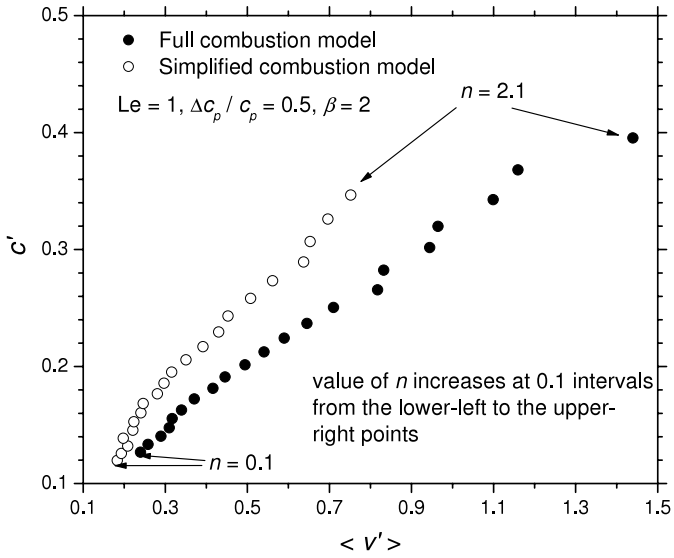

Fig. 6. Dimensionless burning velocity c' as a function of the mean-averaged value of the dimensionless flow velocity $\langle v' \rangle$ arisen in the flame front due to density variations for data shown in Fig. 3. Closed circles correspond to simulations from the full combustion model (as in Figs. 1–5). Open circles use a simplified version of the full combustion model (see text).

taking into consideration a combustion model with both mass and heat transport coefficients dependent on temperature and, in addition, with species with different specific heats. Therefore, we have developed a complete set of new analytical expressions for estimating c' which take into account the above two assumptions.

In essence, the combustion model consists of two components (reactant or fuel and product) with a single-step chemical reaction. Heat and mass diffusivities follow a power law on temperature, and reactants and products differ in their specific heats. We allow for flow velocity changes across the flame due to density variations, with background flow at rest in those zones with homogeneous density. For realistic not very large values of the Zeldovich number β, the numerical integration of this model leads to front propagation, from which the value of c' is obtained. Simulations have been carried out by using a finite difference method with a Crank–Nicholson scheme.

Analytical expressions for c' have been here derived following (1) the Williams burning-rate eigenvalue approximation, (2) the von Kármán approach, (3) the Zeldovich and Frank–Kamenetskii method, (4) the Kolmogorov–Petrovski–Piskunov method, (5) the matching asymptotic expansion method in a two zone model, and the variational principle developed by Benguria and Depassier in order to derive (6) upper and (7) lower bounds. These new expressions account for mass and heat diffusivities as a function of temperature, Lewis number different than unity and reactants and products with different specific heats.

Very recently, upper and lower bounds based on the Benguria and Depassier method have been used in the analysis of the front speed in a simplified combustion model with constant transport coefficients and without taking into consideration changes in flow velocities due to density variations across de flame [8,9]. Our results reveal that among the multiple analytical expressions that may be used for estimating the burning velocity c', the upper bound based on the Benguria and Depassier variational principle gives us the better agreement in comparison with simulated values. In contrast, the asymptotic expansion method, which has been widely used in the recent studies (see Refs. [7,6,17]), provides poorer estimates. Indeed, at large values of n, and even for high values of β, the asymptotic expansion method clearly fails and the upper bound method provides better results. However, in comparison with other analytical expressions that require a numerical integration of the reaction term (i.e., c'_W, c'_K and c'_{ZFK}), the asymptotic expansion method often provides a better estimate, which is very remarkable.

Although the upper bound c'_{UB} here found is rigorous for the $\Delta c_p = 0$ case, it gives us an excellent approach for a combustion process with different specific heats for reactants and products (i.e. $\Delta c_p \neq 0$ case, see Fig. 5). The rigorous lower bound here found also provides good estimates for the front speed for high values of β.

Although the results here found are very encouraging since they generalize former expressions deduced in Refs. [3–5, 8], and shed light into the behavior of widely used methods, additional studies should be made in order to corroborate the accuracy of these expressions, especially those involving experimental data. Of particular interest would be to derive some useful approximations when energy losses (radiation as well as conduction) are included in the combustion process so, then, pulses rather than fronts propagate.

Acknowledgments

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Appendix A

In a moving reference frame attached to the front, where $s = z + ct$, with c the front speed ($c' = c\sqrt{\alpha^2 A D_{H0}/\beta}$ and c' being the dimensionless front speed), integrating Eqs. (1) and (3) on s leads to

$$m \equiv \rho(c + v) = \text{ constant}, \tag{25}$$

where m is known as the mass burning velocity,

$$\rho(c + v) \sum_i h_i \varepsilon_i - \lambda \frac{\mathrm{d}T}{\mathrm{d}s} = \text{ constant}, \tag{26}$$

where the new variable ε_i is

$$\varepsilon_i = Y_i - \frac{D_M}{(c + v)} \frac{\mathrm{d}Y_i}{\mathrm{d}s}, \quad i = R, P \tag{27}$$

We implicitly assume that the front propagates at $z < 0$, so $Y_P(s = -\infty) \equiv Y_{P0} = 0$, $T(s = -\infty) = T_0$, $\varepsilon_P(s = -\infty) \equiv \varepsilon_{P0}$, and $Y_P(s = \infty) \equiv Y_{P\infty} = 1$, $T(s = \infty) = T_\infty$, $\varepsilon_P(s = \infty) \equiv \varepsilon_{P\infty} = 1$.

From Eqs. (25) and (27), Eq. (2) reads

$$\frac{\mathrm{d}\varepsilon_i}{\mathrm{d}s} = \frac{w_i}{\rho\,(c + v)}\,. \tag{28}$$

In terms of the dimensionless variables $\varepsilon = (\varepsilon_P - \varepsilon_{P0})\,/\,(\varepsilon_{P\infty} - \varepsilon_{P0})$ and $\theta = (T - T_0)\,/\,(T_\infty - T_0)$, Eqs. (26)–(27) are

$$\varphi^{n-1} \frac{\mathrm{d}\theta}{\mathrm{d}\zeta} = \theta - \varepsilon + \frac{\Delta c_p}{c_p} \theta\,(Y - \varepsilon)\,, \tag{29}$$

$$\frac{\varphi^{n-1}}{Le} \frac{\mathrm{d}Y}{\mathrm{d}\zeta} = Y - \varepsilon, \tag{30}$$

where ζ is the new dimensionless coordinate attached to the front defined as $\mathrm{d}\zeta = m\mathrm{d}s/\,(D_{H0}\rho_0)$. We point out that Eq. (29) has been obtained by evaluating the constant term on the r.h.s. in Eq. (26) at $s = -\infty$.

On the other hand, Eq. (28) in terms of these dimensionless variables reads

$$\frac{\mathrm{d}\varepsilon}{\mathrm{d}\zeta} = \frac{\Lambda r}{\varphi}, \tag{31}$$

where

$$r = (1 - Y)\left(\mathrm{e}^{-\beta\left(\frac{1-\theta}{1-\alpha(1-\theta)}\right)} - \mathrm{e}^{-\beta\frac{1}{1-\alpha}}\right), \tag{32}$$

and

$$\Lambda = \frac{\rho_0^2 D_{H0}}{m^2} A \mathrm{e}^{-\frac{\beta}{\alpha}} = \text{constant}, \tag{33}$$

is known as the burning-rate eigenvalue [4]. Since the mass burning velocity m is constant, at the cold boundary where the background flow is still at rest (i.e., $v = 0$) and the density is ρ_0, we obtain $m = \rho_0 c$. Therefore, the speed of the flame front c from Eq. (33) is

$$c = \sqrt{\frac{D_{H0} A}{\Lambda}} \mathrm{e}^{-\frac{\beta}{2\alpha}}. \tag{34}$$

In terms of the dimensionless front velocity c', Eq. (34) gives

$$c' = \sqrt{\frac{\beta}{\alpha^2}} \frac{1}{\sqrt{\Lambda}} \mathrm{e}^{-\frac{\beta}{2\alpha}}. \tag{35}$$

Williams [4] obtains upper and lower bounds for the burning-rate eigenvalue Λ by working in the phase space with Eqs. (30)–(29) constrained to the case $n = 0$, $\Delta c_p = 0$ and $Le = 1$. Under such circumstances, $Y = \theta$ and, therefore, a single equation is needed in order to represent the combustion model.

Here, taking the derivative of Eq. (29) with respect to ζ, with the assumption $Y \approx \theta$ (which is reasonable from the simulations carried out in Section 1; see Fig. 1) and defining $g = \mathrm{d}\theta/\mathrm{d}\zeta$ (>0 since the front propagates leftwards), we obtain

$$\frac{d\left(\varphi^{n-1} g\right)}{\mathrm{d}\theta} = 1 - \frac{\Lambda r}{g\varphi}\left(1 + \frac{\Delta c_p}{c_p}\theta\right) + \frac{\Delta c_p}{c_p} \frac{\varphi^{n-1} g}{Le} + \frac{\Delta c_p}{c_p}\theta, \tag{36}$$

which is an ODE with a single variable θ. Integrating Eq. (36) from $\theta = 0$ to $\theta = 1$, and rearranging terms, gives

$$\Lambda = \frac{\int_0^1 \mathrm{d}\theta \left[1 + \frac{\Delta c_p}{c_p}\frac{\varphi^{n-1}g}{Le} + \frac{\Delta c_p}{c_p}\theta\right]}{\int_0^1 \mathrm{d}\theta \frac{r}{\varphi g}\left(1 + \frac{\Delta c_p}{c_p}\theta\right)}, \tag{37}$$

since $g(0) = g(1) = 0$. For $\Delta c_p = 0$, integrating Eq. (36) from $\theta = 0$ to θ, gives the inequality $\varphi^{n-1}g \leq \theta$ since $\Lambda r/g\varphi$ is positive for all θ. Williams [4] chooses the upper bound for $\varphi^{n-1}g$ $(=\theta)$, from which the eigenvalue becomes a maximum and, hence, the predicted velocity a minimum. Here, we also use the condition $\varphi^{n-1}g = \theta$ in Eq. (37) that substituted into Eq. (35) gives the expression for the dimensionless velocity c'_W shown in Eq. (13) since $F = \frac{\beta}{\alpha^2}\mathrm{e}^{-\frac{\beta}{\alpha}}r$ from Eq. (10). Note that here, c'_W does not correspond to a rigorous bound due to both $Y \approx \theta$ and $\varphi^{n-1}g \approx \theta$ approximations.

Appendix B

An approximate formula for the burning-rate eigenvalue Λ is found by von Kármán by dividing Eq. (29) by Eq. (31), which gives

$$\frac{\mathrm{d}\theta}{\mathrm{d}\varepsilon} = \frac{\theta - \varepsilon + \frac{\Delta c_p}{c_p}\theta\,(Y - \varepsilon)}{\varphi^{n-2}\Lambda r}. \tag{38}$$

As has been done in Appendix A, we assume $Y \approx \theta$, from which the integration of Eq. (38) from 0 to 1 is

$$\int_0^1 \mathrm{d}\theta\varphi^{n-2}\Lambda r = \int_0^1 \mathrm{d}\varepsilon\left[\theta - \varepsilon + \frac{\Delta c_p}{c_p}\theta\,(\theta - \varepsilon)\right]. \tag{39}$$

Following Williams [4], a linear relationship $(1 - \theta) = d(1 - \varepsilon)$ may be assumed with d constant, that substituted into the r.h.s of Eq. (39) gives

$$\Lambda\int_0^1 \mathrm{d}\theta\varphi^{n-2}r = \frac{1-d}{2} + \frac{\Delta c_p}{c_p}\left[\frac{1}{2} - \frac{5d}{6} + \frac{d^2}{3}\right]. \tag{40}$$

The simplest approximation proposed by von Kármán is to use $d = 0$ in Eq. (40) [4], from which the burning-rate eigenvalue reads

$$\Lambda = \frac{\left(1 + \frac{\Delta c_p}{c_p}\right)}{2\int_0^1 \mathrm{d}\theta\varphi^{n-2}r}. \tag{41}$$

Eq. (41) substituted into Eq. (35) gives the dimensionless burning velocity c'_K Eq. (14).

Appendix C

For large values of the Zeldovich number β, an asymptotic analysis applied to a two zone model for the combustion process predicts a burning-rate eigenvalue Λ that may be used for estimating the front speed [4,7,10,12]. In the outer zone, the regime is essentially convective–diffusive since the reaction term is negligible. On the contrary, the inner zone, much thinner than the outer one, is dominated by reaction–diffusion processes. The dependence of ε and Y on θ in this inner zone may be obtained by dividing Eq. (31) by Eq. (29), (i.e., the inverse of Eq. (38))

$$\frac{\mathrm{d}\varepsilon}{\mathrm{d}\theta} = \frac{\varphi^{n-2}\Lambda r}{\theta - \varepsilon + \frac{\Delta c_p}{c_p}\theta\,(Y - \varepsilon)}, \tag{42}$$

and Eq. (30) by Eq. (29),

$$\frac{\mathrm{d}Y}{\mathrm{d}\theta} = Le\frac{Y - \varepsilon}{\theta - \varepsilon + \frac{\Delta c_p}{c_p}\theta\,(Y - \varepsilon)}. \tag{43}$$

In the reaction zone, $\theta \approx 1$, so we define the new variable $\overline{\theta} = \beta\,(1 - \theta)$. Then, Eqs. (42) and (43) read

$$-\beta\frac{\mathrm{d}\varepsilon}{\mathrm{d}\overline{\theta}} = \frac{\varphi^{n-2}\Lambda(1 - Y)\left(\mathrm{e}^{-\frac{\overline{\theta}}{1-\alpha\overline{\theta}/\beta}} - \mathrm{e}^{-\beta\frac{1}{1-\alpha}}\right)}{1 - \varepsilon - \frac{\overline{\theta}}{\beta} + \frac{\Delta c_p}{c_p}\left(1 - \frac{\overline{\theta}}{\beta}\right)(Y - \varepsilon)} \tag{44}$$

$$-\beta\frac{\mathrm{d}Y}{\mathrm{d}\overline{\theta}} = Le\frac{Y - \varepsilon}{1 - \varepsilon - \frac{\overline{\theta}}{\beta} + \frac{\Delta c_p}{c_p}\left(1 - \frac{\overline{\theta}}{\beta}\right)(Y - \varepsilon)}. \tag{45}$$

In this inner zone, the dimensionless variables ε and Y, and the eigenvalue Λ are expanded in terms of algebraic powers of β [12],

$$\varepsilon = \varepsilon_0 + \frac{\varepsilon_1}{\beta} + O(\beta^{-2}), \tag{46}$$

$$Y = 1 - \frac{Y_1}{\beta} - \frac{Y_2}{\beta^2} + O(\beta^{-3}), \tag{47}$$

$$\Lambda = \Lambda_0\beta^2 + \Lambda_1\beta + O(\beta^0), \tag{48}$$

that substituted into Eqs. (44) and (45) lead to the following equations at order β^0,

$$\frac{\mathrm{d}\varepsilon_0}{\mathrm{d}\overline{\theta}} = -\frac{\left(\frac{1}{1-\alpha}\right)^{n-2}\Lambda_0 Y_1 \mathrm{e}^{-\overline{\theta}}}{(1-\varepsilon_0)\left(1+\frac{\Delta c_p}{c_p}\right)}, \tag{49}$$

order β^{-1},

$$-\frac{\mathrm{d}\varepsilon_1}{\mathrm{d}\overline{\theta}} = \frac{\left(\frac{1}{1-\alpha}\right)^{n-2}\left(\Lambda_1 Y_1 + \Lambda_0 Y_2 - \Lambda_0 Y_1\left(\overline{\theta}^2\alpha + (n-2)\alpha\overline{\theta}\right)\right)\mathrm{e}^{-\overline{\theta}}}{(1-\varepsilon_0)\left(1+\frac{\Delta c_p}{c_p}\right)} + \frac{\left(\frac{1}{1-\alpha}\right)^{n-2}\Lambda_0 Y_1\left[\varepsilon_1 + \overline{\theta} + \frac{\Delta c_p}{c_p}\left(\overline{\theta}\,(1-\varepsilon_0) + Y_1 + \varepsilon_1\right)\right]\mathrm{e}^{-\overline{\theta}}}{(1-\varepsilon_0)^2\left(1+\frac{\Delta c_p}{c_p}\right)^2} \tag{50}$$

$$\frac{\mathrm{d}Y_1}{\mathrm{d}\overline{\theta}} = Le\frac{1}{\left(1+\frac{\Delta c_p}{c_p}\right)} \tag{51}$$

and order β^{-2},

$$\frac{\mathrm{d}Y_2}{\mathrm{d}\overline{\theta}} = Le\left[\frac{\overline{\theta} - Y_1}{(1-\varepsilon_0)\left(1+\frac{\Delta c_p}{c_p}\right)} + \frac{Y_1\frac{\Delta c_p}{c_p}}{(1-\varepsilon_0)\left(1+\frac{\Delta c_p}{c_p}\right)^2}\right]. \tag{52}$$

By applying the boundary conditions in the inner zone, $\varepsilon_0 \to 1$ and $\varepsilon_1, Y_1, Y_2 \to 0$ as $\overline{\theta} \to 0$ (see Ref. [12]), the integration of Eqs. (49)–(52) gives

$$Y_1 = \frac{Le}{\left(1+\frac{\Delta c_p}{c_p}(1-Y_{P0})\right)}\overline{\theta} \tag{53}$$

$$\varepsilon_0 = 1 - \left[\frac{2\left(\frac{1}{1-\alpha}\right)^{n-2}\Lambda_0 Le}{\left(1+\frac{\Delta c_p}{c_p}\right)^2}\left[1-\left(1+\overline{\theta}\right)\mathrm{e}^{-\overline{\theta}}\right]\right]^{1/2} \tag{54}$$

$$Y_2 = Le\frac{\left(1+\frac{\Delta c_p}{c_p}\right)^2 - Le}{\left(1+\frac{\Delta c_p}{c_p}\right)^3}\int_0^{\overline{\theta}}\frac{\overline{\theta}_1}{(1-\varepsilon_0)}\mathrm{d}\overline{\theta}_1 \tag{55}$$

$$\varepsilon_1 = -\frac{1}{2\,(1-\varepsilon_0)}\int_\infty^{\overline{\theta}}\overline{\theta}_1\mathrm{e}^{-\overline{\theta}_1}\times\left(\frac{\Lambda_1}{\Lambda_0} + \frac{Y_2}{Y_1} - \overline{\theta}_1^2\alpha - (n-2)\alpha\overline{\theta}_1 + \frac{\overline{\theta}_1}{(1-\varepsilon_0)} + \frac{\frac{\Delta c_p}{c_p}\left(Y_1 - \overline{\theta}_1\varepsilon_0\right)}{(1-\varepsilon_0)\left(1+\frac{\Delta c_p}{c_p}\right)}\right)\mathrm{d}\overline{\theta}_1. \tag{56}$$

On the other hand, $\varepsilon_1, \varepsilon_0 \to 0$ as $\overline{\theta} \to \infty$ (see Ref. [12]), so this boundary condition applied to Eq. (54) implies that

$$\Lambda_0 = \frac{\left(1+\frac{\Delta c_p}{c_p}\right)^2}{2Le\left(\frac{1}{1-\alpha}\right)^{n-2}} \tag{57}$$

whereas it applied to Eq. (56) implies

$$\frac{\Lambda_1}{\Lambda_0} = 6\alpha - 4.688 + Le\frac{2 - 2.688\frac{\Delta c_p}{c_p}}{\left(1+\frac{\Delta c_p}{c_p}\right)^2} + \frac{1.688\frac{\Delta c_p}{c_p}}{\left(1+\frac{\Delta c_p}{c_p}\right)} + 2\alpha(n-2) \tag{58}$$

Eq. (48), with Eqs. (57) and (58), substituted into Eq. (35) gives the expression for the dimensionless flame speed at first order c'_{TZ1} Eq. (15) and at second order c'_{TZ2} Eq. (16).

Note that, above, Λ_0 and Λ_1 are derived by suitably applying the boundary conditions to the solutions for the inner zone only. The solutions Y and ε for the outer zone, here not shown, contain constants of integration that are identified by asymptotically matching with the Y and ε solutions for the inner zone (see, e.g., Ref. [12]). We omit this derivation since we are interested here in the values for the burning-rate eigenvalue rather than in the Y and ε profiles followed by the two zone model.

Appendix D

The Zeldovich and Frank–Kamenetskii method focuses on the thinner reaction zone, where the thermal gradient is large [3,20]. Therefore, it is expected that, in Eq. (9), both the diffusive and the reaction terms dominate over the temporal derivative and also over the cross term $\partial\theta/\partial z'\partial Y/\partial z'$ for small values of Δc_p. Thus, Eq. (9) reduces to

$$0 = \varphi\frac{\partial}{\partial z'}\left(\varphi^{n-1}\frac{\partial\theta}{\partial z'}\right) + \left(1+\frac{\Delta c_p}{c_p}\theta\right)F. \tag{59}$$

Integrating this equation in the variable $q = \varphi^{n-1}\partial\theta/\partial z'$ ($\mathrm{d}q/\mathrm{d}z' = q/\varphi^{n-1}\mathrm{d}q/\mathrm{d}\theta$) from q to 0 gives

$$q = \sqrt{2\int_\theta^1 \mathrm{d}\theta'\left(1+\frac{\Delta c_p}{c_p}\theta'\right)\varphi^{n-2}F}. \tag{60}$$

Since we assume that the heat flux must equal the energy released by combustion in the reaction zone as the flame propagates (i.e., $\lambda\partial T/\partial z = Qm$), the dimensionless heat flux q is equal to the dimensionless burning velocity c'. Thus, the Zeldovich and Frank–Kamenetskii expression for the front speed c'_{ZFK} shown in Eq. (18) follows from Eq. (60) with $\theta = 0$.

Appendix E

Rigorous lower and upper bounds may be obtained by extending the variational principle formerly developed by Benguria and Depassier [5] for 1D convection–diffusion–reaction equations to the full combustion model here analyzed. Introducing the dimensionless variable $s' = z' + c't'$ in Eq. (9), with the approximation $\theta \approx Y$, gives

$$0 = -(c'+v')\frac{\partial\theta}{\partial s'} + \varphi^n\frac{\partial^2\theta}{\partial s'^2} + \psi\left(\frac{\partial\theta}{\partial s'}\right)^2 + f, \tag{61}$$

where

$$\psi = \frac{n-1}{n}\frac{\mathrm{d}\varphi^n}{\mathrm{d}\theta} - \frac{\Delta c_p}{c_p}\frac{\varphi^n}{Le}, \quad f = \left(1+\frac{\Delta c_p}{c_p}\theta\right)F. \tag{62}$$

Since the mass burning velocity m is constant, we obtain $\rho(c+v) = \rho_0 c$, or, equivalently in dimensionless variables, $c'+v' = c'\varphi$ that used in Eq. (61) leads to

$$0 = -c'\varphi\frac{\partial\theta}{\partial s'} + \varphi^n\frac{\partial^2\theta}{\partial s'^2} + \psi\left(\frac{\partial\theta}{\partial s'}\right)^2 + f. \tag{63}$$

Defining the phase space variable $p = \partial\theta/\partial s'$, which implies $p\mathrm{d}p/\mathrm{d}\theta = \partial^2\theta/\partial s'^2$, Eq. (63) divided by φ reads

$$0 = -c'p + \varphi^{n-1}p\frac{dp}{\mathrm{d}\theta} + \frac{\psi p^2}{\varphi} + \frac{f}{\varphi}, \tag{64}$$

where p is definite positive with $p(0) = p(1) = 0$. Multiplying Eq. (64) by g/p with g an arbitrary positive function, and integrating from $\theta = 0$ to $\theta = 1$, we obtain

$$c'\int_0^1 g\mathrm{d}\theta = \int_0^1\left[p\left(-\frac{\mathrm{d}(\varphi^{n-1}g)}{\mathrm{d}\theta} + \frac{\psi g}{\varphi}\right) + \frac{gf}{p\varphi}\right]\mathrm{d}\theta \tag{65}$$

after integrating by parts the second term on the r.h.s in Eq. (64).

Choosing a function g such that $\left(-d(\varphi^{n-1}g)/\mathrm{d}\theta + \psi g/\varphi\right) > 0$ from $\theta = 0$ to $\theta = 1$, and since g, f, φ and p are positive, Eq. (65) leads to the condition

$$c' \geq \frac{\int_0^1 2\sqrt{gf\varphi^{n-2}\left(-\frac{\mathrm{d}g}{\mathrm{d}\theta} - \frac{\Delta c_p}{c_p}\frac{1}{Le}g\right)}\mathrm{d}\theta}{\int_0^1 g\,\mathrm{d}\theta}, \tag{66}$$

where the use has been made of Eqs. (10) and (62).

The r.h.s. in Eq. (66) corresponds to the lower bound for the dimensionless speed c'_{LB} shown in Eq. (23), where the g function is chosen as

$$g = \sqrt{1-\theta}. \tag{67}$$

Note that Eq. (67) assures a positive value for the term within the parentheses in Eq. (66).

Following Benguria and Depassier [14], the upper bound for the dimensionless speed c'_{UB} is obtained by assuming a set of trial functions $\widehat{g}$ which satisfy

$$p\left(-\frac{\mathrm{d}(\varphi^{n-1}\widehat{g})}{\mathrm{d}\theta} + \frac{\psi\widehat{g}}{\varphi}\right) = \frac{\widehat{g}f}{p\varphi}. \tag{68}$$

This implies that the equality in Eq. (66) holds. Defining c'_* as the supremum of the r.h.s. of Eq. (66) over all the $\widehat{g}$ functions,

$$c'_* = \sup\left[\frac{\int_0^1 2\sqrt{\widehat{g}f\varphi^{n-2}\left(-\frac{\mathrm{d}\widehat{g}}{\mathrm{d}\theta} - \frac{\Delta c_p}{c_p}\frac{1}{Le}\widehat{g}\right)}\mathrm{d}\theta}{\int_0^1 \widehat{g}\,\mathrm{d}\theta}\right]. \tag{69}$$

Since $\widehat{g}$, f and φ are positive functions, Eq. (69) leads to the condition

$$c'_* \leq \sup\left\{\frac{\int_0^1\left[\frac{\widehat{g}f\varphi^{n-2}}{\mu\theta} + \left(-\frac{\mathrm{d}\widehat{g}}{\mathrm{d}\theta} - \frac{\Delta c_p}{c_p}\frac{1}{Le}\widehat{g}\right)\mu\theta\right]\mathrm{d}\theta}{\int_0^1 \widehat{g}\,\mathrm{d}\theta}\right\}. \tag{70}$$

with μ a positive function. Integrating by parts the $d\widehat{g}/\mathrm{d}\theta$ term in Eq. (70), we find

$$c'_* \leq \sup\left[\frac{f\varphi^{n-2}}{\mu\theta} + \mu\left(1 - \frac{\Delta c_p}{c_p}\frac{\theta}{Le}\right)\right], \tag{71}$$

which is used in Eq. (20) for estimating the upper bound c'_{UB}. Note that the existence of well-defined trial functions $\widehat{g}$ may be easily demonstrated by substituting Eq. (68) into Eq. (64) and obtain an expression for $\widehat{g}$ that does not diverge (see, e.g., Refs. [14,8]).

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