Out of Equilibrium Dynamics

A simple strategy to model the effects of thermal expansion on turbulent transports in premixed flames

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A B S T R A C T

The transport of a reactive substance in a turbulent flow is important in many engineering settings. In turbulent reactive flows of premixed reactants, such a substance can exhibit complex dynamic behaviour associated with counter-gradient or non-gradient diffusion as well as flame-generated turbulence. Herein, simple algebraic models for the turbulent scalar flux and the turbulent kinetic energy have been derived, which avoid any resort to the classical – but complicated – set of second order transport equations. The various contributions appearing in these models and depending on the flamelets orientation have been analysed and expressed in closed forms. Comparisons are performed with DNS data of planar turbulent premixed flames for three distinct values of the normalised heat release. The obtained results clearly validate the relevance of the proposed algebraic closure.

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1. Introduction

The complex interaction phenomena involved in turbulent premixed combustion require strong modelling efforts in order to propose relevant closed expressions for the mean chemical rate $\overline{\omega}_c$ and turbulent transport terms $\overline{\rho \boldsymbol{u}'' c''}$ and $\overline{\rho \boldsymbol{u}'' \boldsymbol{u}''}$ appearing in the Favre averaged transport equations for the progress variable, i.e. $\tilde{c} = \overline{\rho c}/\overline{\rho}$ and velocity field $\tilde{\boldsymbol{u}} = \overline{\rho \boldsymbol{u}}/\overline{\rho}$:

$$\frac{\partial \overline{\rho}\tilde{c}}{\partial t} + \nabla \cdot \overline{\rho}\tilde{\boldsymbol{u}}\tilde{c} = \nabla \cdot \left(\overline{\boldsymbol{F_c}} - \overline{\rho \boldsymbol{u}'' c''} \right) + \overline{\omega}_c \tag{1}$$

$$\frac{\partial \overline{\rho}\tilde{\boldsymbol{u}}}{\partial t} + \nabla \cdot \overline{\rho}\tilde{\boldsymbol{u}}\tilde{\boldsymbol{u}} = \nabla \cdot \left(\overline{\boldsymbol{T_u}} - \overline{\rho \boldsymbol{u}'' \boldsymbol{u}''} \right) - \nabla \overline{p} \tag{2}$$

In Eqs. (1) and (2) ρ, $\boldsymbol{u}$, $\boldsymbol{F_c}$, $\boldsymbol{T_u}$ and p are respectively density, flow velocity, molecular diffusion flux of c, the viscous stress tensor and pressure. In second order models, equations for the scalar and the Reynolds fluxes, i.e. $\overline{\rho \boldsymbol{u}'' c''}$ and $\overline{\rho \boldsymbol{u}'' \boldsymbol{u}''}$, introduced by Eqs. (1) and (2) can be closed by assuming a partitioning into flamelet and non-flamelet contributions. However, such a strategy leads to rather complicated final partial differential equations difficult to use for practical applications. Accordingly, the objective of the present work is to propose a fully closed algebraic model for both turbulent transport terms $\overline{\rho \boldsymbol{u}'' c''}$ and $\overline{\rho \boldsymbol{u}'' \boldsymbol{u}''}$ taking into account the thermal expansion induced by chemical reactions and easy to handle once introduced in a CFD code.

With this objective in mind, the present study is based on a description of the velocity field as made of two contributions as described in our previous analyses [1], used to build algebraic models for the fluxes able to represent the full interaction process between turbulence and premixed flames. The velocity field is expressed as the direct sum of two contributions, with one being specifically related to the flamelets induced thermal expansion, a mechanism characterised by a small but

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finite thickness. As shown recently by Robin et al. [1] such a description leads to the identification of effects due solely to thermal expansion in contrast with those due to the existence of local propagating flamelets whose surface is modified by turbulence. The corresponding analysis makes use of an assumed disparity between two scales: one associated with the wrinkling of the flame, which affects the flame geometry at the largest scales, and the other associated with its local thickness considered as vanishingly small.[1] Nevertheless, this new strategy introduces orientation functions that must be properly related to known quantities before they can be used to provide a full closure for the turbulent transport terms.

Principles of the analysis denoted hereafter as the *velocity splitting procedure* are recalled in the first section of the paper. Then, closure models for the orientation functions are provided and validated on DNS databases. Eventually, new models are provided for the terms representing turbulent transport, i.e., scalar flux $\overline{\rho \boldsymbol{u}'' c''}$ and Reynolds stresses components $\overline{\rho \boldsymbol{u}'' \boldsymbol{u}''}$. These terms are related only to classical known quantities and are validated against DNS database.

2. Splitting of the velocity field

We consider here the flamelet regime of turbulent combustion where a turbulent flame is thought as a collection of local reactive interfaces that retain their identifiable laminar flame structure, i.e., the laminar propagating velocity S_L and the laminar flame thickness δ_L. Moreover, using the progress variable c, and considering a low Mach number description of the flow, lead to the well-known equation of state $\rho_f = \rho(1 + \tau c)$, where $\tau = \rho_f/\rho_b - 1$ is the expansion factor, ρ_f and ρ_b denote the density of fresh reactants and combustion products respectively. Then, the increase of velocity associated with thermal expansion through the local flame front, τS_L, is referred to as the *direct thermal expansion effect*. Furthermore, turbulent motions increasing the flame surface are called the *indirect thermal expansion effect* [1]. Accordingly, we consider that these two contributions of thermal expansion can be treated separately so that the total velocity vector $\boldsymbol{u}$ is split as follows [1]:

$$\boldsymbol{u} = \boldsymbol{v} + \boldsymbol{w} \tag{3}$$

where $\boldsymbol{w} = \boldsymbol{m_w}(\tau S_L c + w_0)$ is the velocity field resulting from the acceleration induced by a local flame front (*direct effect*) and $\boldsymbol{v}$ represents the turbulent motion and its consequences on the flame surface (*indirect effect*). The quantity w_0 is a constant that denotes the value of $\boldsymbol{w}$ in the unburned mixture, which is set to be vanishingly small. Finally $\boldsymbol{m_w}$ is the unit vector that characterises the orientation of the acceleration field induced by thermal expansion through the local laminar flames.

The simple relation (3) leads to the following expressions for the turbulent transport terms:

$$\overline{\rho \boldsymbol{u}'' c''} = \overline{\rho \boldsymbol{v}'' c''} + \overline{\rho \boldsymbol{w}'' c''} \tag{4}$$

$$\overline{\rho \boldsymbol{u}'' \boldsymbol{u}''} = \overline{\rho \boldsymbol{v}'' \boldsymbol{v}''} + \overline{\rho \boldsymbol{w}'' \boldsymbol{w}''} + \overline{\rho \boldsymbol{v}'' \boldsymbol{w}''} + \overline{\rho \boldsymbol{w}'' \boldsymbol{v}''} \tag{5}$$

involving contributions related to: (i) turbulence and its *indirect thermal expansion effects*; (ii) local heat release or *direct thermal expansion effect*, and (iii) heat release–turbulence interactions. Eq. (5) leads to the following expression of the turbulent kinetic energy $\overline{\rho k}$:

$$\overline{\rho k} = \frac{1}{2} \overline{\rho \boldsymbol{u}'' \cdot \boldsymbol{u}''} = \overline{\rho k}_{\boldsymbol{v}} + \overline{\rho k}_{\boldsymbol{w}} + 2 \overline{\rho k}_{\boldsymbol{vw}} \tag{6}$$

The splitting procedure and the introduction of $\overline{\rho k}_{\boldsymbol{v}}$ allow one to filter the direct effect of thermal expansion on the turbulent kinetic energy $\overline{\rho k}$. This latter quantity can be calculated afterwards thanks to relation (6). Prior to this, $\overline{\rho k}_{\boldsymbol{v}}$ is solved by a specific transport equation and $\overline{\rho \boldsymbol{v}'' c''}$ is closed following the proposition of Robin et al. [1,3]. Therefore, the only unknown contributions in Eqs. (4) and (6) are those related to the velocity field $\boldsymbol{w}$.

Using Eq. (3) and the definition of the velocity field $\boldsymbol{w}$ lead to the following expression for the flux $\overline{\rho \boldsymbol{w}'' c''}$ and the two contributions $\overline{\rho k}_{\boldsymbol{w}}$ and $\overline{\rho k}_{\boldsymbol{vw}}$:

$$\overline{\rho \boldsymbol{w}'' c''} = \tau S_L \left(\widetilde{\boldsymbol{m}} \overline{\rho c''^2} + \tilde{c} \overline{\rho c'' \boldsymbol{m}''} + \overline{\rho c''^2 \boldsymbol{m}''} \right) \tag{7}$$

$$\overline{\rho k}_{\boldsymbol{w}} = \frac{1}{2} (\tau S_L)^2 \left[\overline{\rho c''^2} + \overline{\rho} \, \tilde{c}^2 \widetilde{\boldsymbol{m}'' \cdot \boldsymbol{m}''} - \overline{\rho c'' \boldsymbol{m}''} \cdot \left(\widetilde{c'' \boldsymbol{m}''} + 2 \tilde{c} \widetilde{\boldsymbol{m}} \right) \right] \tag{8}$$

$$\overline{\rho k}_{\boldsymbol{vw}} = \frac{1}{2} \tau S_L \left[\overline{\rho \boldsymbol{v}'' c''} \cdot \widetilde{\boldsymbol{m}} + \tilde{c} \, \overline{\rho \boldsymbol{v}'' \cdot \boldsymbol{m}''} + \overline{\rho \boldsymbol{v}'' \cdot \boldsymbol{m}'' c''} \right] \tag{9}$$

These turbulent transport terms are related to classical known mean quantities as the mean progress variable and its variance but they also involve terms where the orientation vector $\widetilde{\boldsymbol{m}}$ appears. The objective of the present contribution is to propose closure relations for these terms depending on the orientation vector $\boldsymbol{m}$.

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[1] The readers are referred to the reference work of Clavin and Williams [2] for further details about premixed flames in large scale turbulence.

Table 1
Characteristics of the direct numerical simulation databases.

	τ	S_L (m/s)	δ_L (mm)	u'/S_L	l_T/δ_L	Re_T	Da	Ka
Case H	6.5	0.60	0.22	0.88	15.9	95.5	18.1	0.54
Case M	4.0	0.52	0.19	1.01	18.0	95.5	17.8	0.55
Case L	1.5	0.42	0.16	1.26	21.8	95.5	17.3	0.56

3. DNS databases

To validate the proposed closed form of the turbulent fluxes introduced by Eqs. (7), (8) and (9) we use the DNS database gathered by Nishiki, see for instance [4], that provides calculation of premixed flames for three different values of the thermal expansion factor τ, namely $\tau = 1.5$, $\tau = 4.0$, and $\tau = 6.5$. In these simulations, a single-step irreversible chemical reaction is considered, while the turbulent intensity is comparable to the laminar burning velocity, see Table 1. The Reynolds number based on the integral scale is $Re_T = 95.5$ for the three databases and the resolution is $512 \times 128 \times 128$. The numerical methodology relies on a spectral collocation method for directions x_2 and x_3, whereas a sixth order central finite differences scheme has been used along the direction x_1. A third order Runge–Kutta scheme has been retained for time integration. Main conditions are summarised in Table 1.

These simulations correspond to turbulent flame brush propagating along the direction x_1 and an ensemble averaging is performed by slicing the DNS data in planes normal to the direction of the mean planar flame propagation, i.e. in the (x_2, x_3) planes.[2]

In the following sections profiles of turbulent quantities that vary in both reactive and non-reactive regions of the flow, i.e. the turbulent kinetic energy $\overline{\rho k}$ and orientation functions $\widetilde{\boldsymbol{m}}$ and $\widetilde{\boldsymbol{m}''\boldsymbol{m}''}$, will be given as functions of the physical x_1-direction while profiles of quantities that vary only in the reactive regions of the flow, i.e. scalar turbulent fluxes $\overline{\rho \boldsymbol{u}''c''}$ and cross correlations between c and $\boldsymbol{m}$, will be given as functions of the mean progress variable.

4. Orientation functions

Orientation functions are commonly used in turbulent combustion modelling by considering the mean and fluctuating components of the normal vector $\boldsymbol{n} = -\nabla c/\|\nabla c\|$. As this vector is defined only within the reaction zone, the averaging process is conditioned on a given value of the progress variable $c \in \,]0 : 1[$ retained to identify the flame surface location. Following this, different closure assumptions have been proposed for the mean part $\langle \boldsymbol{n} \rangle_s = \overline{\boldsymbol{n}\Sigma}/\overline{\Sigma}$ and the orientation factors $\langle \boldsymbol{nn} \rangle_s = \overline{\boldsymbol{nn}\Sigma}/\overline{\Sigma}$, where the operator $\langle . \rangle_s$ refers to surface average quantities. The norm of $\boldsymbol{n}$ is unity but as its direction fluctuates the norm of $\langle \boldsymbol{n} \rangle_s$ is not unity. The geometrical property of the unit vector $\boldsymbol{n}$ leads to the exact relation: $\langle \boldsymbol{n} \rangle_s \overline{\Sigma} = -\nabla \bar{c}$ [6], where $\overline{\Sigma} = \overline{\|\nabla c\|}$ is the mean flame surface density. It should be noticed that $\langle \boldsymbol{n} \rangle_s$ has the same direction as $\nabla \bar{c}$ so that introducing a wrinkling factor $\varXi = \overline{\Sigma}/\|\nabla \bar{c}\|$ leads to the following relationship:

$$\langle \boldsymbol{n} \rangle_s = -\frac{1}{\varXi}\frac{\nabla \bar{c}}{\|\nabla \bar{c}\|} \tag{10}$$

Then, the mean part $\langle \boldsymbol{n} \rangle_s$ is obtained from the closure retained for the mean chemical rate which can be written as $\overline{\omega} = \rho_f S_L \varXi \|\nabla \bar{c}\| - \nabla \cdot \overline{\boldsymbol{F_c}}$ where $\boldsymbol{F_c} = \rho D \nabla c$. However, some difficulties remain for the orientation factors $\langle \boldsymbol{nn} \rangle_s$ which still require closure models [6–8].

One of the advantages of the description of the velocity field proposed here is that the velocity $\boldsymbol{w}$ and so its unit orientation vector $\boldsymbol{m} = \boldsymbol{w}/\|\boldsymbol{w}\|$, introduced above, are defined everywhere in the flow. As a consequence, a classical Favre averaging process can be applied to the unit vector $\boldsymbol{m}$ and the quantities of interest can be defined in terms of the mean part $\widetilde{\boldsymbol{m}}$ and the orientation factors $\widetilde{\boldsymbol{m}''\boldsymbol{m}''}$. However, the geometrical properties of $\boldsymbol{m}$ do not provide exact relation similar to Eq. (10). In the direct numerical simulation database used in this study, the flame brush is planar and normal to the incoming flow so that the directions of the mean vectors $\widetilde{\boldsymbol{m}}$, $\widetilde{\boldsymbol{u}}$, $\widetilde{\boldsymbol{v}}$, $\widetilde{\boldsymbol{w}}$, and $\nabla \bar{c}$ are the same:

$$\frac{\widetilde{\boldsymbol{m}}}{\|\widetilde{\boldsymbol{m}}\|} = \frac{\widetilde{\boldsymbol{w}}}{\|\widetilde{\boldsymbol{w}}\|} = \frac{\widetilde{\boldsymbol{u}}}{\|\widetilde{\boldsymbol{u}}\|} = \frac{\widetilde{\boldsymbol{v}}}{\|\widetilde{\boldsymbol{v}}\|} = \frac{\nabla \tilde{c}}{\|\nabla \tilde{c}\|} = \boldsymbol{m}_{\tilde{c}} \tag{11}$$

It must be noticed at this point that the Reynolds averaging process leads to the same conclusions so that, in the case investigated here, we can write $\nabla \bar{c}/\|\nabla \bar{c}\| = \nabla \tilde{c}/\|\nabla \tilde{c}\|$. Consequently, we choose to express the mean orientation vector as:

$$\widetilde{\boldsymbol{m}} = \lambda \boldsymbol{m}_{\tilde{c}} \tag{12}$$

where $\lambda = \|\widetilde{\boldsymbol{m}}\|$ is a scalar parameter that characterises the fluctuations of orientation. In the absence of any fluctuations, i.e. in the case of planar and laminar flame, we have $\lambda = 1$, whereas λ vanishes if the fluctuations of $\boldsymbol{m}$ are isotropically distributed ($\|\widetilde{\boldsymbol{m}}\| = 0$). It should be also noticed that it is not possible to obtain $\|\widetilde{\boldsymbol{m}}\| = 0$ for a propagating flame brush.

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[2] Complementary details concerning this set of DNS databases can be found in Refs. [1,4,5].
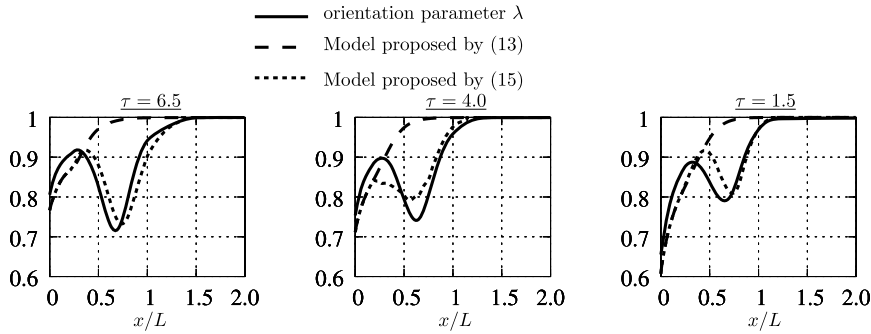
Fig. 1. Comparison between the orientation parameter λ and the models proposed by (13) and (15) for three distinct values of the expansion factor $\tau = 6.5$ (left), $\tau = 4.0$ (middle), and $\tau = 1.5$ (right).

The orientation parameter λ must be modelled carefully since it is a key factor in the whole description of the flow presented herein. Considering the BML analysis based on the existence of a quasi-bimodal PDF of the progress variable c, we can write $\widetilde{\boldsymbol{m}} = (1-\tilde{c})\overline{\boldsymbol{m}}_f + \tilde{c}\overline{\boldsymbol{m}}_b$. In the case investigated here, the directions of the mean vectors are all the same so that $\lambda = (1-\tilde{c})\lambda_f + \tilde{c}\lambda_b$, where $\lambda_f = \|\overline{\boldsymbol{m}}_f\|$ and $\lambda_b = \|\overline{\boldsymbol{m}}_b\|$ are the conditional orientation parameters and the subscripts f and b stand for fresh and burnt gases respectively. On the colder side of the flame brush where there is a very small amount of burnt gases, we consider that the *indirect thermal expansion effect* has not yet affected the velocity orientation conditioned in burnt gases so that the fluctuations of velocity orientation in fresh and burnt gases are nearly the same: $\lambda_b \approx \lambda_f$. However, on the burnt gas side of the flame brush the *indirect thermal expansion effect* in burnt gases is maximum and may even lead to a re-orientation of all the velocity vectors in the same direction so that λ_b may reach unity. Consequently, we conclude that λ_b is a function of the mean progress variable and we propose the following relation: $\lambda_b = \lambda_f + (1-\lambda_f)f_1(\tilde{c})$, where $f_1(\tilde{c}) = C_2 \tilde{c}^{\theta}$ and $0 < f_1 < 1$. Thus, we obtain:

$$\lambda = \lambda_f + \tilde{c}(1-\lambda_f)f_1 \tag{13}$$

The values of the model constants C_2 and θ are respectively zero and infinity in the case of very small values of the Bray number (cold flames) so that $f_1 = 0$ and $\lambda = \lambda_b = \lambda_f$ everywhere in the flow. On the contrary, in the limiting situation of very large values of the Bray number, the limiting values of C_2 and θ are respectively unity and zero so that $f_1 = 1$ and λ_b reaches unity everywhere in the flow. In this limiting case, the expansion effects are so strong that all the local velocity vectors in burnt gases have the same direction, namely the mean direction. In the DNS cases considered in the present paper, the values of the Bray number are not small and we retain $C_2 = 0.95$ and $\theta = 0.4$.

Relation (13) provides a useful expression for the orientation parameter λ from the orientation parameter conditioned in fresh gases λ_f. Then, we can only consider the behaviour λ_f conditioned in a non-reactive region of the flow. Thus, in a non-reactive flow $\lambda_f = \lambda = \|\overline{\boldsymbol{m}}\|$. Considering now the definition of $\boldsymbol{m}$ used in our previous study [1], i.e. $\boldsymbol{m} = \boldsymbol{u}/\|\boldsymbol{u}\|$ outside local flames and using the following assumption: $\overline{\boldsymbol{u}/\|\boldsymbol{u}\|} \approx \overline{\boldsymbol{u}}/\|\overline{\boldsymbol{u}}\|$. Accordingly, if $\bar{k} \ll \overline{\boldsymbol{u}} \cdot \overline{\boldsymbol{u}}$, the first order expansion of $\overline{\|\boldsymbol{u}\|}/\|\overline{\boldsymbol{u}}\|$ gives: $1 + \bar{k}/\overline{\boldsymbol{u}} \cdot \overline{\boldsymbol{u}}$, and in non-reactive flow we obtain: $\lambda \approx (1 + \bar{k}/\overline{\boldsymbol{u}} \cdot \overline{\boldsymbol{u}})^{-1}$. Finally, by analogy with this relation, and since $\boldsymbol{u} = \boldsymbol{v}$ in the fresh reactants we propose the following closure for the orientation parameter conditioned in fresh gases:

$$\lambda_f \approx (1 + \widetilde{k_{\boldsymbol{v}}}/\widetilde{\boldsymbol{u}} \cdot \widetilde{\boldsymbol{u}})^{-1} \tag{14}$$

The orientation parameter obtained through (13) and (14) is now compared to the orientation parameter extracted from the DNS databases, see Fig. 1. One can see that the proposed model leads to fairly satisfactory results in the non-reactive part of the flow (fresh reactants and burnt products) but overestimates the orientation parameter in the flame brush. The observed behaviour of the orientation parameter is the following: (i) in fresh reactants, the orientation parameter increases because the turbulent intensity decreases and thus leads to smaller orientation fluctuations; (ii) in the first part of the flame brush the orientation parameter decreases because the local flame orientation fluctuates more than the velocity orientation induced by turbulence, leading to an increase of the orientation fluctuations; (iii) in the second part of the flame brush the orientation parameter increases again because the velocity vectors are redirected by the *indirect thermal expansion* leading to a decrease of orientation fluctuations; (iv) in the burnt gases the orientation parameter reaches unity because all vectors have the same direction. The unity orientation parameter in burnt gases means that in the cases considered in this work all the vortices have been destroyed by thermal expansion. Consequently, the turbulence that still exists in burnt gases is only induced by the shear phenomenon. Moreover, as shown in Fig. 1, the decrease of the orientation parameter observed in the flame brush cannot be recovered using the bimodal PDF approximation. To improve this point we propose to introduce an inner PDF the shape of which is determined through the use of a laminar flamelet inner structure so that now $\widetilde{\boldsymbol{m}} = \alpha\overline{\boldsymbol{m}}_f + \beta\overline{\boldsymbol{m}}_b + \gamma\overline{\boldsymbol{m}}_i$, where subscript i denotes the inner structure of the local flames. Then, the orientation parameter expressed by (13) can be now written as:

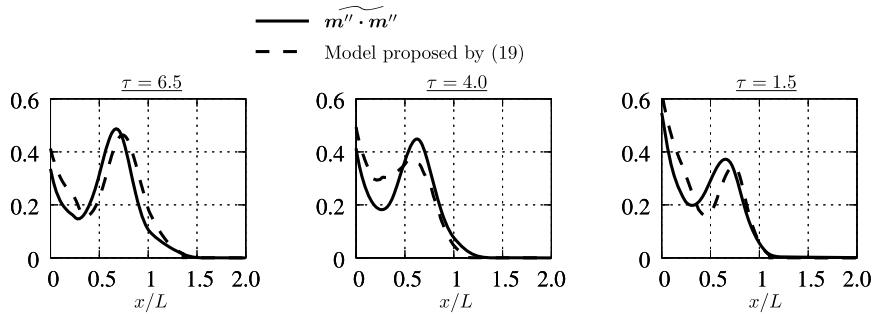$$\lambda = (1-\gamma)\lambda_f + \beta(1-\lambda_f)f_1 + \gamma\lambda_i \tag{15}$$

Fig. 2. Comparison between $\widetilde{m''\cdot m''}$ and the model proposed by (19) for three distinct values of the expansion factor $\tau = 6.5$ (left), $\tau = 4.0$ (middle), and $\tau = 1.5$ (right).

where the coefficients β and γ are related to the mean and variance of the progress variable by [9]:

$$\gamma = \frac{\tilde{c}(1-\tilde{c}) - \widetilde{c''^2}}{I_1 - I_2} \tag{16}$$

$$\beta = \tilde{c} - \gamma I_1 \tag{17}$$

The constant I_1 and I_2 are integral quantities that can be evaluated from flamelets properties. Following the methodology proposed by Bray et al. [9], we have evaluated $I_1 = 0.43$ and $I_2 = 0.28$ in all cases.

To model the orientation parameter conditioned inside the local flames we use again the thin flame hypothesis that leads to $\widetilde{m}_i = -\langle n \rangle_s$, so that the following relation is obtained:

$$\lambda_i = 1/\Xi = \|\nabla \bar{c}\|/\overline{\Sigma} \tag{18}$$

The flame surface density is evaluated from the DNS databases using: $\nabla \cdot \overline{F_c} + \overline{\omega} = \rho_f S_L \overline{\Sigma}$. Fig. 1 shows that the model given by (15) associated with (14) and (18) gives results in good agreement with DNS for all three values of the expansion factor τ.

We now focus our attention on the orientation tensor $\widetilde{m''m''}$. The trace of this tensor can be obtained analytically by making use of the properties of the unit vector m:

$$\widetilde{m'' \cdot m''} = (1 - \widetilde{m} \cdot \widetilde{m}) = 1 - \lambda^2 \tag{19}$$

Fig. 2 compares $\widetilde{m'' \cdot m''}$ extracted from the DNS databases to Eq. (19) where λ is modelled by (15). As (19) is obtained analytically, Fig. 2 leads to the same conclusions as those deduced from Fig. 1 and results are again very satisfactory.

However, (19) does not provide information about the anisotropy of the flow described by the orientation factors. We may assume that this anisotropy is directly related to the anisotropy of the velocity field v:

$$\widetilde{m''m''} = \frac{\widetilde{v}\widetilde{v} + \widetilde{v''v''}}{\widetilde{v}\cdot\widetilde{v} + 2\widetilde{k_v}} - \widetilde{m}\widetilde{m} \tag{20}$$

This assumption is similar to the one made previously by Mantel and Borghi [7] in their derivation of a closure for the scalar dissipation rate transport equation, namely $\langle nn \rangle_s = \widetilde{u''u''}/2k$. However these authors consider the anisotropy of the velocity field u instead of v. Moreover, the closure proposed by Mantel and Borghi [7] is probably even more adapted to our analysis because the anisotropy of the velocity field is defined everywhere in the flow, as is $\widetilde{m''m''}$, whereas $\langle nn \rangle_s$ is only defined within the flame brush.

The analytical relationships (7) and (8) also involve quantities related to the orientation: $\widetilde{c''m''}$ and $\widetilde{c''^2m''}$. For the sake of simplicity we consider only the bimodal PDF limit which yields:

$$\widetilde{c''m''} = \tilde{c}(1-\tilde{c})(\overline{m}_b - \overline{m}_f) \tag{21}$$

$$\widetilde{c''^2m''} = \tilde{c}(1-\tilde{c})(1-2\tilde{c})(\overline{m}_b - \overline{m}_f) \tag{22}$$

In the case of very low values of the Bray number, the effects of thermal expansion on the flow can be neglected so that c and m can be considered as statistically independent; thus $\overline{m}_f \approx \overline{m}_b$ and then $\widetilde{c''m''} = \widetilde{c''^2m''} \approx 0$. However, in the case investigated here, these correlations are not negligible, see [1]. This means that the expansion factor has a strong influence on the orientation of the velocity. By using (13), which is consistent with the bimodal PDF limit, we obtain:

$$(\overline{m}_b - \overline{m}_f) = \frac{1-\lambda}{f_1^{-1} - \tilde{c}}\, m_{\tilde{c}} \tag{23}$$

$$\text{———}\quad \tau S_L(\tilde{c}\,\overline{\rho c''m_1''} + \overline{\rho c''^2 m_1''})$$

$$\text{– – –}\quad \text{Model proposed by (24)}\times(\tau S_L)$$
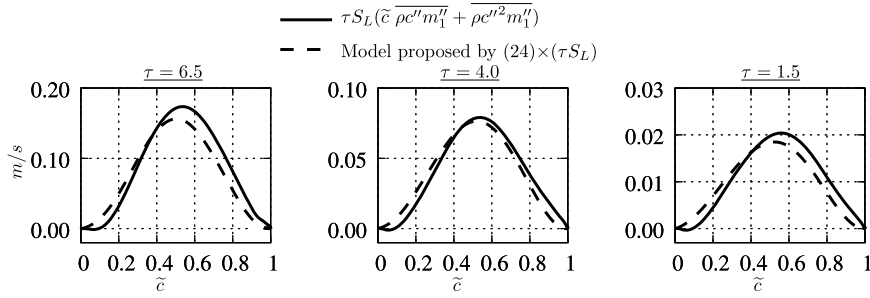

Fig. 3. Comparison between the cross correlations involved in (7) and the model proposed by (24) for three distinct values of the expansion factor $\tau = 6.5$ (left), $\tau = 4.0$ (middle), and $\tau = 1.5$ (right).
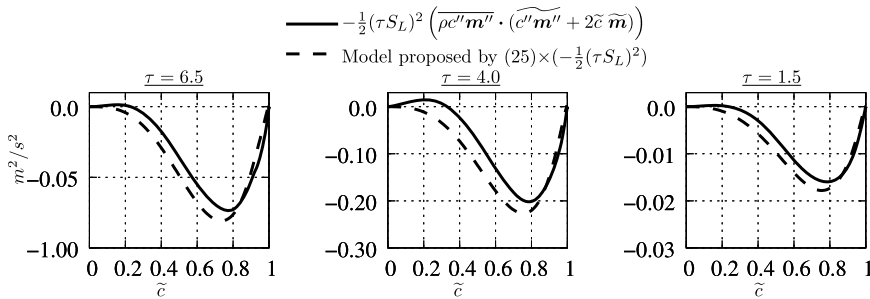
$$\text{———}\quad -\tfrac{1}{2}(\tau S_L)^2\left(\overline{\rho c''\boldsymbol{m}''}\cdot(\widetilde{c''\boldsymbol{m}''} + 2\tilde{c}\,\widetilde{\boldsymbol{m}})\right)$$

$$\text{– – –}\quad \text{Model proposed by (25)}\times(-\tfrac{1}{2}(\tau S_L)^2)$$

Fig. 4. Comparison between the cross correlations involved in (8) and the model proposed by (25) for three distinct values of the expansion factor $\tau = 6.5$ (left), $\tau = 4.0$ (middle), and $\tau = 1.5$ (right).

Finally, the cross correlations involved in (7) and (8) write:

$$\tilde{c}\,\overline{\rho c''\boldsymbol{m}''} + \overline{\rho c''^2\boldsymbol{m}''} = \bar{\rho}\frac{\tilde{c}(1-\tilde{c})^2}{f_1^{-1}-\tilde{c}}(1-\lambda)\,\boldsymbol{m}_{\tilde{c}} \tag{24}$$

$$\overline{\rho c''\boldsymbol{m}''}\cdot(\widetilde{c''\boldsymbol{m}''} + 2\tilde{c}\widetilde{\boldsymbol{m}}) = \bar{\rho}\frac{\tilde{c}(1-\tilde{c})}{f_1^{-1}-\tilde{c}}(1-\lambda)\left(\frac{\tilde{c}(1-\tilde{c})}{f_1^{-1}-\tilde{c}}(1-\lambda) + 2\tilde{c}\lambda\right) \tag{25}$$

Figs. 3 and 4 show that a very good agreement is obtained between the model proposed by (24) and (25) with the same terms evaluated from the DNS database, for the three values of τ. To perform this comparison λ is evaluated from (12). It is important to notice that the same set of constants, i.e. $C_2 = 0.95$ and $\theta = 0.4$, is used for the three distinct cases under consideration.

5. Algebraic models for the scalar flux and turbulent kinetic energy

When using the velocity splitting procedure introduced by (3), the objective is not only to analyse in detail the physical mechanisms associated with thermal expansion as previously done in details in Ref. [1], but also to propose simplified strategies to describe them in closed form as proposed herein. The corresponding strategies make use of the relationship that exists between the velocity field $\boldsymbol{w}$ and the progress variable. This relationship allows one to relate the average and fluctuating velocity fields to the mean value of the progress variable thus favouring the obtention of algebraic closures for the unknown terms that involve the velocity field $\boldsymbol{w}$. In this respect, the objective of this last section is to assess the models introduced in previous sections by evaluating the turbulent transports of mass $\overline{\rho\boldsymbol{u}''c''}$ and momentum *via* $\overline{\rho k}$. Accordingly, the modelling of these terms must be related to known or resolved mean quantities. In the present modelling strategy based on the velocity splitting procedure, we consider that the following mean quantities are solved by their transport equation: the mean density $\bar{\rho}$, the total mean velocity $\tilde{\boldsymbol{u}}$, the mean scalar variable $\tilde{c}$ and the turbulent kinetic energy $\overline{\rho k_{\boldsymbol{v}}}$ related to the velocity field $\boldsymbol{v}$. This velocity field does not take the *direct* thermal expansion effect into account so that classical non-reactive closures can be used for $\overline{\rho k_{\boldsymbol{v}}}$ transport equation. Moreover, we consider that the following mean quantities are calculated by other specific known models: the mean chemical rate $\bar{\omega}_c$ and the scalar variance $\overline{\rho c''^2}$. Eventually, in order to validate the proposed algebraic models for the turbulent transports of mass $\overline{\rho\boldsymbol{u}''c''}$ and turbulent kinetic energy $\overline{\rho k}$, only these classically known mean quantities ($\bar{\rho}$, $\tilde{\boldsymbol{u}}$, $\tilde{c}$, $\overline{\rho k_{\boldsymbol{v}}}$, $\bar{\omega}_c$ or Σ, $\overline{\rho c''^2}$) are extracted from the DNS databases.
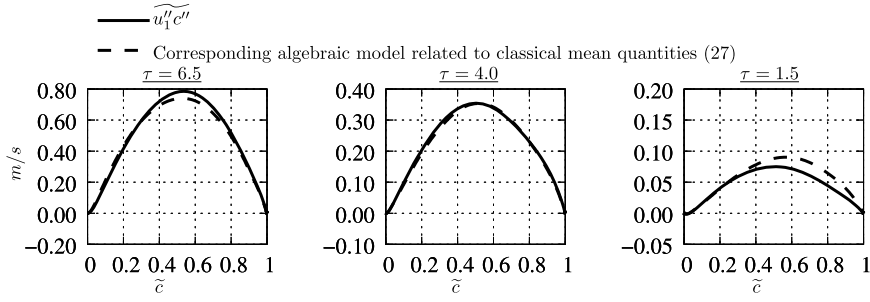
Fig. 5. Comparison between the scalar turbulent fluxes $\widetilde{u_1''c''}$ and the corresponding algebraic model only related to classical mean quantities $\widetilde{\boldsymbol{u}}$, $\tilde{c}$, $\overline{\rho c''^2}$, $\overline{\omega_c}$, $\overline{\rho k_{\boldsymbol{v}}}$ for three distinct values of the expansion factor $\tau = 6.5$ (left), $\tau = 4.0$ (middle), and $\tau = 1.5$ (right).
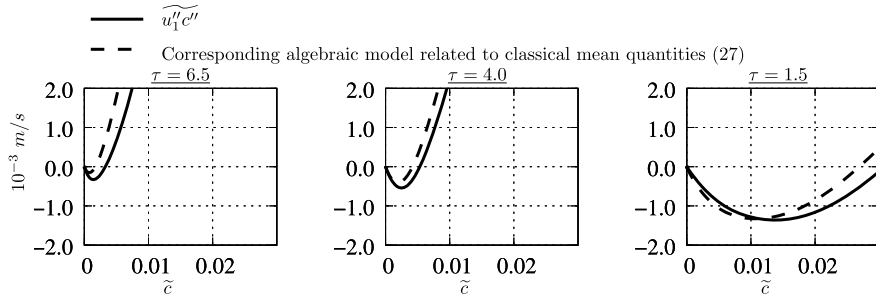

Fig. 6. Zoom of Fig. 5. Comparison between the scalar turbulent fluxes $\widetilde{u_1''c''}$ and the corresponding algebraic model only related to classical mean quantities $\widetilde{\boldsymbol{u}}$, $\tilde{c}$, $\overline{\rho c''^2}$, $\overline{\omega_c}$, $\overline{\rho k_{\boldsymbol{v}}}$ for three distinct values of the expansion factor $\tau = 6.5$ (left), $\tau = 4.0$ (middle), and $\tau = 1.5$ (right).

Turbulent transport of mass $\overline{\rho \boldsymbol{u}''c''}$ is first split using Eq. (4) where $\overline{\rho \boldsymbol{v}''c''}$ is given by the previous proposal of Robin et al. [1]:

$$\overline{\rho \boldsymbol{v}''c''} = \overline{\rho}\big(-\tilde{c}(1-\tilde{c})\sqrt{\tilde{k}_{\boldsymbol{v}}} + C_{ae}\tau S_L \tilde{c}\overline{\rho c''^2}\big)\boldsymbol{m}_{\tilde{c}} \tag{26}$$

where the effects of turbulent motions (first term of the right-hand side) as well as the effects of the indirect thermal expansion (second term of the right-hand side) are taken into account. The model constant C_{ae} has been assigned the same value 0.45 in all cases [1]. The turbulent flux $\overline{\rho \boldsymbol{w}''c''}$ is obtained thanks to (7) where the mean orientation vector $\widetilde{\boldsymbol{m}}$ and the cross correlations are modelled through Eqs. (12) and (24) so that the final algebraic closure for the turbulent transport of mass is:

$$\overline{\rho \boldsymbol{u}''c''} = \overline{\rho}\left[-\tilde{c}(1-\tilde{c})\sqrt{\tilde{k}_{\boldsymbol{v}}} + \tau S_L\left(C_{ae}\tilde{c}\overline{\rho c''^2} + \lambda\overline{\rho c''^2} + \overline{\rho}\frac{\tilde{c}(1-\tilde{c})^2}{(C_2\tilde{c}^\theta)^{-1} - \tilde{c}}(1-\lambda)\right)\right]\boldsymbol{m}_{\tilde{c}} \tag{27}$$

with

$$\lambda = (1-\gamma)(1+\tilde{k}_{\boldsymbol{v}}/\widetilde{\boldsymbol{u}}\cdot\widetilde{\boldsymbol{u}})^{-1} + (\tilde{c} - \gamma I_1)\big(1 - (1+\tilde{k}_{\boldsymbol{v}}/\widetilde{\boldsymbol{u}}\cdot\widetilde{\boldsymbol{u}})^{-1}\big)(C_2\tilde{c}^\theta) + \gamma\|\nabla\bar{c}\|/\Sigma \tag{28}$$

Eq. (16) is used to calculate γ from known quantities and the parameters are all set constant for all databases: $C_{ae} = 0.45$, $C_2 = 0.95$, $\theta = 0.4$, $I_1 = 0.43$, $I_2 = 0.28$.

Then $\overline{\rho \boldsymbol{u}''c''}$ is compared to its value calculated from DNS data. Results are shown in Figs. 5 and 6 and it can be seen that an excellent agreement is achieved, even on the fresh gas side where the turbulent fluxes $\overline{\rho \boldsymbol{u}''c''}$ become negative. In particular, the size of the gradient-like diffusion zone on the fresh gas side is very well evaluated by the model, for the three values of the expansion factor τ. Inside the flame brush, approximately at $\tilde{c} = 0.6$, the turbulent fluxes are slightly underestimated for the largest value of the expansion factor whereas they are slightly overestimated for the smallest value.

The same strategy is used to validate the model for the turbulent kinetic energy $\overline{\rho k}$ which is split by using Eq. (6). The turbulent kinetic energy $\overline{\rho k_{\boldsymbol{v}}}$ is extracted from the DNS database because it is supposed to be solved in practical numerical simulations. The two other contributions of the turbulent kinetic energy, i.e. $\overline{\rho k_{\boldsymbol{w}}}$ and $\overline{\rho k_{\boldsymbol{vw}}}$, are calculated thanks to Eqs. (8) and (9) where the cross correlations between $\boldsymbol{m}$ and $\boldsymbol{v}$ have been neglected whereas the cross correlations between $\boldsymbol{m}$ and c are modelled from (25) and the scalar turbulent flux $\overline{\rho \boldsymbol{v}''c''}$ is modelled from (26). The final algebraic closure for the turbulent kinetic energy is:
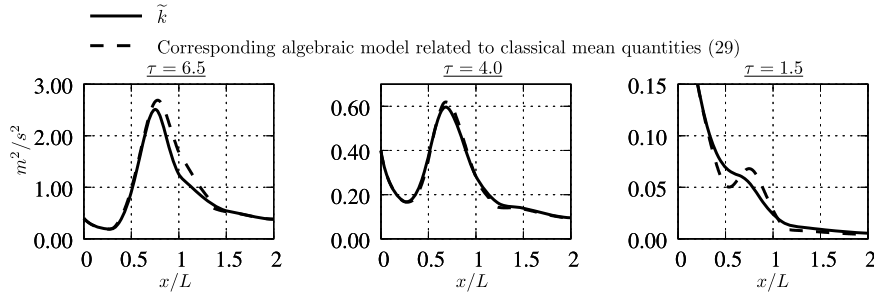
Fig. 7. Comparison between the turbulent kinetic energy $\widetilde{k}$ and the corresponding algebraic model only related to classical mean quantities $\widetilde{\boldsymbol{u}}$, $\tilde{c}$, $\overline{\rho c''^2}$, $\overline{\omega_c}$, $\overline{\rho k_{\boldsymbol{v}}}$ for three distinct values of the expansion factor $\tau = 6.5$ (left), $\tau = 4.0$ (middle), and $\tau = 1.5$ (right).

$$\overline{\rho k} = \overline{\rho k_{\boldsymbol{v}}} + \frac{1}{2}(\tau S_L)^2 \left[\overline{\rho c''^2} + \overline{\rho}\tilde{c}^2\left(1 - \lambda^2\right) - \overline{\rho}\frac{\tilde{c}(1-\tilde{c})}{(C_2\tilde{c}^\theta)^{-1} - \tilde{c}}(1-\lambda)\left(\frac{\tilde{c}(1-\tilde{c})}{(C_2\tilde{c}^\theta)^{-1} - \tilde{c}}(1-\lambda) + 2\tilde{c}\lambda \right) \right]$$
$$+ \tau S_L \lambda \overline{\rho}\left(-\tilde{c}(1-\tilde{c})\sqrt{\widetilde{k_{\boldsymbol{v}}}} + C_{ae}\tau S_L \tilde{c}\,\overline{\rho c''^2} \right) \tag{29}$$

The model is compared to $\overline{\rho k}$ extracted from the DNS databases in Fig. 7. Once again very good results are obtained for the three values of the expansion factor despite a slight overestimation by the model of the maximum of turbulence within the flame brush for the smallest value of the expansion factor $\tau = 1.5$. This discrepancy is to be related to the overestimation of the flux $\overline{\rho \boldsymbol{v}''c''}$ given by (26), see [1].

6. Conclusion

Simple algebraic expressions describing the turbulent scalar flux and the turbulent kinetic energy have been derived by using a specific velocity splitting procedure. The various contributions appearing in these models and depending on the flamelets orientations have been analysed and expressed in closed forms. These models have been validated through comparisons with DNS data of three premixed flames characterised by different rates of heat release.

Acknowledgements

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