A simple method to evaluate the eigenvalue of premixed flame propagation

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Abstract
The Lewis number is the ratio of thermal diffusivity to molecular diffusion coefficient, and its influence on premixed-flame propagation has been a topic of extensive combustion research. Diffusive-thermal model, which neglects density variation caused by temperature increase due to combustion, has been frequently used to examine the effect of the Lewis number. Major advantages of the diffusive-thermal model are that it allows computation with a given flow field and that the sole effect of the Lewis number can be investigated. The diffusive-thermal model includes a dimensionless parameter, hereafter denoted by $\lambda$, which corresponds to the pre-exponential factor of reaction rate constant. Its value must be determined such that the correct burning velocity can be reproduced. Although a number of studies use the lowest-order asymptotic expression for evaluating the value of $\lambda$, the expression causes errors as much as several tens of percent depending on the condition. In this study, the value of $\lambda$ is numerically determined by seeking a traveling wave solution in a one-dimensional moving coordinate system. The method is simple enough to be implemented in Microsoft Excel using its solver add-in. It was found that even two-term asymptotic expansion of $\lambda$ resulted in errors more than 10% in some cases. It is therefore recommended to numerically evaluate the value of $\lambda$ under every condition of interest. As an alternative means, this paper proposes an empirical formula that yields the value of $\lambda$ with errors less than 1% in most cases (less than 2% in all the cases) tested in this study.

Keywords: Diffusive-thermal model, Traveling wave solution, Burning velocity, Eigenvalue, Empirical formula

1. Introduction

Premixed flame propagation is significantly influenced by the Lewis number, $Le = \bar{a}/\bar{D}$, where $\bar{a}$ is the thermal diffusivity, and $\bar{D}$ is the molecular diffusion coefficient (Kadowaki and Hasegawa, 2005; Okuno et al., 2018; Dejoan et al., 2019; Cai et al., 2020); an overline ($\bar{\cdot}$) is used in this paper to denote a dimensional quantity. To specifically study the effects of the Lewis number, the so-called diffusive-thermal model that ignores density variation due to temperature change has been widely used (Bayliss and Matkowsky, 1991; Kurdyumov and Jiménez, 2016; Iizuka et al., 2017; Okuno et al., 2018; Lu and Matalon, 2019). The basic equations of the diffusive-thermal models can be written as

$$\frac{\partial T}{\partial t} + \nu \cdot \nabla T = \nabla^2 T + \lambda Y \exp \left[ \frac{\beta(T - 1)}{y(T - 1) + 1} \right]$$

(1)

$$\frac{\partial Y}{\partial t} + \nu \cdot \nabla Y = \frac{1}{Le} \nabla^2 Y - \lambda Y \exp \left[ \frac{\beta(T - 1)}{y(T - 1) + 1} \right]$$

(2)

where $T$ and $Y$ are dimensionless temperature and mass fraction, respectively. $T$ and $Y$ are normalized such that $T = 0$ and $Y = 1$ in the fresh unburnt mixture, whereas $T = 1$ and $Y = 0$ in the burnt, equilibrium mixture.
length scale in Eqs. (1) and (2) is in units of the width of the thermal flame structure \( \bar{T}_T = \bar{a}/\bar{s}_u \), where \( \bar{s}_u \) is the laminar burning velocity, whereas the time scale is in units of \( \bar{T}_T/\bar{s}_u \). Consequently, velocity \( v \) is in units of \( \bar{s}_u \).

Equations (1) and (2) include three parameters, namely, the Lewis number \( Le \), the Zel’dovich number \( \beta = E(\bar{T}_b - \bar{T}_w)/\bar{R} \bar{T}_b^2 \), and \( \gamma = (\bar{T}_b - \bar{T}_w)/\bar{T}_w^2 \). Here, \( \bar{T}_w \) and \( \bar{T}_b \) are the temperatures of unburnt and burnt mixtures, respectively, \( E \) is the activation energy, and \( \bar{R} \) is the universal gas constant.

The major advantages of the diffusive-thermal model are that (i) \( v \) can be treated as a given flow field not affected by combustion reactions, and that (ii) the sole effect of the Lewis number can be examined because the buoyancy and Darrieus-Landau effects (Kadowaki and Hasegawa, 2005) caused by the density difference between unburnt and burnt mixtures are excluded.

\( A \) is the value of \( A \) that must be determined such that the resultant laminar burning velocity is equal to unity. The lowest-order asymptotic analysis in the limit of large activation energy leads to the following expression for \( A \) (Bush and Fendell, 1970):

\[
A = \frac{\beta^2}{2Le} \quad (3)
\]

This value is adopted in a number of numerical studies, e.g., Bayliss and Matkowsky (1991), Kagan et al. (2004), Iizuka et al. (2017), and Okuno et al. (2018). As we shall see later in this paper, however, use of Eq. (3) causes errors as much as several tens of percent. Adding the next-order corrections to Eq. (3), one obtains the following two-term asymptotic expansion (Bush and Fendell, 1970; Takeno, 1989):

\[
A = \beta^2 \left[ \frac{1}{2Le} + \frac{1}{\beta} \frac{Le + 3\gamma - 1 - 1}{Le} \right] \quad (4)
\]

Here, \( I = 1.344 \ldots \) is a constant whose value must be numerically evaluated. It is found that use of Eq. (4) still causes errors more than 10% (see Section 3) when the Zel’dovich number is relatively small. As the burning velocity is roughly proportional to the square root of \( A \), a 10% error in \( A \) would cause an error of approximately 5% in burning velocity. The activation energies of some combustion systems are not sufficiently large, so that the accuracy of asymptotic analysis is limited. For example, Coffee et al. (1983) estimated that the overall activation energy of stoichiometric methane/air flame was 29 kcal/mol, giving a Zel’dovich number \( \beta \approx 6 \).

Further asymptotic expansion of \( A \) is not straightforward. This study therefore adopts a different approach and numerically determines the values of \( A \) under a wide range of conditions. Differences between the obtained values and Eqs. (3) and (4) are examined, and an empirical formula is proposed by fitting the obtained values. The results are reported herein.

2. Numerical methods

Constant-speed flame propagation in a 1-D system can be expressed by a steady state in a moving coordinate system that is attached to flame front. Traveling wave solutions (i.e., stationary solutions in the moving coordinate) are sought in the following way.

Equations (1) and (2) are rewritten in the 1-D moving coordinate as

\[
s \frac{dT}{dx} = \frac{d^2T}{dx^2} + A \exp \left[ \frac{\beta(T - 1)}{\gamma(T - 1) + 1} \right], \quad (5)
\]

\[
s \frac{dY}{dx} = \frac{1}{Le} \frac{d^2Y}{dx^2} - A \exp \left[ \frac{\beta(T - 1)}{\gamma(T - 1) + 1} \right], \quad (6)
\]

where \( s \) is the speed of moving coordinate that is equal to the burning velocity. In this study, \( s > 0 \) is considered, meaning that flame propagates in the \( -x \) direction. The boundary conditions are therefore \( T = 0 \) and \( Y = 1 \) at \( x = -\infty \), whereas \( T = 1 \) and \( Y = 0 \) at \( x = \infty \).

Traveling wave solutions are sought such that \( s = 1 \). In other words, the value of \( A \) is so determined that the dimensionless burning velocity is equal to unity. Equations (5) and (6) thus define a nonlinear eigenvalue problem, in which \( A \) plays a role as the eigenvalue.
This study adopts a similar method to Bush and Fendell (1970), and second-order differential equations (5) and (6) are converted into the following system of first-order differential equations.

\[
\frac{dT}{dx} = s(T - 1) + \Omega, \tag{7}
\]
\[
\frac{dY}{dx} = Le(sY - \Omega), \tag{8}
\]
\[
\frac{d\Omega}{dx} = -AY\exp\left[\frac{\beta(T - 1)}{Y(T - 1) + 1}\right], \tag{9}
\]

which can be integrated using a numerical method such as the Runge-Kutta method. Here, \(\Omega = sY - (1/Le)dY/dx\) is the mass-flux fraction.

In Bush and Fendell (1970), Eqs. (7)–(9) were further converted to two equations for \(dY/dT\) and \(d\Omega/dT\), which were then integrated. Although the number of equations can be reduced this way, spatial distributions \(T(x)\) and \(Y(x)\) are yet to be determined. Profiles \(T(x)\) and \(Y(x)\) are often needed as an initial condition in 2-D or 3-D diffusive-thermal computation. Hence, Eqs. (7)–(9) were directly solved in this study. In so doing, the range of \(x\) was set to be \(-50 \leq x \leq 10\) with the position of flame front being at \(x = 0\).

Following Funashima et al. (2019), the domain is divided into a reaction region (inner region) in the vicinity of \(x = 0\) and outer regions where the reaction rate is negligibly small. The following analytical solution is available in the outer regions:

\[
T = \begin{cases} 
1 & (x > 0) \\
\exp(s \times) & (x < 0)
\end{cases}, \tag{10}
\]

\[
Y = \begin{cases} 
Y^* & (x > 0) \\
1 - \exp(Le \times) & (x < 0)
\end{cases}, \tag{11}
\]

\[
\Omega = \begin{cases} 
0 & (x > 0) \\
1 & (x < 0)
\end{cases}, \tag{12}
\]

where \(Y^*\) is a small value to be determined as part of solution. Equations (7)–(9) were integrated using the 4th-order Runge-Kutta method from \(x = 10\) to \(x = -50\) with a fixed step size of \(\Delta x = 0.01\). Note that the initial value of \(Y\), i.e., \(Y^*\), must not be zero to avoid the trivial solution of \(Y(x) = 0\). The values of \(Y^*\) and eigenvalue \(\Lambda\) were determined such that \(T, Y,\) and \(\Omega\) converge to the outer solution, Eqs. (10)–(12), in the region of \(x < 0\). Specifically, \(Y^*\) and \(\Lambda\) were sought by minimizing the sum of the squares of the differences between outer solutions, Eqs. (10)–(12), and the corresponding numerical values. The numerical method outlined thus far can be implemented in Microsoft Excel using its solver add-in. Solution in a typical condition can be obtained in several minutes using a standard personal computer. The ranges of parameters varied in this study are 0.1 \(\leq Le \leq 5.0\), 6.0 \(\leq \beta \leq 20.0\), and 0.5 \(\leq \gamma \leq 0.95\); a total of 3,450 conditions were tested.

In addition to steady-state computations in a moving coordinate system, unsteady calculations were performed in a laboratory coordinate system to confirm whether eigenvalues \(\Lambda\) obtained by steady-state computations yield the correct burning velocity, i.e., \(s = 1\). The basic equations solved in unsteady calculations are

\[
\frac{dT}{dt} = d^2T/dx^2 + AY\exp\left[\frac{\beta(T - 1)}{Y(T - 1) + 1}\right], \tag{13}
\]

\[
\frac{dY}{dt} = \frac{1}{Le} \frac{d^2Y}{dx^2} - AY\exp\left[\frac{\beta(T - 1)}{Y(T - 1) + 1}\right]. \tag{14}
\]

The size of computational domain in unsteady calculations was set to be 300. As the width of the regions where a significant temperature gradient exists is less than approximately 10 (see Fig. 1), this size of computational domain is large enough to simulate steady flame propagation. Figure 1 demonstrates that steady propagation is achieved within the computational domain. Equations (13) and (14) were solved by a finite difference method. Time integration was performed by a first-order explicit Euler method, while a second-order central-difference scheme was used for the diffusive terms. The size of
computational cell was varied from 0.05 to 0.8 for a grid-convergence test, while the time step was fixed at $1 \times 10^{-6}$.

3. Results and discussion

It should be first confirmed that the values of $\Lambda$ obtained from steady-state Eqs. (7)–(9) by the method described above actually reproduce the correct burning velocity, $s = 1$, in corresponding unsteady calculations. As an example, $\Lambda = 59.36$ obtained for $Le = 1$, $\beta = 10$, and $\gamma = 0.8$ was used in a series of unsteady calculations, in which Eqs. (13) and (14) were numerically solved. Figure 2 plots the burning velocity computed by unsteady calculations with varied computational cell sizes, confirming that the burning velocity approached unity with the decrease in $\Delta x$. Further, Fig. 3 compares the profiles of $T$, $Y$, and reaction term $\omega = AY \exp[\beta(T - 1)/[\gamma(T - 1) + 1]]$ between those obtained from steady-state Eqs. (7)–(9) and unsteady calculations. Both solutions were nearly identical when $\Delta x = 0.1$, while differences were appreciable when $\Delta x = 0.5$, for which the burning velocity predicted by unsteady calculation was approximately 10% less than the correct value. Clearly, the thin structure of reaction zone was not captured by the coarse cells. The step size $\Delta x$ in steady calculation is equal to 0.01, and profiles obtained by steady calculation (lines) are smoother than those obtained by unsteady calculation (symbols) in Fig. 3.

Results shown in Figs. 2 and 3 confirm that unity burning velocity can be reproduced by using $\Lambda$ obtained from steady-state Eqs. (7)–(9). Consequently, values of $\Lambda$ obtained from Eqs. (7)–(9) are treated as the true values in the following discussion. Note that solving steady-state Eqs. (7)–(9) is computationally much less expensive than unsteady
Next, an empirical expression was obtained by fitting the obtained values of $A$ with the following formula:

$$A = \beta^2 \left[ \frac{1}{2Le} + \frac{Le + 3\gamma - 1 - l}{\beta} + \sum_{n=2}^{5} \frac{C_{\beta,n}}{\beta^n} \times \left( \sum_{n=0}^{1} \frac{C_{Le,n}}{Le^n} \right) \times \left( \sum_{n=-3}^{6} C_{\gamma,n} \gamma^n \right) \right].$$

Equation (15) is a natural extension of asymptotic Eq. (4). Proposed values of constant coefficients $C_{\beta,n}$, $C_{Le,n}$, and $C_{\gamma,n}$ are listed in Table 1. Ten terms were necessary for the polynomial of $\gamma$ because the difference between Eq. (4) and the true value was found to depend on $\gamma$ in a rather complicated manner as shown in Fig. 4.
Figure 5 compares values of $\Lambda$ calculated using asymptotic Eqs. (3), (4), and empirical Eq. (15) with the true values. It is obvious that lowest-order asymptotic Eq. (3) cannot account for the effect of $\gamma$ on $\Lambda$, and its error can be as much as several tens of percent. It is also observed that proposed Eq. (15) yields $\Lambda$ with better accuracy than Eqs. (3) and (4). In Fig. 5(a), the maximum error of Eq. (4) is 8.3%, while that of empirical Eq. (15) is less than 1.4%. As a general trend, regardless of the value of $\mu$, the error of Eq. (4) increased with a decrease in $\beta$ because Eq. (4) was asymptotically obtained in the limit of $\beta \to \infty$. Overall, the error of empirical Eq. (15) was 0.5% on average with the maximum error less than 2%; the number of test cases that resulted in errors greater than 1% was 193 out of the total of 3,450 cases. On the other hand, the average error of Eq. (4) was approximately 2% with the maximum being 11%, and the number of test cases that resulted in errors greater than 1% was 2,341 out of the total of 3,450 cases.

In the discussion thus far, Eqs. (7)–(9) were solved to find $\Lambda$ that yields $s = 1$. The same Eqs. (7)–(9) can be used to obtain burning velocity $s$ for a given value of $\Lambda$. There is no need to conduct unsteady calculations to predict burning velocity; as mentioned above, numerical integration of Eqs. (7)–(9) is computationally less expensive than unsteady calculation of Eqs. (13) and (14). Figure 6(a) compares burning velocity obtained with $\Lambda$ given by asymptotic Eqs. (3) and (4), and empirical Eq. (15); the values of $\Lambda$ in the same conditions are shown in Fig. 6(b), which shows the data only for small $\beta$ to emphasize the difference between Eqs. (4) and (15). Use of lowest-order Eq. (3) resulted in significant errors (more than 10%) in burning velocity. Although use of two-term asymptotic Eq. (4) can
greatly reduce the error as compared with Eq. (3), the error tends to increase with a decrease in $\beta$. It is confirmed that the proposed empirical Eq. (15) yielded burning velocity with better accuracy than Eqs. (3) and (4).

In summary, use of Eq. (3) is not recommended as it causes errors of more than 10% in predicting burning velocity. Use of Eq. (4) is recommended if the Zel'dovich number $\beta$ is roughly greater than 10 because the error in predicting burning velocity is then less than approximately 1%. However, use of Eq. (4) can result in errors greater than 1% when the Zel'dovich number is smaller. As pointed out in Section 1, the Zel'dovich numbers in typical combustion systems are often less than 10, and it should be avoided that mere choice of a parameter value causes an error over 1%. Consequently, it is ideal to determine the value of $A$ in every condition of interest by seeking a traveling wave solution using the method described in Section 2. Alternatively, empirical Eq. (15) may be used for simple estimation if the condition of interest is within the range tested in this study. Empirical Eq. (15) yields burning velocity with an error less than approximately 0.5%.

4. Conclusions

The diffusive-thermal model of premixed combustion is widely used to examine the effect of the Lewis number on flame propagation. Then, the value of parameter $A$ that corresponds to the pre-exponential factor of reaction rate constant must be determined such that the correct burning velocity is obtained.

The values of $A$ under a wide range of conditions were numerically obtained by seeking traveling wave solutions in a moving coordinate system. The obtained values were then compared with the values given by lowest-order and two-term asymptotic approximations. It was found that the lowest-order approximation resulted in errors as much as several tens of percent in evaluating the value of $A$. Use of the lowest-order approximation is therefore not recommended. Although two-term asymptotic approximation is more accurate than that of the lowest order, its error in estimating $A$ exceeds 10% when the Zel'dovich number is relatively small. Use of the two-term asymptotic approximation is thus recommended only when the activation energy is sufficiently large and the Zel'dovich number is greater than about 10. As the activation energies of typical combustion systems are often not so high that the Zel'dovich number is less than 10, it is ideal to determine the value of $A$ under every condition of interest. The numerical method described in this paper is simple and can be implemented in Microsoft Excel using its solver add-in. It is computationally much less expensive than determining $A$ by a trial-and-error method using an unsteady model. Alternatively, an empirical formula proposed in this study can be used when the condition of interest is within the range tested in this study. Errors in calculating the value of $A$ by the empirical formula are less than 1% in most cases.

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