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Observation, analysis and modelling in complex fluid media

Scalar dissipation and flame surface density in premixed turbulent combustion

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Abstract

A new closed version of the transport equation for the flame surface density in premixed turbulent combustion is derived, on the basis of an equation for the scalar dissipation that has previously been proposed by the present authors. As in this earlier work, volume expansion due to heat release is found to have an important role in determining the flame surface density. An algebraic approximation to the transport equation is obtained, on the basis of an order-of-magnitude analysis, and is found to be in good agreement with data from DNS. Finally, laminar flame calculations are used to estimate a key parameter in the new model. ***To cite this article: K.N.C. Bray, N. Swaminathan, C. R. Mecanique 334 (2006).***

Résumé

Dissipation du scalaire et densité de surface de flamme en combustion turbulente prémélangée. Une nouvelle version modélisée de l'équation de transport pour la densité de surface de flamme en combustion turbulente prémélangée est obtenue, sur la base d'une équation pour la dissipation du scalaire qui avait été préalablement obtenue par les mêmes auteurs. Comme pour ce précédent travail, l'expansion volumique due au dégagement de chaleur est trouvée jouer un rôle important dans la détermination de la densité de surface de flamme. Une approximation algébrique de l'équation de transport est obtenue, sur la base d'une analyse d'ordre de grandeur, qui se révèle être en très bon accord avec des données obtenues par DNS. Finalement, des calculs de flamme laminaire sont utilisés pour estimer l'un des paramètres principaux du nouveau modèle. ***Pour citer cet article : K.N.C. Bray, N. Swaminathan, C. R. Mecanique 334 (2006).***

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Mots-clés : Turbulence ; Flammes turbulentes de prémélange ; Micro-mélange ; Mélange de scalaire ; Taux de dissipation du scalaire

1. Introduction

Roland Borghi was among the first to understand the importance of the relationship between scalar dissipation and mean reaction rates in premixed turbulent combustion. This important insight led him, with co-workers, to derive and propose closure approximations for the transport equation for the scalar dissipation [1–4]. The mean scalar dissipation

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is $\bar{\rho}\tilde{\varepsilon}_c = \overline{\rho\alpha(\nabla c'' \cdot \nabla c'')}$, where α is the molecular diffusivity of the reaction progress variable $c(\mathbf{x}, t)$, which is defined as a normalised temperature. The overbar implies an appropriate averaging. The Favre average or density weighted average of c is $\tilde{c}$ and its fluctuation is c''. With the above definition, $\tilde{\varepsilon}_c$ is one half of the molecular dissipation term in the transport equation for the scalar variance, $\tilde{c}''^2$, and represents the reciprocal of a time scale for the mean rate of small-scale mixing between cold reactants and hot products. In one form or another, scalar dissipation plays a central role in most mean reaction rate formulations for premixed systems, including transported and presumed pdfs, conditional moment closure, and flame surface density methods.

In deriving their governing equation for $\tilde{\varepsilon}_c$, Borghi et al. [1–4] introduce the simplifying assumption of constant density and consequently neglect volume expansion due to heat release. More recently, Swaminathan and Bray [5] revisited this problem, taking into account effects of volume expansion, which are shown to be significant. Comparison with DNS data provides support for the analysis.

The aim of the present work is to apply the results of Swaminathan and Bray [5] to the flame surface density $\Sigma(\mathbf{x}, t)$. A closed version of the transport equation is presented for this quantity in the context of RANS methodology. An order-of-magnitude analysis leads to an algebraic expression for Σ. This simple expression is used to discuss the choice of an appropriate length scale to normalise Σ. Also, the prediction of the flame surface density by this model is compared to previous models [6,7] and direct numerical simulation (DNS) results. The derivation of a closed transport equation for $\tilde{\varepsilon}_c$ is reviewed first.

2. Transport equation for $\tilde{\varepsilon}_c$ [5]

The unclosed transport equation for $\tilde{\varepsilon}_c$, including effects of volume expansion due to heat release, may be written as [5]

$$\frac{\partial \bar{\rho}\tilde{\varepsilon}_c}{\partial t} + \frac{\partial}{\partial x_j}\left(\bar{\rho}\widetilde{U}_j\tilde{\varepsilon}_c\right) - \frac{\partial}{\partial x_j}\left(\overline{\rho\alpha}\frac{\partial \tilde{\varepsilon}_c}{\partial x_j}\right) + \overline{2\rho\alpha\alpha\left[\frac{\partial}{\partial x_j}\left(\frac{\partial c''}{\partial x_k}\right)\right]^2} = T_1 + T_2 + T_3 + T_4 \tag{1}$$

where

$$T_1 \equiv \underbrace{-\frac{\partial \overline{\rho u_j'' \varepsilon_c}}{\partial x_j}}_{T_{11}} \underbrace{-2\overline{\rho\alpha\left(u_j''\frac{\partial c''}{\partial x_k}\right)}\frac{\partial}{\partial x_j}\left(\frac{\partial \tilde{c}}{\partial x_k}\right)}_{T_{12}}$$

$$T_2 \equiv 2\bar{\rho}\tilde{\varepsilon}_c\frac{\partial \widetilde{U}_l}{\partial x_l} + \overline{2\rho\alpha\left(\frac{\partial c''}{\partial x_k}\frac{\partial c''}{\partial x_k}\frac{\partial u_l''}{\partial x_l}\right)} = \overline{2\rho\varepsilon_c\frac{\partial u_l}{\partial x_l}}$$

$$T_3 \equiv \underbrace{\overline{-2\rho\alpha\left(\frac{\partial c''}{\partial x_k}\frac{\partial u_j''}{\partial x_k}\right)}\frac{\partial \tilde{c}}{\partial x_j}}_{T_{31}} \underbrace{\overline{-2\rho\alpha\left(\frac{\partial c''}{\partial x_j}e_{jk}''\frac{\partial c''}{\partial x_k}\right)}}_{T_{32}} \underbrace{\overline{-2\rho\alpha\left(\frac{\partial c''}{\partial x_j}\frac{\partial c''}{\partial x_k}\right)}\tilde{e}_{jk}}_{T_{33}}$$

$$T_4 \equiv 2\overline{\left(\alpha\frac{\partial c''}{\partial x_k}\frac{\partial \dot{\omega}''}{\partial x_k}\right)}$$

where $e_{jk} = 0.5(u_{j,k} + u_{k,j})$ represents a component of the rate of strain and T_2 describes effects due to dilatation. If this latter term is set equal to zero, and density is held constant, Eq. (1) reduces to the equation of Mura and Borghi [4].

An order-of-magnitude analysis [5] establishes the relative magnitude of terms in this equation. The turbulence Reynolds and Damköhler numbers are respectively defined as $Re \equiv u'\Lambda/\nu_u$ and $Da \equiv (\tau_f/\tau_c) = \Lambda s_L^o/(u'\delta_L^o)$, where u' is the root mean square value of turbulence velocity, Λ is the integral length scale of the turbulence field, δ_L^o is the thermal thickness of unstrained laminar flame propagating at speed s_L^o and ν_u is the kinematic viscosity of reactant mixture. Also, it is assumed that $\nu_u \simeq \alpha_u$. In the case of thin flamelets, the gradient of c is zero outside the flamelet. Thus, the laminar flame scales are used to scale the quantities involving or multiplied by the gradient of c in the order of magnitude analysis. The spatial derivatives of mean quantities are scaled by the integral length scale and the evolution time t is scaled by the eddy turn over time. Dropping some small terms, adopting models from Borghi

et al. [3,4], and introducing laminar flamelet assumptions to model T_2 [5], Eq. (1) may be written in modelled form, for conditions where Da and Re are both large, as

$$\frac{\partial \bar{\rho}\tilde{\varepsilon}_c}{\partial t} + \frac{\partial \bar{\rho}\widetilde{U}_j\tilde{\varepsilon}_c}{\partial x_j} = \underbrace{\frac{\partial}{\partial x_j}\left(\frac{\mu_t}{Sc_{\varepsilon_c}}\frac{\partial \tilde{\varepsilon}_c}{\partial x_j}\right)}_{T_1} + \underbrace{\frac{4K_c}{(2C_m-1)}\left(\frac{s_L^o}{\delta_L^o}\right)\bar{\rho}\tilde{\varepsilon}_c}_{T_2} \underbrace{- C_{p_c}\bar{\rho}\left(\frac{\tilde{\varepsilon}}{\tilde{k}}\right)\widetilde{u_j''c''}\frac{\partial \tilde{c}}{\partial x_j}}_{T_{31}}$$
$$\underbrace{+ A_e\bar{\rho}\left(\frac{\tilde{\varepsilon}}{\tilde{k}}\right)\tilde{\varepsilon}_c}_{T_{32}} \underbrace{- C_{p_u}\bar{\rho}\tilde{\varepsilon}_c\frac{\widetilde{u_j''u_k''}}{\tilde{k}}\tilde{e}_{jk}}_{T_{33}} \underbrace{- \frac{2}{3}\beta\bar{\rho}\frac{\tilde{\varepsilon}_c^2}{\widetilde{c''^2}}\left(\frac{3}{2} - C_{\varepsilon_c}\frac{s_L}{\sqrt{\tilde{k}}}\right)}_{T_4^*} \tag{2}$$

where $C_{p_c}, A_e, C_{p_u}, C_{\varepsilon_c}$ and β are model constants introduced by Borghi and colleagues [1–4], while K_c and C_m can be evaluated from the properties of a planar unstrained laminar flame. s_L is the local laminar flame speed and T_4^* is defined below. The Favre mean of turbulence kinetic energy and its dissipation rate are denoted by $\tilde{k}$ and $\tilde{\varepsilon}$ respectively. The dynamic viscosity of the turbulence is μ_t.

The order-of-magnitude estimates [5] show that the three dominant terms in Eq. (1) are T_2, T_{32} and T_4^*, where

$$T_4^* = T_4 - 2\overline{\rho\alpha\alpha\left(\frac{\partial c_{,k}''}{\partial x_j}\frac{\partial c_{,k}''}{\partial x_j}\right)} + \frac{\partial}{\partial x_j}\left(\overline{\rho\alpha}\frac{\partial \tilde{\varepsilon}_c}{\partial x_j}\right)$$

Hence, Eq. (1) can be approximated by $T_2 + T_{32} + T_4^* \simeq 0$. A simple model for the dissipation rate can now be obtained by retaining only these three leading order terms from Eq. (2), leading to

$$\tilde{\varepsilon}_c \simeq \left(1 + \frac{2}{3}C_{\varepsilon_c}\frac{s_L^o}{\sqrt{\tilde{k}}}\right)\left(C_{D_c}\frac{s_L^o}{\delta_L^o} + C_D\frac{\tilde{\varepsilon}}{\tilde{k}}\right)\widetilde{c''^2}, \tag{3}$$

where $C_D = A_e/\beta$ and it has been assumed that $(\sqrt{\tilde{k}}/s_L^o) > 2C_{\varepsilon_c}/3$; C_{D_c} is a constant for a given thermochemistry and it is equal to the ratio of $4K_c$ to $(2C_m - 1)\beta$. If C_{ε_c} and C_{D_c} are both set to zero, the classical scalar dissipation model for nonreactive turbulent flows is recovered. The term containing C_{ε_c} describes effect of flamelet curvature, while the factor including C_{D_c} introduces a chemical time scale. The local laminar flame speed s_L is taken to be approximately equal to s_L^o in this study. Strictly, s_L is related to s_L^o via an appropriate Markstein number.

3. Flame surface density

If the Damköhler number Da is sufficiently large, combustion occurs in the so-called laminar flamelets regime [8,9], in which burning is confined to thin reaction surfaces, whose internal structure is similar to that of a laminar flame. The surface area per unit volume or surface density function of an isosurface on which $c = \zeta$ is denoted by $\Sigma(\zeta; \mathbf{x}, \mathbf{t})$. If $Da \gg 1$, $\Sigma(\zeta; \mathbf{x}, t)$ is essentially independent of ζ and we may define a flame surface density either as the value of Σ at a specified value of ζ or from

$$\Sigma(\mathbf{x}, t) = \int_0^1 \mathbf{\Sigma}(\zeta; \mathbf{x}, t)\,\mathbf{d}\zeta \tag{4}$$

The mean heat release rate, $\bar{\dot{\omega}}$, which appears as a source term in the transport equation for $\tilde{c}$, can be calculated as the product of the flame surface density, Σ, and the rate of conversion of reactants into products per unit flame area, i.e., $\bar{\dot{\omega}} = \rho_u s_L \Sigma$. In the limit $Da \gg 1$, $\bar{\dot{\omega}}$ is also related to $\tilde{\varepsilon}_c$ by equation [10]

$$\bar{\dot{\omega}} = \frac{2\bar{\rho}\tilde{\varepsilon}_c}{2C_m - 1} \tag{5}$$

where $C_m = \overline{c\dot{\omega}}/\bar{\dot{\omega}}$, and it follows that Σ is proportional to $\tilde{\varepsilon}_c$. We also have

$$\Sigma(\mathbf{x}, t) = \frac{\bar{\rho}\tilde{\varepsilon}_c}{K_\Sigma s_L} \tag{6}$$

with $K_\Sigma = \rho_u(2C_m - 1)/2$. By substituting for $\tilde{\varepsilon}_c$ in Eq. (2), one gets

$$\frac{\partial \Sigma}{\partial t} + \frac{\partial}{\partial x_j}\left[\left(\widetilde{U}_j - n_j\widetilde{s_L}\right)\Sigma\right] = \frac{\partial}{\partial x_j}\left(\mathcal{D}_\Sigma \frac{\partial \Sigma}{\partial x_j}\right) - C_{p_c}\left(\frac{\tilde{\varepsilon}}{\tilde{k}}\right)\frac{\bar{\rho}\widetilde{u_j''c''}}{K_\Sigma s_L}\frac{\partial \tilde{c}}{\partial x_j} + A_e\left(\frac{\tilde{\varepsilon}}{\tilde{k}}\right)\Sigma - C_{p_u}\left(\frac{\widetilde{u_j''u_k''}}{\tilde{k}}\right)\tilde{e}_{jk}\Sigma + \frac{4K_c}{(2C_m-1)}\left(\frac{s_L^0}{\delta_L^0}\right)\Sigma - \frac{2}{3}\beta\frac{K_\Sigma s_L}{\bar{\rho}\tilde{c}''^2}\left(\frac{3}{2} - C_\varepsilon\frac{s_L}{\sqrt{\tilde{k}}}\right)\Sigma^2 \tag{7}$$

as a transport equation for Σ. This equation with $K_c = 0$ is exactly the same as summarized in [11]. It is also worth noting that the above equation is closed in the context of RANS calculation. However, a simple algebraic expression is attractive for Large Eddy Simulation (LES) of turbulent premixed flames. The derivation of a simple algebraic model for Σ is attempted next.

3.1. Algebraic approximation

An algebraic expression for Σ can be derived by taking the three dominant terms from the transport equation for $\tilde{\varepsilon}_c$. It follows from Eqs. (3) and (6) that

$$\Sigma \simeq 2\frac{\bar{\rho}}{\rho_u}\left(1 + \frac{2}{3}C_{\varepsilon_c}\frac{s_L^o}{\sqrt{\tilde{k}}}\right)\left(C_{D_c}\frac{s_L^o}{\delta_L^o} + C_D\frac{\sqrt{\tilde{k}}}{\Lambda}\right)\frac{\tilde{c}''^2}{s_L(2C_m-1)} \tag{8}$$

in which the turbulence time $\Lambda/\sqrt{\tilde{k}}$ and the laminar flame time δ_L^0/s_L^0 both appear. However, this can be rearranged as

$$\Sigma^+ \equiv \Sigma\delta_L^0 \simeq \frac{2C_{D_c}}{(2C_m-1)}\frac{\bar{\rho}}{\rho_u}\left(1 + \frac{2}{3}C_{\varepsilon_c}\frac{1}{\sqrt{\tilde{k}^+}}\right)\left(1 + \frac{C_D}{C_{D_c}}\frac{\tilde{\varepsilon}^+}{\tilde{k}^+}\right)\tilde{c}''^2. \tag{9}$$

The ratio $\tilde{k}^+/\tilde{\varepsilon}^+$ can be defined to be a local Damköhler number $Da = \Lambda s_L^o/\sqrt{\tilde{k}}\delta_L^0$. Here and in the following discussion the superscript + denotes the quantities appropriately normalised using the unburnt mixture density, ρ_u, s_L^o and δ_L^o.

Also, if one uses the data in [5] then

$$\frac{C_D}{C_{D_c}} = \frac{A_e(2C_m-1)}{4K_c} = 0.9$$

It follows that $\frac{C_D}{C_{D_c}Da} \ll 1$ under conditions of present interest. Hence, Eq. (9) states that the flame surface density scales with δ_L^o rather than Λ. Chen and Bilger [12] showed this while analysing their experimental data on turbulent premixed flames. Earlier algebraic models for the flame surface density generally assume that Σ scales with the integral length scale, Λ, of turbulence—see, for example [6,7,13].

Using Eq. (162) of [7] an algebraic model, which is referred to as VV-model in the following discussion, for the flame surface density can be written as

$$\Sigma^+ = \frac{2}{(2C_m-1)}\frac{\bar{\rho}}{\rho_u}\left(\frac{\tilde{\varepsilon}^+}{\tilde{k}^+}\right)\tilde{c}(1-\tilde{c}) \tag{10}$$

in our notations. Also the model of Bray and Peters [6], referred to as BP model below, can be written as

$$\Sigma^+ = 4.05K\frac{(1+\tau)}{(1+\tau\tilde{c})}\frac{\bar{\rho}}{\rho_u}\left(\frac{\tilde{\varepsilon}^+}{\tilde{k}^+}\right)\tilde{c}(1-\tilde{c}) \tag{11}$$

where $\tau = (T_b/T_u) - 1$, is the heat release parameter and K is a constant of order unity.

It is interesting to note the similarity in the models given by Eqs. (9)–(11) for the flame surface density although their starting points of derivation are different. The VV and BP models include the effect of turbulence on the flame surface density. But the model derived in this study includes the effects of flame propagation, dilatation and turbulence on the flame surface density. The terms inside the first bracket in Eq. (9) represent the effect of flame propagation while the terms inside the second bracket represent the combined effects of turbulence and dilatation. If effects of flame

propagation and dilatation are ignored by setting C_{ε_c} and K_c to zero and expressing the variance as $\tilde{c}(1-\tilde{c})$, one get an expression for Σ which is the same as in Eq. (10) except for the constant C_D. We will compare the predictions of the above algebraic models with results from a direct numerical simulation (DNS) of turbulent premixed flame [14]. The pertinent details of the DNS data are given below.

4. Attributes of DNS data

The problem of premixed flame propagating inside a cubic computational domain containing homogeneous isotropic turbulence in the unburnt mixture was directly simulated by Rutland and Cant [14]. The computational domain had turbulence inflow and outflow boundary conditions in the mean flame propagation direction while the other two directions had periodic boundary condition (see Fig. 1). The turbulence was decaying spatially as the simulation progressed and the fluid transport properties are treated to be invariant in space and time. The combustion kinetics was simulated using a single irreversible reaction with large activation energy. However, to make the simulation practical the temperature rise across the flame front was set to be 3.3 while its typical value is about six to seven. The simulation was initialized with a planar laminar flame having these attributes and the conditions chosen for turbulence were to be representative of flamelet combustion. The value of the ratio of root mean square of turbulence velocity, u', to the planar laminar flame speed, s_l^o, is about 1.4. The length scale ratio between Λ and δ_L^o is about 6.1.

Fig. 1 shows the three-dimensional iso-surface of $c = 0.5$ at $t^+ = 19.4$. This value of t^+ corresponds to about 4.4 initial eddy turn over time. Hence, one can say that a considerable interaction of the turbulence with the scalar field and the initial laminar flame has happened. This is also clear from the level of corrugation and contortion of $c = 0.5$ iso-surface shown in Fig. 1. The turbulent flame brush is statistically planar because of the periodic boundary conditions in the cross stream and spanwise directions. Thus one can obtain average quantities of interest by ensemble averaging the data collected from a sample volume shown in Fig. 1 using the thin lines. The Favre average of c constructed thus is uniquely related to x. Hence, in the following discussion $\tilde{c}$ is used to denote the spatial position inside the turbulent flame brush.

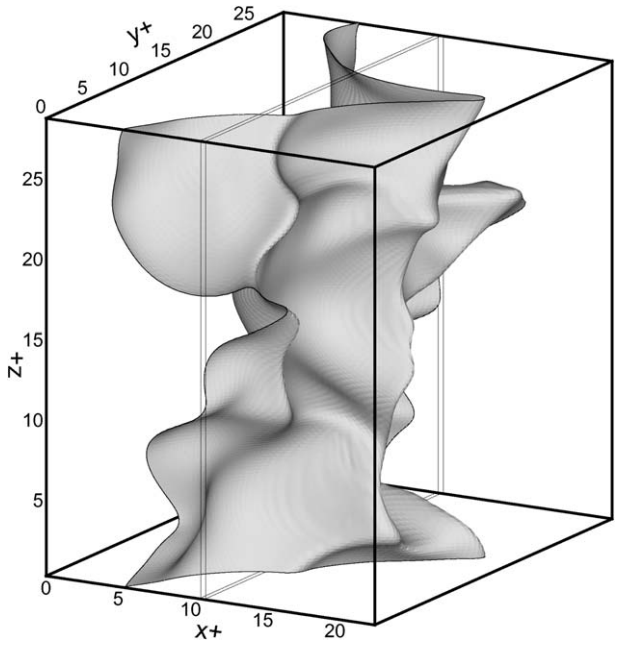

Fig. 1. Iso-surface of $c = 0.5$ at $t^+ = 19.5$ from the DNS [14]. The turbulent flow of cold reactants enters the domain via the left boundary and leaves through the right boundary. The flow is periodic in y and z directions. The thin slab represents the sample volume.

Fig. 1. Iso-surfaces de $c = 0{,}5$ à $t^+ = 19{,}5$ obtenues par DNS par [14]. L'écoulement turbulent de réactifs froids entre dans le domaine par sa frontière gauche et le quitte par sa frontière droite. L'écoulement est périodique selon les directions y et z. La tranche fine indique le volume échantillon.

5. Results and discussion

The flame surface density, $\Sigma(\zeta; \mathbf{x}, t)$, can be obtained by two methods. In the first method, the area of an iso-surface can be calculated by tracking the particular iso-surface $c = \zeta$. In the second method, Σ is calculated via $\Sigma(\zeta; \mathbf{x}) = \langle |\nabla c| | c = \zeta \rangle P_\zeta$ [15]. The conditional average, which is defined as the average of the ensemble satisfying the condition $c = \zeta$, of the magnitude of the progress variable gradient is denoted as $\langle |\nabla c| | c = \zeta \rangle$. The marginal pdf of c is P_ζ. Here, we follow the second approach to obtain Σ because of its inherent accuracy. The typical variation of normalised $\Sigma(\zeta; \mathbf{x})$ with ζ in the DNS is shown in Fig. 2. The results are shown for five different locations inside the turbulent flame brush as marked in Fig. 2. Since the combustion occurs in the thin flamelets regime one would expect Σ^+ to be independent of ζ. The results in Fig. 2 indeed show this behavior except for ζ near zero and unity. The sharp increase in Σ^+ near $\zeta = 0$ and 1 is because a very small number, the conditional dissipation rate, multiplies a very large number, the marginal pdf of c. Also, at all the locations inside the flame brush considered here Σ^+ is insensitive to ζ. Such an observation was also made in an experimental investigation [12] of turbulent premixed flame.

Because of the insensitivity of Σ^+ to the value of ζ observed in Fig. 2, we will consider $\zeta = 0.75$ for further analysis. This value of ζ corresponds to the location of peak reaction rate. A close study of Fig. 2 also shows that Σ^+ varies with the location inside the flame brush. This variation is shown in Fig. 3 for ζ equal to 0.75. The line with circles denote the DNS results. The width of the vertical bars on the circles corresponds to twice the standard

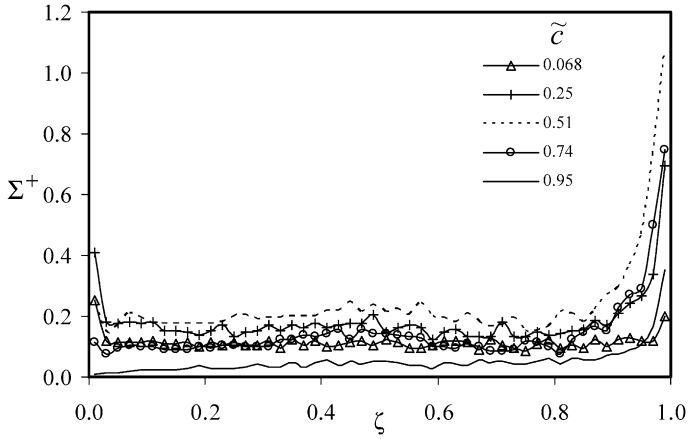

Fig. 2. Behavior of Σ^+ with ζ at various locations inside the flame brush simulated in the DNS.

Fig. 2. Comportement de Σ^+ avec ζ en différentes positions à l'intérieur de la flamme simulée par DNS.

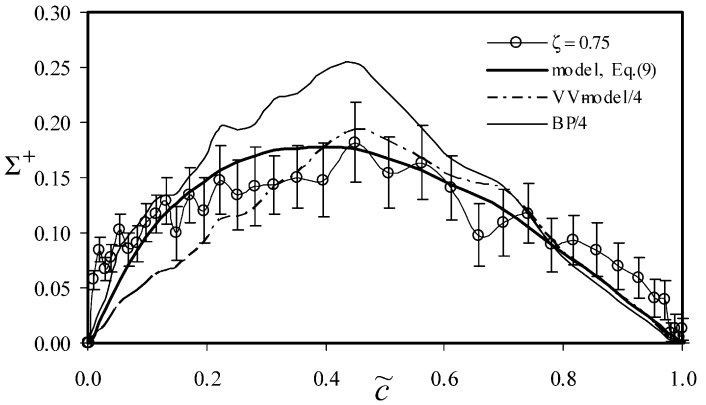

Fig. 3. Variation of Σ^+ with $\tilde{c}$ in the DNS (-o-) and the model predictions. The size of vertical bars denote two standard deviation in the DNS result.

Fig. 3. Variation de Σ^+ avec $\tilde{c}$ dans la DNS (-o-) et les prédictions du modèle. La taille des barres verticales correspond à deux écarts–types pour les résultats obtenus par DNS.

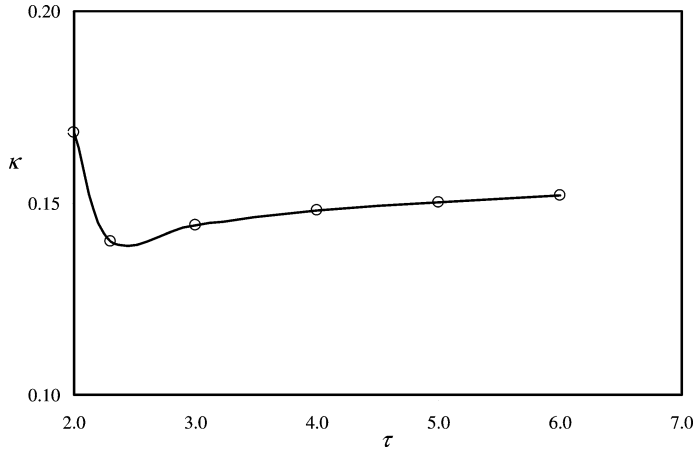

Fig. 4. Variation of κ, defined by Eq. (13), with τ.

Fig. 4. Variation de κ, défini par l'Éq. (13), avec τ.

deviation in Σ^+ observed in the DNS results. The values of normalised flame surface density predicted by the three models are also shown in Fig. 3. It is important to note that only the one fourth of the predicted values are shown in Fig. 3 for VV and BP models. It is clear that these models over predict the DNS results. A value of $K = 1$ is used for BP model given in Eq. (11). For the model obtained here, see Eq. (9), the values of model constants given in [5] are used and its prediction is very good. The values of these constants are $C_D = 0.05$, $C_{D_c} = 0.24$, $C_{\varepsilon_c} = 0.1$ and $C_m = 0.7$. The value of C_D is obtained from the DNS as explained in [5].

As one can see in Fig. 3, including the effects of dilatation and flame propagation is important. Since the flame propagation phenomenon depends on the Damköhler and Karlovitz numbers, it is possible that some of the constants in the present model will have some dependence on them. As pointed out earlier, the constant related to dilatation is an important one and we explore its behavior next.

5.1. Scaling of K_c

We now consider the scaling of C_{D_c} which is the most important model parameter in Eq. (9). It is defined [5] as $4K_c/(2C_m - 1)\beta$ where

$$K_c = \frac{\delta_L^o}{s_L^o} \frac{\int_0^1 [\rho N(\nabla.u)]_L^o f(c)\,\mathrm{d}c}{\int_0^1 \omega_L^o f(c)\,\mathrm{d}c} \tag{12}$$

In the laminar flamelet burning regime the internal pdf $f(c)$ is inversely proportional to the gradient of c in a planar unstrained laminar flame. Thus, $f(c) = C_1/y$, where y is the gradient of c normalised using the Zeldovich flame thickness, $\delta \equiv \alpha_u/s_l^o$. Also, $\nabla \cdot \mathbf{u} = \tau s_L^o y/\delta$ and $\int \omega f\,\mathrm{d}c = \rho_u s_L^o C_1$ in a planar laminar flame with a thermal thickness of δ_L^o. The scalar dissipation rate in the laminar flame can be written as $N = \alpha y^2/\delta^2$. Substituting these expression into Eq. (12) and assuming $\rho\alpha = \rho_u\alpha_u$, one gets

$$\frac{K_c}{\tau}\left(\frac{\delta}{\delta_L^o}\right)^2 = \frac{\delta}{\delta_L^o}\int_0^1 y^2\,\mathrm{d}c \equiv \kappa \tag{13}$$

where $C_1^{-1} = \int \mathrm{d}c/y$ and one should be cautious in obtaining C_1 because of the singularity at the cold and hot boundaries. Also, one can expect κ to be a weak function of τ. Fig. 4 shows the variation of κ with τ for activation energy parameter $\beta^* = \tau(T_a/T_b)/(1+\tau)$ of 6. The value of κ remains almost constant for meaningful values of τ. It is not surprising that K_c and hence also C_{D_c} are proportional to τ as these coefficients represent effects of dilatation which is zero when $\tau = 0$. However, the above modelling also suggests that K_c and C_{D_c} will be less sensitive to changes in the laminar flame and turbulence time scales and this remains to be explored.

6. Summary

The proposed transport equation for the flame surface density Σ is Eq. (7). The term containing K_c represents the influence of volume expansion due to heat release and, if this term is absent, Eq. (7) reduces to an equation previously summarised in [11]. The three dominant terms in Eq. (7) provide an algebraic approximation for Σ, namely Eq. (9), and this is shown to have features in common with earlier algebraic models [6,7], which describe effects of turbulence and spatial inhomogeneity. However, unlike these earlier models, Eq. (9) also includes terms describing influences due to volume expansion and flame propagation that are found to be essential in order to obtain agreement with the DNS data of Rutland and Cant [14]. Predictions from the new model depend crucially on a parameter, K_c, describing the influence of heat release which appears in the flame surface density equation and also in the algebraic closure for the flame surface density through the ratio C_D/C_{D_c}. The parameter K_c is shown to be proportional to the heat release parameter, τ. It is also shown that flame surface density scales with the laminar flame thermal thickness rather than the integral length scale of turbulence when combustion occurs in the flamelets regime.

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