Towards the development of an evolution equation for flame turbulence interaction in premixed turbulent combustion

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Abstract Flame turbulence interaction is one of the leading order terms in the scalar dissipation ($\tilde{\epsilon}_c$) transport equation [35] and is thus an important phenomenon in premixed turbulent combustion. Swaminathan and Grout [36] and Chakraborty and Swaminathan [15, 16] have shown that the effect of strain rate on the transport of $\tilde{\epsilon}_c$ is dominated by the interaction between the fluctuating scalar gradients and the fluctuating strain rate, denoted here by $\bar{\rho}\tilde{\Delta}_c = \overline{\rho\alpha\nabla c''S_{ij}''\nabla c''}$; this represents the flame turbulence interaction. In order to obtain an accurate representation of this phenomenon, a new evolution equation for $\tilde{\Delta}_c$ has been proposed. This equation gives a detailed insight into flame turbulence interaction and

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provides an alternative approach to model the important physics represented by $\tilde{\Delta}_c$. The $\tilde{\Delta}_c$ evolution equation is derived in detail and an order of magnitude analysis is carried out to determine the leading order terms in the $\tilde{\Delta}_c$ evolution equation. The leading order terms are then studied using a Direct Numerical Simulation (DNS) of premixed turbulent flames in the corrugated flamelet regime. It is found that the behaviour of $\tilde{\Delta}_c$ is determined by the competition between the source terms (pressure gradient and the reaction rate), diffusion/dissipation processes, turbulent strain rate and the dilatation rate. Closures for the leading order terms in $\tilde{\Delta}_c$ evolution equation have been proposed and compared with the DNS data.

Keywords Flame turbulence interaction · Scalar turbulence interaction · Premixed turbulent combustion · Scalar dissipation

1 Introduction

In premixed turbulent combustion modelling, the closure for the reaction rate is challenging. The problem can be simplified under the thin flamelet assumption, according to which the reaction zone is assumed to be thin compared to the Kolmogorov length scale [7]. In the flamelet approach it is assumed that the flame consists of a very thin sheet, and its local structure is the same as that of a laminar flame [8,9]. A laminar flamelet consists of a thin and highly wrinkled interface separating products from reactants. This interface contains all the effects of the combustion chemistry associated with heat release and all of the related molecular transport effects, thus making it possible to decouple the chemistry from the turbulence. The thin flamelet assumption makes it possible to approximate the probability density function (pdf) of a reaction progress variable (c) (usually defined as a normalised product mass fraction Y), through a double delta function, representing the unburnt and burnt mixtures [8]. This approximation leads to simple closures for the turbulent transport and the

reaction rate. Usually in engineering applications, a transport equation for the Favre averaged progress variable $\tilde{c}$ is solved. The transport equation for $\tilde{c}$ requires closures for mean reaction rate $(\bar{\omega}_c)$ and the turbulent transport $(\widetilde{u''c''})$ of $\tilde{c}$. Several approaches to close the reaction rate are available in the literature, although two approaches are widely used under the thin flamelet assumption; the flame surface density (Σ) approach and the scalar dissipation ($\tilde{\epsilon}_c$) approach. Borghi has shown that Σ and $\tilde{\epsilon}_c$ are algebraically related to each other [4], thus representing the same physical phenomenon. In the Σ approach $\bar{\omega}_c$ is closed as [12]:

$$\bar{\omega}_c \simeq \Sigma \rho_u u_L^0 I_0, \quad (1)$$

where ρ_u is the density of the reactants, u_L^0 is the unstrained laminar flame speed, and I_0 represents a correction factor to account for strain rate and curvature effects on the local laminar flame speed [12]. In the $\tilde{\epsilon}_c$ approach $\bar{\omega}_c$ is usually closed as [6]:

$$\bar{\omega}_c \simeq \frac{2}{2C_m - 1} \bar{\rho} \tilde{\epsilon}_c, \quad (2)$$

where $\tilde{\epsilon}_c$ is the scalar dissipation, $\bar{\rho} \tilde{\epsilon}_c = \overline{\rho \alpha (\nabla c'' \nabla c'')}$ (double primes denote the Favre fluctuations), α represents the diffusivity of the progress variable and C_m is a model constant. Both Σ and $\tilde{\epsilon}_c$ transport equations have been developed in previous studies and details are available in [35, 12, 5, 13, 30, 10]. Here our aim is to develop an evolution equation for flame turbulence interaction, hence the scalar dissipation approach is only used from here onwards.

A transport equation for $\tilde{\epsilon}_c$ has been proposed by Swaminathan and Bray [35]:

$$\bar{\rho} \frac{D\tilde{\epsilon}_c}{Dt} = D_1 - D_2 + T_1 + T_2 + T_3 + T_4 \quad (3)$$

where the nomenclature of the right-hand side of Eq (3) reflects the most common usage [35, 15, 25]. Each of the terms in Eq. (3) represent a particular physical process; for example

$$T_3 = \underbrace{-2\bar{\rho}\bar{\alpha}\frac{\partial\bar{c}}{\partial x_i}\left(\frac{\partial\bar{c}''}{\partial x_j}\frac{\partial\bar{u}_i''}{\partial x_j}\right)}_{T_{31}} \underbrace{-2\bar{\rho}\bar{\alpha}\left(\frac{\partial\bar{c}''}{\partial x_i}\frac{\partial\bar{S}_{ij}''}{\partial x_j}\right)}_{T_{32}} \underbrace{-2\bar{\rho}\bar{\alpha}\left(\frac{\partial\bar{c}''}{\partial x_i}\frac{\partial\bar{c}''}{\partial x_j}\right)\bar{S}_{ij}}_{T_{33}} \quad (4)$$

represents the combined effects of flame turbulence interaction. In Eq. (4) $\bar{S}_{ij}''$ represents the fluctuating strain rate and is defined as $\bar{S}_{ij}'' = 0.5 \left(\partial\bar{u}_i''/\partial x_j + \partial\bar{u}_j''/\partial x_i \right)$.

An order of magnitude analysis (OMA) under joint assumptions of high turbulent Reynolds (Re_t) and Damköhler (Da) numbers shows term T_{32} to be of leading order [35]; the behaviour of T_3 is thus dominated by the behaviour of T_{32} [36].

The flame turbulence interaction phenomenon presents a major difficulty in obtaining an accurate closure for both the scalar dissipation ($\bar{\epsilon}_c$) and the flame surface density (Σ), and thus the mean reaction rate ($\bar{\omega}_c$). Here we present an alternative way for the prediction of flame turbulence interaction in premixed flames.

The paper is organised as follows: in the next section we derive the transport equation for flame turbulence interaction. The order of magnitude analysis is carried out in section 3. The details of the DNS data set are discussed in section 4 along with the data processing method followed in this study. The results are discussed in section 5 and the conclusions are summarised in the last section.

2 Flame turbulence interaction evolution equation

In the case of statistically multidimensional flames T_{32} can be decomposed using an eigen-decomposition and written as [25,27]:

$$T_{32} = -\overline{2\rho\alpha|\nabla c''|^2(e_\alpha\cos^2\theta_\alpha + e_\beta\cos^2\theta_\beta + e_\gamma\cos^2\theta_\gamma)}, \quad (5)$$

where e_α, e_β and e_γ are the eigenvalues of the turbulent strain rate tensor $\bar{S}_{ij}''$. The eigenvalues are ranked as $e_\alpha > e_\beta > e_\gamma$, with e_α being the most extensive principal strain rate and e_γ

being the most compressive principal strain rate. The angle between the scalar gradient and the eigenvector associated with e_α is denoted by θ_α . The source or sink behaviour of T_{32} is thus dependent on the statistics of the alignment between the scalar gradient and the directions of the principal strain rates [13, 25]. It is well known that in case of the cold turbulence, the scalar gradient preferentially aligns with the most compressive principal strain rate [2, 3], thus giving a source contribution from T_{32} . In case of flows with intense heat release, it has been shown by Chakraborty and Swaminathan [15], Swaminathan and Grout [36], Kim and Pitsch [24] and Hartung et al [22] that the scalar gradient preferentially aligns with the most extensive principal strain rate. The variation between the alignment characteristics is due to the competition between dilatation rate and turbulent strain rate [36]. In case of strong heat release, the dilatation mostly occurring in the local normal direction overcomes the turbulence effects thus causing the scalar gradient to align with the most extensive strain rate e_α [13, 24]; T_{32} becomes negative and dissipates the scalar gradient [13, 22, 24].

In order to capture the physical phenomenon mentioned above, an evolution equation for flame turbulence interaction can be used. In this section we derive the evolution equation in detail and do an order of magnitude analysis for the evolution equation. The evolution equation can be found by taking the total derivative of :

$$\rho \frac{D}{Dt} \left(\alpha \frac{\partial c}{\partial x_i} S_{ij} \frac{\partial c}{\partial x_j} \right), \quad (6)$$

where α is assumed to be constant to reduce the complexity of the problem. Applying the Reynolds decomposition to Eq. (6) and then Favre averaging leads to:

$$\begin{aligned}
\rho \frac{D}{Dt} \left(\alpha \frac{\partial c}{\partial x_i} S_{ij} \frac{\partial c}{\partial x_j} \right) &= \underbrace{\rho \alpha \frac{D}{Dt} \left(\frac{\partial c''}{\partial x_i} S_{ij}'' \frac{\partial c''}{\partial x_j} \right)}_{\text{Term 1}} + \underbrace{\rho \alpha \frac{D}{Dt} \left(\frac{\partial c''}{\partial x_i} \widetilde{S_{ij}} \frac{\partial c''}{\partial x_j} \right)}_{\text{Term 2}} \\
&+ \underbrace{\rho \alpha \frac{D}{Dt} \left(\frac{\partial \widetilde{c}}{\partial x_i} S_{ij}'' \frac{\partial c''}{\partial x_j} \right)}_{\text{Term 3}} + \underbrace{\rho \alpha \frac{D}{Dt} \left(\frac{\partial c''}{\partial x_i} S_{ij}'' \frac{\partial \widetilde{c}}{\partial x_j} \right)}_{\text{Term 4}} \\
&+ \underbrace{\rho \alpha \frac{D}{Dt} \left(\frac{\partial \widetilde{c}}{\partial x_i} \widetilde{S_{ij}} \frac{\partial \widetilde{c}}{\partial x_j} \right)}_{\text{Term 5}}
\end{aligned} \tag{7}$$

An order of magnitude analysis under the joint assumptions of high Re_l and Da (similar to that of Swaminathan and Bray [35]) is used to find the leading order terms in Eq. (7).

The order of magnitude analysis is carried out based on the following scaling arguments. The spatial derivatives are scaled by the integral length scale l_t . The ratio of the integral length scale l_t and the root mean square velocity u' is used to scale the time derivative. The density is scaled by the density of the reactants ρ_u . The mean velocities are scaled by a reference velocity u_{ref} . The thermal diffusivity of the mixture is scaled by the laminar flame scales $u_L^0 \delta_L^0$, where u_L^0 is the unstretched laminar flame speed and δ_L^0 is the laminar flame thermal thickness. The quantities involving or multiplied by the gradient of progress variable are also scaled with the laminar flame quantities.

According to the scaling arguments the terms in Eq. (7) scale as:

Term 1 :

$$\overline{\rho \alpha} \frac{\partial c''}{\partial x_i} \widetilde{S_{ij}''} \frac{\partial c''}{\partial x_j} \simeq \mathcal{O} \left(\rho_u \left(\frac{u_L^0}{\delta_L^0} \right)^2 ; 1 \right), \tag{8}$$

Term 2 :

$$\overline{\rho \alpha} \frac{\partial c''}{\partial x_i} \frac{\partial c''}{\partial x_j} \widetilde{S_{ij}} \simeq \mathcal{O} \left(\rho_u \left(\frac{u_L^0}{\delta_L^0} \right)^2 ; \left(\frac{u' Da}{u_{ref}} \right)^{-1} \right), \tag{9}$$

Term 3 :

$$\overline{\rho \alpha} \frac{\partial c''}{\partial x_j} S_{ij}'' \frac{\partial \widetilde{c}}{\partial x_i} \simeq \mathcal{O} \left(\rho_u \left(\frac{u_L^0}{\delta_L^0} \right)^2 ; (Re_l Da)^{-1/2} \right), \tag{10}$$

Term 4 :

$$\overline{\rho \alpha} \frac{\partial \widetilde{c''}}{\partial x_i} S_{ij}'' \frac{\partial \widetilde{c}}{\partial x_j} \simeq \mathcal{O} \left(\rho_u \left(\frac{u_L^0}{\delta_L^0} \right)^2 ; (Re_L Da)^{-1/2} \right), \quad (11)$$

Term 5 :

$$\overline{\rho \alpha} \left(\frac{\partial \widetilde{c}}{\partial x_i} S_{ij}'' \frac{\partial \widetilde{c}}{\partial x_j} \right) \simeq \mathcal{O} \left(\rho_u \left(\frac{u_L^0}{\delta_L^0} \right)^2 ; \left(\frac{Re_L Da^2 u'}{u_{ref}} \right)^{-1} \right). \quad (12)$$

The above order of magnitude analysis suggests that in the thin flamelet limit, $\overline{\rho} \left(\overline{\alpha c''_{,i} S_{ij}'' c''_{,j}} \right)$

is a dominant term, and, thus an evolution equation for $\overline{\rho} \left(\overline{\alpha c''_{,i} S_{ij}'' c''_{,j}} \right)$ will provide a useful first approximation. Introducing the definition:

$$\tilde{\rho \Delta_c} \equiv \overline{\rho \alpha \frac{\partial c''}{\partial x_i} S_{ij}'' \frac{\partial c''}{\partial x_j}}, \quad (13)$$

The total derivative of the fluctuating part of flame turbulence interaction term is :

$$\begin{aligned} \rho \frac{D}{Dt} \left(\alpha \frac{\partial c''}{\partial x_i} S_{ij}'' \frac{\partial c''}{\partial x_j} \right) &= \overline{\rho \alpha \frac{\partial c''}{\partial x_i} S_{ij}'' \frac{D}{Dt} \left(\frac{\partial c''}{\partial x_j} \right)} + \overline{\rho \alpha \frac{\partial c''}{\partial x_j} \frac{\partial c''}{\partial x_i} \frac{D}{Dt} (S_{ij}'')} \\ &\quad + \overline{\rho \alpha \frac{\partial c''}{\partial x_j} S_{ij}'' \frac{D}{Dt} \left(\frac{\partial c''}{\partial x_i} \right)}. \end{aligned} \quad (14)$$

Using the definition of S_{ij}'' and some algebraic simplification leads to :

$$\begin{aligned} \rho \frac{D}{Dt} \left(\alpha \frac{\partial c''}{\partial x_i} S_{ij}'' \frac{\partial c''}{\partial x_j} \right) &= \underbrace{2 \overline{\rho \alpha \frac{\partial c''}{\partial x_i} S_{ij}'' \frac{D}{Dt} \left(\frac{\partial c''}{\partial x_j} \right)}}_{\text{Term 1}} + \underbrace{\overline{\rho \alpha \frac{\partial c''}{\partial x_j} \frac{\partial c''}{\partial x_i} \frac{D}{Dt} \left(\frac{\partial u_i''}{\partial x_j} \right)}}_{\text{Term 2}}. \end{aligned} \quad (15)$$

Term 1 and Term 2 in Eq. (15) can be simplified to give the final transport equation for $\tilde{\Delta_c}$.

The details for the complete derivation are given in Appendix-A. After some algebra the

transport equation for $\tilde{\Delta_c}$ can be obtained as:

$$\begin{aligned} \overline{\rho} \frac{D \tilde{\Delta_c}}{Dt} &= - \frac{\partial}{\partial x_n} \left(\overline{\rho \alpha u_n'' \frac{\partial c''}{\partial x_i} S_{ij}'' \frac{\partial c''}{\partial x_j}} \right) + \underbrace{2 \frac{\partial c''}{\partial x_i} S_{ij}'' \frac{\partial}{\partial x_j} \left(\frac{\partial}{\partial x_n} \left(\overline{\rho \alpha \alpha \frac{\partial c''}{\partial x_n}} \right) \right)}_{D_{f1}} \\ &\quad + \underbrace{\overline{\alpha \frac{\partial c''}{\partial x_i} \frac{\partial c''}{\partial x_j} \frac{\partial}{\partial x_n} \left(\frac{\partial \tau_{in}''}{\partial x_j} \right)}}_{D_{f2}} + F_1 + F_2 + F_3 + F_4, \end{aligned} \quad (16)$$

where D_{f1} and D_{f2} represent diffusion/dissipation terms, F_1 represents source terms due to pressure gradient and reaction rate :

$$F_1 = 2\alpha \underbrace{\frac{\partial c''}{\partial x_i} S_{ij}'' \frac{\partial \dot{\omega}_c''}{\partial x_j}}_{F_{11}} - \alpha \underbrace{\frac{\partial c''}{\partial x_i} \frac{\partial c''}{\partial x_j} \frac{\partial}{\partial x_i} \left(\frac{\partial p'}{\partial x_j} \right)}_{F_{12}}, \quad (17)$$

F_2 represents terms arising due to turbulent transport :

$$F_2 = 2 \underbrace{\frac{\partial}{\partial x_n} \left(\overline{\rho \alpha u_n'' \frac{\partial c''}{\partial x_j}} \right) \frac{\partial c''}{\partial x_i} S_{ij}''}_{F_{21}} - 2 \underbrace{\overline{\rho \alpha} \frac{\partial c''}{\partial x_i} S_{ij}'' u_n'' \frac{\partial}{\partial x_n} \left(\frac{\partial \tilde{c}}{\partial x_j} \right)}_{F_{22}} \\ + \underbrace{\frac{\partial}{\partial x_n} \left(\overline{\rho \alpha u_n'' \frac{\partial u_i''}{\partial x_j}} \right) \frac{\partial c''}{\partial x_i} \frac{\partial c''}{\partial x_j}}_{F_{23}} - \underbrace{\overline{\rho \alpha} \frac{\partial c''}{\partial x_i} \frac{\partial c''}{\partial x_j} u_n'' \frac{\partial}{\partial x_n} \left(\frac{\partial \tilde{u}_i}{\partial x_j} \right)}_{F_{24}}, \quad (18)$$

F_3 represents the dilatation terms:

$$F_3 = 2 \underbrace{\overline{\rho \alpha} \frac{\partial c''}{\partial x_i} S_{ij}'' \frac{\partial c''}{\partial x_j} \frac{\partial u_l''}{\partial x_l}}_{F_{31}} + 2 \underbrace{\overline{\rho \alpha} \frac{\partial \tilde{u}_l}{\partial x_l} \tilde{\Delta}_c}_{F_{32}} + 2 \underbrace{\overline{\rho \alpha} \frac{\partial \tilde{c}}{\partial x_j} \frac{\partial c''}{\partial x_i} S_{ij}'' \frac{\partial u_l''}{\partial x_l}}_{F_{33}} - 2 \underbrace{\overline{\rho \alpha} \frac{\partial c''}{\partial x_j} \frac{\partial u_l''}{\partial x_l} \frac{\partial c''}{\partial x_i} S_{ij}''}_{F_{34}} \\ + \underbrace{\alpha \frac{\partial \rho}{\partial x_j} \frac{\partial p'}{\partial x_i} \frac{\partial c''}{\partial x_j} \frac{\partial c''}{\partial x_i} \frac{1}{\rho}}_{F_{35}} - \underbrace{\alpha \frac{\partial \rho}{\partial x_j} \frac{\partial \tau_{in}''}{\partial x_n} \frac{\partial c''}{\partial x_i} \frac{\partial c''}{\partial x_j} \frac{1}{\rho}}_{F_{36}}, \quad (19)$$

and F_4 represents turbulent straining terms :

$$F_4 = -2 \underbrace{\overline{\rho \alpha} \frac{\partial c''}{\partial x_i} S_{ij}'' \frac{\partial c''}{\partial x_n} \frac{\partial u_n''}{\partial x_j}}_{F_{41}} - 2 \underbrace{\overline{\rho \alpha} \frac{\partial c''}{\partial x_i} S_{ij}'' \frac{\partial c''}{\partial x_n} \frac{\partial \tilde{u}_n}{\partial x_j}}_{F_{42}} - 2 \underbrace{\overline{\rho \alpha} \frac{\partial \tilde{c}}{\partial x_n} \frac{\partial c''}{\partial x_i} S_{ij}'' \frac{\partial u_n''}{\partial x_j}}_{F_{43}} \\ + 2 \underbrace{\overline{\rho \alpha} \frac{\partial c''}{\partial x_n} \frac{\partial u_n''}{\partial x_j} \frac{\partial c''}{\partial x_i} S_{ij}''}_{F_{44}} - \underbrace{\overline{\rho \alpha} \frac{\partial c''}{\partial x_i} \frac{\partial c''}{\partial x_j} \frac{\partial u_n''}{\partial x_j} \frac{\partial u_i''}{\partial x_n}}_{F_{45}} - \underbrace{\overline{\rho \alpha} \frac{\partial c''}{\partial x_i} \frac{\partial c''}{\partial x_j} \frac{\partial u_n''}{\partial x_j} \frac{\partial \tilde{u}_i}{\partial x_n}}_{F_{46}} \\ - \underbrace{\overline{\rho \alpha} \frac{\partial \tilde{u}_n}{\partial x_j} \frac{\partial c''}{\partial x_i} \frac{\partial c''}{\partial x_j} \frac{\partial u_i''}{\partial x_n}}_{F_{47}} + \underbrace{\overline{\rho \alpha} \frac{\partial c''}{\partial x_i} \frac{\partial c''}{\partial x_j} \frac{\partial u_n''}{\partial x_j} \frac{\partial u_i''}{\partial x_n}}_{F_{48}}, \quad (20)$$

3 Leading order terms in the $\tilde{\Delta}_c$ evolution equation

Repeating the order of magnitude analysis described in section 2 Eq. (16) leads to :

$$D_f + F_1 + F_D + F_{TS} \simeq 0, \quad (21)$$

where D_f represents the leading order diffusion/dissipation terms as :

$$\begin{aligned} D_f = & \overline{-2\rho\alpha\alpha \frac{\partial}{\partial x_n} \left(\frac{\partial c''}{\partial x_j} \right) \frac{\partial}{\partial x_n} \left(\frac{\partial c''}{\partial x_i} S''_{ij} \right)} - \overline{2\rho\alpha\alpha \frac{\partial}{\partial x_n} \left(\frac{\partial c''}{\partial x_i} \frac{\partial c''}{\partial x_j} \frac{\partial}{\partial x_n} S''_{ij} \right)} \\ & - \overline{2\rho\alpha\alpha \frac{\partial}{\partial x_n} \left(\frac{\partial c''}{\partial x_j} S''_{ij} \frac{\partial}{\partial x_n} \left(\frac{\partial c''}{\partial x_i} \right) \right)} + \overline{\alpha \frac{\partial c''}{\partial x_i} \frac{\partial c''}{\partial x_j} \frac{\partial}{\partial x_n} \left(\frac{\partial \tau''_{in}}{\partial x_j} \right)}, \end{aligned} \quad (22)$$

F_D represents the leading order dilatation terms as:

$$F_D = F_{31} + F_{34} + F_{35} + F_{36}, \quad (23)$$

and F_{TS} represents the leading order turbulent straining terms as:

$$F_{TS} = F_{41} + F_{44} + F_{45} + F_{48}. \quad (24)$$

Note that all the leading order terms in Eq. (16) scale as :

$$\mathcal{O} \left(\rho_u \left(\frac{u_L^0}{\delta_L^0} \right)^3 ; 1 \right).$$

A detailed order of magnitude analysis for all the terms in Eq. (16) is given in Appendix-B.

Here our interest is to close the leading order terms by suitable approximations. This is achieved via detailed interrogation of a Direct Numerical Simulation (DNS) data set of turbulent premixed V-flame in the corrugated flamelet regime. The details of the DNS are discussed in the next section.

4 Direct Numerical Simulation data

In this study, the DNS data produced by Dunstan et al [21] for a turbulent premixed V-flame has been used. In the V-flame configuration, a stationary, non-planar flame is produced which is oblique to the mean flow, and subject to mean shear, strong tangential convection by the mean flow and flow divergence [20]. This type of configuration is characterised by a continuously developing flame in a statistically two dimensional mean flow field; the turbulence intensity along the leading edge of the flame brush decreases significantly while the individual flame elements are convected in the stream wise direction [20].

The V-flame in the DNS is representative of a lean, unit Lewis number flame with pre-heated reactants. The combustion kinetics are approximated by a single step reaction [21, 20]. DNS of the V-flame was carried out using a code called SENG2, in which the conservation equations for mass, momentum, energy and reacting species are solved for compressible flow [21,20,23,11,18]. The spatial derivatives for interior grid points are calculated by using a 10th order central difference scheme, which gradually reduce to a 2nd order scheme for all outflow boundaries, and 4th order scheme at the inlet boundary. The solution is evolved in time by using a 4th order explicit Runge-Kutta scheme. The transport coefficients have a temperature dependence approximated by 5th order polynomials following the CHEMKIN formats. Navier-Stokes Characteristic Boundary Conditions (NSCBC) have been applied to all non-periodic boundaries. The standard NSCBC has been modified to accommodate the steep thermal and compositional gradients when the flame crosses the boundary. This has been done to avoid large pressure perturbations which can have a significant influence on the interior solution. Further details on the boundary conditions can be found in [21,31,32,34,37]. Similar DNS data sets have been used in several modelling stud-

ies for scalar dissipation rate, turbulent flame speed and flame generated noise in premixed turbulent combustion [21, 20, 19, 26].

The domain for the V-flame simulation is a cube of side $29.69\delta_L^0$. The domain is discretised by a $512 \times 512 \times 512$ node uniform grid, ensuring a minimum resolution of about 10 grid points is maintained to resolve the laminar flame thermal thickness δ_L^0 . The flame is stabilised by a flame holder positioned at $3.49\delta_L^0$ from the inlet plane; this is achieved by fixing the mass fraction through a Gaussian weighting function and restricting velocities to their mean values (further details on the flame holder can be found in [21, 20]). The schematic of the computational domain is given in figure 1. The simulation is run for one flow through, to allow for the transients to decay before collecting data for analysis.

The global thermochemical parameters used in the DNS are; planar, unstretched laminar flame speed $u_L^0 = 0.6034 \text{ m/s}$; laminar flame thermal thickness $\delta_L^0 = (T_{ad} - T_0)/\max|\nabla T| = 0.43 \text{ mm}$ (where $T_{ad} = 2113.3 \text{ K}$ is the adiabatic flame temperature and $T_0 = 600.0 \text{ K}$ is the inlet reactant temperature); heat release parameter $\tau = (T_{ad} - T_0)/T_0 = 2.52$; Zeldovitch number $\beta = 7.13$; characteristic laminar flame time is given by $\tau_f = \delta_L^0/u_L^0 = 0.71 \text{ ms}$ and the laminar diffusive thickness $\delta_L = \alpha/u_L^0 = 0.1207 \text{ mm}$. For the purpose of comparison with real air-fuel mixture flames, the Zeldovitch number and the heat release parameter are representative of a pre-heated premixed methane-air flame with an equivalence ratio $\phi \approx 0.6$ [21].

The values of the inlet turbulent Reynolds number (Re_l), Karlovitz number (Ka) and Damköhler number (Da) based on the laminar flame diffusive thickness and inlet flow conditions are summarised in table 1, where u'_{in} is the rms velocity at the inlet, $\bar{u}_{in}$ is the mean inlet velocity in the y – direction as shown in figure 1, ν is the kinematic viscosity and l_t is the integral length scale.

Figure 2 show the contours of $0.1 \leq \tilde{c} \leq 0.9$ in the V-flame DNS, where the x^+ and y^+ represent the directions normalised by the thermal thickness of the flame δ_L^0 .

4.1 Post-processing and numerical resolution

During the post processing of the DNS, the data was averaged in time over 21 instantaneous realisations of the flow (over a total sample time corresponding to one flow through), and space averaged in the periodic (z) direction. Spatial derivatives of fluctuating quantities required by the terms in Eq. (21) are calculated using the same numerical algorithm as used in the DNS. The present analysis is restricted to $y^+ > 20$, beyond which the flame has sufficient time to develop after ignition at the flame holder [21, 19]. Three sampling locations downstream of the flame holder at $y^+ \approx 23$, $y^+ \approx 25$ and $y^+ \approx 27$ are used, labelled as a, b, and c in figure 2. The flame is influenced by the level of turbulence upstream of the flame, hence non-dimensional parameters such as Ka , Da and Re_l are reported for all the sampling locations at $\tilde{c} \approx 0.001$ in table 2. It can be observed in table 2 that the flame lies in the corrugated flamelet regime, and Re_l remains close to approximately 20 at all the sampling locations used for this study. All the results have been normalised using ρ_u, u_L^0 and δ_L^0 . As the thickness of $\tilde{c}$ changes along the mean flow direction and $\tilde{c}$ varies monotonically from the flame centreline, $\tilde{c}$ is used to denote the location inside the flame brush in the results discussed below.

As mentioned earlier a resolution of minimum 10 grid points is used to resolve the laminar flame thickness; in the regions where the data is extracted, the number of grid points in the flame structure have increased to almost 30. This can be noted in figure 3 where the different time realisations for the instantaneous progress variable are shown for all sampling locations. This level of spatial resolution is assumed to be sufficient for the evaluation of the

higher order (i.e. 4th or 5th order) correlations with high order derivatives of the fluctuating quantities. Sufficiency can be further established by the numerical resolution criterion of Poinso et al [29]:

$$Re_t Da < 2(1 + \tau)^{0.7} \left(\frac{N_x}{n_g} n_e \right)^2, \quad (25)$$

where N_x represents the number of grid points in the direction of flame gradients, n_g represents the number of grid points in the flame structure and n_e represents the number of large scale eddies in the domain. The values of n_e have been calculated using the turbulence characteristics upstream of the flame as reported in table 2. Table 3 shows the results obtained by using Eq. (25) for all sampling locations; the inequality in Eq. (25) is satisfied for all the sampling locations.

The statistical convergence of the Reynolds/Favre averaged quantities is tested by comparing the average data from all 21 realisations against the average data from 10,12,15 and 18 realisations. The time evolution of D_f (one of the highest moments with the highest order of derivatives in Eq. (22)) is shown in figure 4 for all sampling locations. Statistical convergence has been achieved for D_f after 15 averaged realisations. Sample size of 21 instantaneous realisations is thus deemed sufficient for calculating the leading order terms in the flame turbulence interaction transport equation.

5 Results and discussion

5.1 Eigenvector analysis and alignment statistics

The behaviour of the flame turbulence interaction relies on the alignment of the strain rate eigenvectors with the scalar gradient, hence an eigenvector analysis has been undertaken for the V-flame DNS.

The eigenvectors for the strain rate have been calculated by using LAPACK libraries for FORTRAN [1]. Figures 5, 6 and 7 show the pdfs of direction cosines between the strain rate eigenvectors and the flame gradient at $y^+ \approx 23$, $y^+ \approx 25$ and $y^+ \approx 27$ respectively for different iso-surfaces of c . It can be observed in figures 5(a), 6(a) and 7(a) that the most probable inner product tending towards unity is the inner product between e_α and ∇c , which implies that the extensive strain rate eigenvector aligns preferentially with the flame gradient for $0.3 \leq c \leq 0.7$ at all the sampling locations in the DNS. It should be noted here however that the direct interpretation of strain rate orientation from direction cosines can be obscured by the non-linearity of the cosine function. In case of a uniformly distributed angle between two vectors, the pdf of $\cos\theta$ shows higher probabilities of unity [33], and caution must be taken when interpreting alignment pdfs based on direction cosines.

Steinberg et al [33] argue that the actual physical orientation of the strain rate field with the flame gradient can be better represented by the pdfs of the angle between the two vectors directly. Figures 5(b), 6(b) and 7(b) show the pdfs of the angles between the extensive strain rate eigenvector and the flame gradient at $y^+ \approx 23$, $y^+ \approx 25$ and $y^+ \approx 27$ respectively for different iso-surfaces of c . It can be observed that the most probable alignment between e_α and ∇c occurs at $0 \leq \theta_\alpha \leq 0.5$ for $0.3 \leq c \leq 0.7$ at all sampling locations, which again implies that e_α preferentially aligns with ∇c for $0.3 \leq c \leq 0.7$. This is in agreement with the earlier studies [15,22] as the chemical reactions releasing heat compete with the local fluid dynamic processes, thus causing the flame gradient to align with the most extensive strain rate eigenvector.

The non-linearity induced by the cosine function can be noticed by comparing the pdfs of direction cosines between e_α and ∇c and the pdfs for the resulting angles between e_α and ∇c . The pdfs for the direction cosines between e_α and ∇c show a bias towards higher prob-

ability of unity as shown in figures 5(a), 6(a) and 7(a); whereas the pdfs for the associated angles show a range of angles with lower probability as shown in figures 5(b), 6(b) and 7(b).

Note that e_α and ∇c are not completely aligned for $c = 0.1$ and $c = 0.9$ iso-surfaces at all sampling locations. The dilatation due to heat release is low near $c = 0.1$ and $c = 0.9$ iso-surfaces, as shown in figure 8 for all the sampling locations in the V-flame. The mean shear overcomes the dilatation effects and enters the flame structure at $c = 0.1$ and $c = 0.9$, thus causing the flame gradients to move away from the extensive strain rate eigenvector and towards the compressive strain rate eigenvector as shown in figures 5(b), 6(b), 7(b), 5(f), 6(f) and 7(f). This phenomenon has been noted in the earlier studies by Minamoto et al [27] in case of reacting flows and by Ashurst et al [2] in case of non reacting flows. These changes in alignment characteristics across the flame structure signify the importance of the transport equation for $\tilde{\Delta}_c$, as the transport equation allows for a more flexible approach to incorporate the correct physics and flow history effects into the modelling strategy.

5.2 Leading order terms in the $\tilde{\Delta}_c$ evolution equation

Figures 9(a) - 9(c) show the profiles for the leading order terms in the $\tilde{\Delta}_c$ transport equation at $y^+ \approx 23$, $y^+ \approx 25$ and $y^+ \approx 27$. The over all behaviour of $\tilde{\Delta}_c$ transport equation is strongly controlled by a competition between the source terms (F_1), diffusion/dissipation process (D_f), turbulent strain rate (F_{TS}) and the dilatation rate (F_D) as shown in figure 9.

It can be seen in figure 10 that there is a competition between the turbulent strain rate (F_{TS}) and the dilatation rate (F_D) at all the sampling locations, which is in agreement with theories proposed in earlier studies [13,36]. These earlier studies further suggest that the competition between F_{TS} and F_D significantly influences the evolution of $\tilde{\Delta}_c$ and is considered to be an important phenomenon [13,36]. We argue here that the source terms (F_1) and

diffusion/dissipation processes (D_f) are the main contributing terms in the evolution of $\tilde{\Delta}_c$ as shown in figure 9.

5.3 Model for F_{TS}

Expanding the expression for F_{TS} in Eq. (24) leads to :

$$F_{TS} = \underbrace{\rho\alpha \frac{\partial c''}{\partial x_i} S_{ij}'' \frac{\partial c''}{\partial x_n} \frac{\partial u_n''}{\partial x_j}}_{Term1} + \underbrace{2\rho\alpha \frac{\partial c''}{\partial x_n} \frac{\partial u_n''}{\partial x_j} \frac{\partial c''}{\partial x_i} S_{ij}''}_{Term2} - \underbrace{\rho\alpha \frac{\partial c''}{\partial x_i} \frac{\partial c''}{\partial x_j} \frac{\partial u_n''}{\partial x_j} \frac{\partial u_i''}{\partial x_n}}_{Term3} + \underbrace{\rho\alpha \frac{\partial c''}{\partial x_i} \frac{\partial c''}{\partial x_j} \frac{\partial u_n''}{\partial x_j} \frac{\partial u_i''}{\partial x_n}}_{Term4} \quad (26)$$

All the terms in Eq. (26) require closures. The scalar gradient and strain rate contribution in term 1, Eq. (26) can be scaled as :

$$\rho\alpha \frac{\partial c''}{\partial x_i} S_{ij}'' \frac{\partial c''}{\partial x_n} \sim \bar{\rho} \tilde{\Delta}_c,$$

and the turbulent straining represented by the fluctuating velocity gradients can be scaled by a turbulent time scale as :

$$\frac{\partial u_i''}{\partial x_j} \sim \frac{\tilde{\epsilon}}{\tilde{k}}.$$

Similar scaling arguments are used to scale the rest of the terms in Eq. (26), thus leading to :

$$F_{TS} \approx C_b \bar{\rho} \frac{\tilde{\epsilon}}{\tilde{k}} \tilde{\Delta}_c, \quad (27)$$

where C_b is a scaling factor for the model.

The value of C_b is of key importance. Following earlier modelling strategies used in the $\tilde{\epsilon}_c$ transport equation [16, 14, 17] a functional form of C_b is proposed as :

$$C_b = - \left[3.5 + \frac{0.01 \operatorname{erf}(Ka_L)}{0.01 + \sqrt{\operatorname{erf}(Re_{lt})}} \right], \quad (28)$$

where Re_{l_t} is defined as [28]:

$$Re_{l_t} = \frac{u' l_t}{\nu_u}, \quad (29)$$

and Ka_L is defined as [28]:

$$Ka_L = \left(u' / u_L^0 \right)^{3/2} (\delta_L / l_t)^{1/2}. \quad (30)$$

u' and l_t in Eq (29) and Eq (30) are defined as :

$$u' = \sqrt{\frac{2\tilde{k}}{3}} \text{ and } l_t = \frac{u'^3}{\tilde{\epsilon}}. \quad (31)$$

The function for C_b is one of several possible empirical relations which lead to a physically plausible result. It should be noted that the turbulent strain rate increases with an increase in small scale turbulence represented by Karlovitz number; this phenomenon is captured by the functional form of C_b presented in Eq. (28). The function in Eq. (28) reaches an asymptotic value as $u' \rightarrow \infty$. Similar scaling factors have been proposed by Chakraborty and Swaminathan [17] for the closures of the $\tilde{\epsilon}_c$ transport equation.

Comparisons of the model against the DNS data set at all the sampling locations are given in figure 11. Throughout, the model performance improves as the distance of the sampling location from the flame holder increases. The scaling factor C_b in Eq. (28) is only valid for high Damköhler number flames, and further tests need to be carried out to check the validity of the model for different combustion conditions.

5.4 Model for F_D

It can be observed in Eq. (23) that :

$$\begin{aligned}
F_D = & \underbrace{2\bar{\rho}\alpha \frac{\partial c''}{\partial x_i} S_{ij}'' \frac{\partial c''}{\partial x_j} \frac{\partial u_l''}{\partial x_l}}_{Term1} - \underbrace{2\bar{\rho}\alpha \frac{\partial c''}{\partial x_j} \frac{\partial u_l''}{\partial x_l} \frac{\partial c''}{\partial x_i} S_{ij}''}_{Term2} + \underbrace{\alpha \frac{\partial \rho}{\partial x_j} \frac{\partial p'}{\partial x_i} \frac{\partial c''}{\partial x_j} \frac{\partial c''}{\partial x_i} \frac{1}{\rho}}_{Term3} \\
& - \underbrace{\alpha \frac{\partial \rho}{\partial x_j} \frac{\partial \tau_{in}''}{\partial x_n} \frac{\partial c''}{\partial x_i} \frac{\partial c''}{\partial x_j} \frac{1}{\rho}}_{Term4}.
\end{aligned} \tag{32}$$

We propose that the contributions involving the scalar gradients and the strain rate in term 1

Eq. (32) scale as :

$$\rho \alpha \frac{\partial c''}{\partial x_i} S_{ij}'' \frac{\partial c''}{\partial x_j} \sim \bar{\rho} \tilde{\Delta}_c,$$

while the contributions involving the dilatation represented by the divergence of the velocity

field scale as :

$$\frac{\partial u_l''}{\partial x_l} \sim \tau \frac{u_L^0}{\delta_L}.$$

Similar scaling arguments apply to term 2 in Eq. (32). Term 3 in Eq. (32) includes the effects of pressure gradient which is a source term for the transport of momentum and thus containing the effects of the strain rate; the density gradients include the effects of dilatation, and hence combining the two observations term 3 in Eq. (32) scales as :

$$\alpha \frac{\partial \rho}{\partial x_j} \frac{\partial p'}{\partial x_i} \frac{\partial c''}{\partial x_j} \frac{\partial c''}{\partial x_i} \frac{1}{\rho} \sim \bar{\rho} \tilde{\Delta}_c \tau \frac{u_L^0}{\delta_L}.$$

Term 4 in Eq. (32) can be simplified by substituting τ_{in}'' as $\tau_{in}'' \approx 2\mu S_{in}''$, where $\mu \approx \rho \alpha$, and assuming that the density gradients associated with τ_{in}'' are small, thus leading to :

$$-\rho \alpha \alpha \frac{\partial \rho}{\partial x_j} \frac{\partial S_{in}''}{\partial x_n} \frac{\partial c''}{\partial x_i} \frac{\partial c''}{\partial x_j} \frac{1}{\rho}. \tag{33}$$

Following the earlier scaling arguments the expression in Eq. (33) scales as :

$$\sim \bar{\rho} \tilde{\Delta}_c \tau \frac{u_L^0}{\delta_L}.$$

Thus leading to the model :

$$F_D \approx C_c Da_L \bar{\rho} \tilde{\Delta}_c \tau \frac{u_L^0}{\delta_L}, \tag{34}$$

where Da_L represents the local Damköhler number and is defined as :

$$Da_L = \frac{(u_L^0/\delta_L)}{(\tilde{\varepsilon}/\tilde{k})}, \quad (35)$$

and C_c is a scaling factor for the model. Note that an expression for the local Damköhler number has been proposed by Chakraborty and Swaminathan [16], but their definition is based on the laminar flame thermal thickness δ_L^0 where as the definition in Eq. (35) is based on the laminar flame diffusive thickness δ_L . The model proposed in Eq. (34) has an explicit dependence on the heat release parameter τ and the local Damköhler number Da_L , thus allowing the model to account for the changes in heat release and turbulence and their influence on dilatation in the $\tilde{\Delta}_c$ evolution. It can be observed in Eq. (34) that in the limiting case of $u' \rightarrow \infty$ and $Da \rightarrow 0$ the influence of dilatation vanishes. Furthermore an explicit dependence of the model on τ allows the model to vanishes in the limiting case of cold flow turbulence.

The accuracy of the model in Eq. (34) relies on the choice of the scaling factor C_c ; here we include the effects of turbulent Reynolds number into our modelling strategy and define C_c as :

$$C_c = \frac{0.01 + 3.5 \operatorname{erf}(Ka_L)}{13 \operatorname{erf}\left(\left(Re_{t_i}^3/17.5\right) + 0.01\right)}. \quad (36)$$

Note that C_c decreases as u' increases, eventually reducing to an asymptotic value as $Re_{t_i} \rightarrow \infty$ and $Ka_L \rightarrow \infty$. This has been done because the dilatation rate decreases with increasing u' values. The Karlovitz number effects have been included in Eq. (36) to account for the changes in the dilatation rate due to small scale turbulence. Furthermore in case of cold flows where $Ka_L \rightarrow 0$ the function in Eq. (36) reduces to a very small number along with the contributions from the actual model in Eq. (34) going to zero. The results from the model are in good agreement with the DNS data as shown in figure 12. The scaling factor C_c

presented in Eq. (36) is one of many possible empirical functions; and is only valid for $Da > 1$ and $Ka < 1$ flames. More DNS data in the thin reaction zone regime is needed to extend the modelling further and obtain more robust scaling factors.

5.5 Model for diffusion D_f and F_1 source terms

$$\begin{aligned}
 D_f + F_1 = & -2\rho\alpha\alpha\overline{\frac{\partial}{\partial x_n}\left(\frac{\partial c''}{\partial x_j}\right)\frac{\partial}{\partial x_n}\left(\frac{\partial c''}{\partial x_i}S''_{ij}\right)} - 2\rho\alpha\alpha\overline{\frac{\partial}{\partial x_n}\left(\frac{\partial c''}{\partial x_i}\frac{\partial c''}{\partial x_j}\frac{\partial}{\partial x_n}S''_{ij}\right)} \\
 & - 2\rho\alpha\alpha\overline{\frac{\partial}{\partial x_n}\left(\frac{\partial c''}{\partial x_j}S''_{ij}\frac{\partial}{\partial x_n}\left(\frac{\partial c''}{\partial x_i}\right)\right)} + \alpha\overline{\frac{\partial c''}{\partial x_i}\frac{\partial c''}{\partial x_j}\frac{\partial}{\partial x_n}\left(\frac{\partial \tau''_{in}}{\partial x_j}\right)} \\
 & + 2\alpha\overline{\frac{\partial c''}{\partial x_i}S''_{ij}\frac{\partial \dot{\omega}''_c}{\partial x_j}} - \alpha\overline{\frac{\partial c''}{\partial x_i}\frac{\partial c''}{\partial x_j}\frac{\partial}{\partial x_i}\left(\frac{\partial p'}{\partial x_j}\right)}. \tag{37}
 \end{aligned}$$

It can be seen in figure 9 that term F_1 is dominantly a source and D_f is dominantly a sink for $\tilde{\Delta}_c$ evolution. The combined terms in Eq. (37) scale as a product of flame normal strain rate $\tilde{\Delta}_c/\tilde{\epsilon}_c$ and flame turbulence interaction $\tilde{\Delta}_c$ as :

$$\sim \tilde{\Delta}_c^2/\tilde{\epsilon}_c,$$

thus leading to :

$$D_f + F_1 \approx -C_a\bar{\rho}\frac{\tilde{\Delta}_c^2}{\tilde{\epsilon}_c}. \tag{38}$$

C_a is a scaling factor in Eq. (38), and the negative sign is used due to the (over all) sink nature of $D_f + F_1$ as shown in figure 13. The sum of terms D_f and F_1 has a dominant effect in $\tilde{\Delta}_c$ evolution, thus the ratio $\tilde{\Delta}_c^2/\tilde{\epsilon}_c$ in Eq. (38) represents the rate of change of flame turbulence interaction, $\tilde{\Delta}_c^2/\tilde{\epsilon}_c \approx d\tilde{\Delta}_c/dt$.

The value of C_a in Eq. (38) is a matter of calibration and is dependent on the DNS data set used for model calibration. Here we propose a value of C_a based on the ratio of turbulent Reynolds number and local Karlovitz number, thus accounting for the changes in the local flow conditions :

$$C_a = \left[4 + \frac{1.9 \operatorname{erf}(Re_l)}{\operatorname{erf}((Ka_L + 1)/50)} \right]. \quad (39)$$

This has been done because the flame normal strain rate decreases with increasing strength of the small scale turbulence represented by Karlovitz numbers [15]. It can be seen in Eq. (39) that the value of C_a reaches an asymptotic value as $Re_l \rightarrow \infty$ and $Ka_L \rightarrow \infty$. Note that the exact behaviour of $D_f + F_1$ at higher Re_l and Ka conditions is not known and more DNS data in the thin reaction zone regime is needed to extend the modelling further. The model proposed for $D_f + F_1$ are in qualitative agreement with the DNS data as shown in figure 13.

6 Summary and Conclusions

Flame turbulence interaction is an important quantity in turbulent premixed combustion modelling. It has been shown in previous studies that the effect of strain rate on the transport of scalar dissipation is dominated by the interaction between the fluctuating scalar gradients and the fluctuating strain rate (here denoted by $\tilde{\Delta}_c$). An accurate representation of the flame turbulence interaction can be obtained from the leading order terms in the evolution equation for $\tilde{\Delta}_c$. In this paper an evolution equation for $\tilde{\Delta}_c$ has been derived and an order of magnitude analysis under the joint assumption of high Reynolds and Damköhler numbers has been done to identify the leading order terms. The leading order terms have been analysed via the DNS results of Dunstan et al [21]. It has been found that the turbulent strain rate and the dilatation rate compete in $\tilde{\Delta}_c$ evolution, which is in agreement with the theories proposed in earlier studies [13, 36]. It has also been found that there is also competition between the source terms (pressure gradient and reaction rate) and the diffusion/dissipation processes. It is argued in this study that the overall behaviour of $\tilde{\Delta}_c$ evolution equation is determined by the competition between source and diffusion/dissipation terms.

Closures for the leading order terms have been proposed and compared against the DNS data set at different locations. The comparisons of modelled predictions and the DNS values are in good agreement for the combustion conditions considered in this study. In the light of a recent study by Chakarborty and Swaminathan [17] the closures for the leading order terms have been made functions of turbulent Reynolds and local Karlovitz numbers. The present modelling strategy is only able to capture the flame turbulence interaction in the wrinkled/corrugated flamelet regime ($Da > 1$ and $Ka < 1$). More investigations of DNS data sets with different combustion conditions and turbulent Reynolds number are needed to fully understand the behaviour of the leading order terms in $\tilde{\Delta}_c$ evolution equation, which would lead to more robust modelling strategies applicable to a wide range of combustion conditions. This forms part of the on going work.

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Appendix-A

In order to resolve Term 1 in Eq. (14), a transport equation for the gradient of c'' is required. That is achieved by using the definition $c'' = c - \tilde{c}$ and taking the derivative of the instantaneous progress variable transport equation to write :

$$\begin{aligned} \rho\alpha \frac{\partial}{\partial t} \left(\frac{\partial c}{\partial x_j} \right) + \rho\alpha u_n \frac{\partial}{\partial x_n} \left(\frac{\partial c}{\partial x_j} \right) &= \alpha \frac{\partial}{\partial x_j} \left(\frac{\partial}{\partial x_n} \left(\rho\alpha \frac{\partial c}{\partial x_n} \right) \right) + \frac{\partial \dot{\omega}_c}{\partial x_j} \\ &\quad - \rho\alpha \frac{\partial c}{\partial x_n} \frac{\partial u_n}{\partial x_j} + \rho\alpha \frac{\partial c}{\partial x_j} \left(\frac{\partial u_l}{\partial x_l} \right). \end{aligned} \quad (40)$$

Applying the Reynolds decomposition and Favre averaging Eq. (40) leads to:

$$\begin{aligned} \overline{\rho\alpha} \frac{\partial}{\partial t} \left(\frac{\partial \tilde{c}}{\partial x_j} \right) + \overline{\rho\alpha \tilde{u}_n} \frac{\partial}{\partial x_n} \left(\frac{\partial \tilde{c}}{\partial x_j} \right) &= \frac{\partial}{\partial x_j} \left(\frac{\partial}{\partial x_n} \left(\overline{\rho\alpha\alpha} \frac{\partial \tilde{c}}{\partial x_n} \right) \right) - \frac{\partial}{\partial x_n} \left(\overline{\rho\alpha u_n''} \frac{\partial \tilde{c}}{\partial x_j} \right) \\ &+ \overline{\alpha} \frac{\partial}{\partial x_j} \overline{\tilde{c}} + \overline{\rho\alpha} \frac{\partial \tilde{c}}{\partial x_j} \frac{\partial u_l''}{\partial x_l} + \overline{\rho\alpha} \frac{\partial \tilde{c}}{\partial x_j} \frac{\partial \tilde{u}_l}{\partial x_l} - \overline{\rho\alpha} \frac{\partial \tilde{c}}{\partial x_n} \frac{\partial u_n''}{\partial x_j} + \overline{\rho\alpha} \frac{\partial \tilde{c}}{\partial x_n} \frac{\partial \tilde{u}_n}{\partial x_j}. \end{aligned} \quad (41)$$

Subtracting the mean equation from the instantaneous equation and then multiplying the resulting equation with $\frac{\partial c''}{\partial x_i} S_{ij}''$ and Favre averaging leads to:

$$\begin{aligned} \overline{\rho\alpha} \frac{\partial c''}{\partial x_i} S_{ij}'' \frac{D}{Dt} \left(\frac{\partial c''}{\partial x_j} \right) &= \overline{\frac{\partial c''}{\partial x_i} S_{ij}'' \frac{\partial}{\partial x_j} \left(\frac{\partial}{\partial x_n} \left(\rho\alpha\alpha \frac{\partial c''}{\partial x_n} \right) \right)} \\ &+ \overline{\frac{\partial c''}{\partial x_i} S_{ij}'' \frac{\partial}{\partial x_n} \left(\overline{\rho\alpha u_n''} \frac{\partial c''}{\partial x_j} \right)} - \overline{\rho\alpha} \frac{\partial c''}{\partial x_i} S_{ij}'' u_n'' \frac{\partial}{\partial x_n} \left(\frac{\partial \tilde{c}}{\partial x_j} \right) \\ &+ \overline{\alpha} \frac{\partial c''}{\partial x_i} S_{ij}'' \frac{\partial}{\partial x_j} \overline{\tilde{c}} + \overline{\rho\alpha} \frac{\partial c''}{\partial x_i} S_{ij}'' \frac{\partial \tilde{c}}{\partial x_j} \frac{\partial u_l''}{\partial x_l} + \overline{\rho\alpha} \frac{\partial \tilde{u}_l}{\partial x_l} \frac{\partial c''}{\partial x_i} S_{ij}'' \frac{\partial \tilde{c}}{\partial x_j} \\ &+ \overline{\rho\alpha} \frac{\partial \tilde{c}}{\partial x_j} \frac{\partial c''}{\partial x_i} S_{ij}'' \frac{\partial u_l''}{\partial x_l} - \overline{\rho\alpha} \frac{\partial c''}{\partial x_j} \frac{\partial u_l''}{\partial x_l} \frac{\partial c''}{\partial x_i} S_{ij}'' \\ &- \overline{\rho\alpha} \frac{\partial c''}{\partial x_i} S_{ij}'' \frac{\partial \tilde{c}}{\partial x_n} \frac{\partial u_n''}{\partial x_j} - \overline{\rho\alpha} \frac{\partial c''}{\partial x_i} S_{ij}'' \frac{\partial \tilde{u}_n}{\partial x_n} \frac{\partial \tilde{c}}{\partial x_j} \\ &- \overline{\rho\alpha} \frac{\partial \tilde{c}}{\partial x_n} \frac{\partial c''}{\partial x_i} S_{ij}'' \frac{\partial u_n''}{\partial x_j} + \overline{\rho\alpha} \frac{\partial \tilde{u}_n}{\partial x_n} \frac{\partial c''}{\partial x_i} S_{ij}'' \frac{\partial \tilde{c}}{\partial x_j}. \end{aligned} \quad (42)$$

Term 2 in Eq. (14) can be obtained by using the transport equation for the gradient of u_i'' .

Using a similar procedure to above and taking the derivative of the instantaneous momentum transport equation to write:

$$\begin{aligned} \rho\alpha \frac{\partial}{\partial t} \left(\frac{\partial u_i}{\partial x_j} \right) + \rho\alpha u_n \frac{\partial}{\partial x_n} \left(\frac{\partial u_i}{\partial x_j} \right) &= -\alpha \frac{\partial}{\partial x_i} \left(\frac{\partial p}{\partial x_j} \right) + \alpha \frac{\partial}{\partial x_n} \left(\frac{\partial \tau_{in}}{\partial x_j} \right) \\ &- \rho\alpha \frac{\partial u_n}{\partial x_j} \frac{\partial u_i}{\partial x_n} - \alpha \frac{\partial \rho}{\partial x_j} \left(-\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{in}}{\partial x_n} \right) \frac{1}{\rho}. \end{aligned} \quad (43)$$

Applying the Reynolds decomposition and Favre averaging Eq. (43) leads to:

$$\begin{aligned}
& \overline{\rho \alpha} \frac{\partial}{\partial t} \left(\frac{\partial \tilde{u}_i}{\partial x_j} \right) + \overline{\rho \alpha \tilde{u}_n} \frac{\partial}{\partial x_n} \left(\frac{\partial \tilde{u}_i}{\partial x_j} \right) = -\overline{\alpha} \frac{\partial}{\partial x_i} \left(\frac{\partial \bar{p}}{\partial x_j} \right) - \frac{\partial}{\partial x_n} \left(\overline{\rho \alpha u_n''} \frac{\partial u_i''}{\partial x_j} \right) \\
& + \overline{\alpha} \frac{\partial}{\partial x_n} \left(\frac{\partial \tau_{in}}{\partial x_j} \right) - \overline{\rho \alpha} \frac{\partial u_n''}{\partial x_j} \frac{\partial u_i''}{\partial x_n} - \overline{\rho \alpha} \frac{\partial \tilde{u}_n}{\partial x_j} \frac{\partial \tilde{u}_i}{\partial x_n} + \frac{\overline{\alpha \partial \rho}}{\rho} \frac{\partial \bar{p}}{\partial x_i} - \frac{\overline{\alpha \partial \rho}}{\rho} \frac{\partial \tau_{in}}{\partial x_j} \frac{\partial \tau_{in}}{\partial x_n}. \quad (44)
\end{aligned}$$

Subtracting Eq. (44) from Eq. (43) then multiplying the resulting equation with $\frac{\partial c''}{\partial x_i} \frac{\partial c''}{\partial x_j}$ and

Favre averaging leads to:

$$\begin{aligned}
& \overline{\rho \alpha} \frac{\partial c''}{\partial x_i} \frac{\partial c''}{\partial x_j} \frac{D}{Dt} \left(\frac{\partial u_i''}{\partial x_j} \right) = -\overline{\rho \alpha} \frac{\partial c''}{\partial x_i} \frac{\partial c''}{\partial x_j} u_n'' \frac{\partial}{\partial x_n} \left(\frac{\partial \tilde{u}_i}{\partial x_j} \right) \\
& - \overline{\alpha} \frac{\partial c''}{\partial x_i} \frac{\partial c''}{\partial x_j} \frac{\partial}{\partial x_i} \left(\frac{\partial \bar{p}'}{\partial x_j} \right) + \overline{\alpha} \frac{\partial c''}{\partial x_i} \frac{\partial c''}{\partial x_j} \frac{\partial}{\partial x_n} \left(\frac{\partial \tau_{in}}{\partial x_j} \right) + \overline{\frac{\partial c''}{\partial x_i} \frac{\partial c''}{\partial x_j} \frac{\partial}{\partial x_n} \left(\overline{\rho \alpha u_n''} \frac{\partial u_i''}{\partial x_j} \right)} \\
& - \overline{\rho \alpha} \frac{\partial c''}{\partial x_i} \frac{\partial c''}{\partial x_j} \frac{\partial u_n''}{\partial x_j} \frac{\partial u_i''}{\partial x_n} - \overline{\rho \alpha} \frac{\partial c''}{\partial x_i} \frac{\partial c''}{\partial x_j} \frac{\partial u_n''}{\partial x_j} \frac{\partial \tilde{u}_i}{\partial x_n} \\
& - \overline{\rho \alpha} \frac{\partial \tilde{u}_n}{\partial x_j} \frac{\partial c''}{\partial x_j} \frac{\partial c''}{\partial x_i} \frac{\partial u_i''}{\partial x_n} + \overline{\rho \alpha} \frac{\partial c''}{\partial x_i} \frac{\partial c''}{\partial x_j} \frac{\partial u_n''}{\partial x_j} \frac{\partial u_i''}{\partial x_n} \\
& + \overline{\alpha} \frac{\partial \rho}{\partial x_j} \frac{\partial P'}{\partial x_i} \frac{\partial c''}{\partial x_j} \frac{\partial c''}{\partial x_i} \frac{1}{\rho} - \overline{\alpha} \frac{\partial \rho}{\partial x_j} \frac{\partial \tau_{in}}{\partial x_n} \frac{\partial c''}{\partial x_i} \frac{\partial c''}{\partial x_j} \frac{1}{\rho}. \quad (45)
\end{aligned}$$

Replacing terms 1 and 2 in Eq. (14) leads to $\tilde{\Delta}_c$ transport equation as given in Eq. (16).

Appendix-B

The scaling arguments explained in section 2 are applied to Eq. (14) to identify leading order terms. A number of simplifications have been made while carrying out the analysis. It is assumed that in the high Re limit, the contributions from the viscous tensor will be small. Hence it is assumed that $\tau_{in} \approx 2\mu S_{in}$, $\mu \approx \rho \alpha$ and the spatial gradients of density associated with τ_{in} are very small when compared with other terms.

The first term on the left-hand side of Eq. (16) can be decomposed into two parts as :

$$\bar{\rho} \frac{D}{Dt} \left(\overline{\alpha \frac{\partial c''}{\partial x_i} S_{ij}'' \frac{\partial c''}{\partial x_j}} \right) = \underbrace{\frac{\partial}{\partial t} \left(\overline{\rho \alpha \frac{\partial c''}{\partial x_i} S_{ij}'' \frac{\partial c''}{\partial x_j}} \right)}_{\text{Term 1}} + \underbrace{\frac{\partial}{\partial x_n} \left(\overline{\rho \alpha \tilde{u}_n \frac{\partial c''}{\partial x_i} S_{ij}'' \frac{\partial c''}{\partial x_j}} \right)}_{\text{Term 2}}, \quad (46)$$

where

$$\frac{\partial}{\partial t} \left(\overline{\rho \alpha \frac{\partial c''}{\partial x_i} S_{ij}'' \frac{\partial c''}{\partial x_j}} \right) \simeq \mathcal{O} \left(\rho_u \left(\frac{u_L^0}{\delta_L^0} \right)^3 ; Da^{-1} \right)$$

and

$$\frac{\partial}{\partial x_n} \left(\overline{\rho \alpha \tilde{u}_n \frac{\partial c''}{\partial x_i} S_{ij}'' \frac{\partial c''}{\partial x_j}} \right) \simeq \mathcal{O} \left(\rho_u \left(\frac{u_L^0}{\delta_L^0} \right)^3 ; \left(\frac{u' Da}{u_{ref}} \right)^{-1} \right).$$

The first term on the right-hand side of Eq. (16) scales as:

$$\frac{\partial}{\partial x_n} \left(\overline{\rho \alpha u_n'' \frac{\partial c''}{\partial x_i} S_{ij}'' \frac{\partial c''}{\partial x_j}} \right) \simeq \mathcal{O} \left(\rho_u \left(\frac{u_L^0}{\delta_L^0} \right)^3 ; (Re_l Da)^{-1/2} \right).$$

D_{f1} represents the diffusion/dissipation terms arising from the scalar part of the $\tilde{\Delta}_c$ transport equation. Following Swaminathan and Bray [35] term D_{f1} can be expanded and simplified based on the assumption that the second gradient of ρ is small compared with the other terms, thus leading to:

$$\begin{aligned} \overline{\frac{\partial c''}{\partial x_i} S_{ij}'' \frac{\partial}{\partial x_j} \left(\frac{\partial}{\partial x_n} \left(\rho \alpha \frac{\partial c''}{\partial x_n} \right) \right)} &= \underbrace{\frac{\partial}{\partial x_n} \left(\overline{\rho \alpha \frac{\partial}{\partial x_n} \left(\alpha \frac{\partial c''}{\partial x_i} S_{ij}'' \frac{\partial c''}{\partial x_j} \right)} \right)}_{Df11} \\ &\quad - \underbrace{\overline{\rho \alpha \alpha \frac{\partial}{\partial x_n} \left(\frac{\partial c''}{\partial x_j} \right) \frac{\partial}{\partial x_n} \left(\frac{\partial c''}{\partial x_i} S_{ij}'' \right)}}_{Df12} - \underbrace{\overline{\rho \alpha \alpha \frac{\partial}{\partial x_n} \left(\frac{\partial c''}{\partial x_i} \frac{\partial c''}{\partial x_j} \frac{\partial}{\partial x_n} S_{ij}'' \right)}}_{Df13} \\ &\quad - \underbrace{\overline{\rho \alpha \alpha \frac{\partial}{\partial x_n} \left(\frac{\partial c''}{\partial x_j} S_{ij}'' \frac{\partial}{\partial x_n} \left(\frac{\partial c''}{\partial x_i} \right) \right)}}_{Df14}. \end{aligned}$$

Terms D_{f1i} scale as :

$$D_{f11} \simeq \mathcal{O} \left(\rho_u \left(\frac{u_L^0}{\delta_L^0} \right)^3 ; (Da u')^{-1} \right),$$

$$D_{f12}, D_{f13}, D_{f14} \simeq \mathcal{O} \left(\rho_u \left(\frac{u_L^0}{\delta_L^0} \right)^3 ; 1 \right),$$

Term D_{f2} represents the diffusion/dissipation from the momentum part of the $\tilde{\Delta}_c$ transport equation and scales as:

$$D_{f2} \simeq \mathcal{O} \left(\rho_u \left(\frac{u_L^0}{\delta_L^0} \right)^3 ; 1 \right).$$

Terms F_{1i} representing the source terms scale as :

$$F_{11}, F_{12} \simeq \mathcal{O} \left(\rho_u \left(\frac{u_L^0}{\delta_L^0} \right)^3 ; 1 \right),$$

Terms F_{2i} representing the terms arising due to the turbulent transport of $\tilde{\Delta}_c$ scale as :

$$F_{21}, F_{23} \simeq \mathcal{O} \left(\rho_u \left(\frac{u_L^0}{\delta_L^0} \right)^3 ; \frac{u_L^0 Da^{-1}}{u'} \right),$$

$$F_{22} \simeq \mathcal{O} \left(\rho_u \left(\frac{u_L^0}{\delta_L^0} \right)^3 ; (Re_l Da)^{-1} \right),$$

$$F_{24} \simeq \mathcal{O} \left(\rho_u \left(\frac{u_L^0}{\delta_L^0} \right)^3 ; \left(\frac{u_{ref} Da^{-3/2} Re_l^{-1/2}}{u'} \right) \right).$$

Terms F_{3i} representing the dilatation terms scale as :

$$F_{31}, F_{34}, F_{35}, F_{36} \simeq \mathcal{O} \left(\rho_u \left(\frac{u_L^0}{\delta_L^0} \right)^3 ; 1 \right),$$

$$F_{32} \simeq \mathcal{O} \left(\rho_u \left(\frac{u_L^0}{\delta_L^0} \right)^3 ; \left(\frac{u' Da}{u_{ref}} \right)^{-1} \right),$$

$$F_{33} \simeq \mathcal{O} \left(\rho_u \left(\frac{u_L^0}{\delta_L^0} \right)^3 ; (Re_l Da)^{-1/2} \right),$$

Terms F_{4i} representing the turbulent straining terms scale as :

$$F_{41}, F_{44}, F_{45}, F_{48} \simeq \mathcal{O} \left(\rho_u \left(\frac{u_L^0}{\delta_L^0} \right)^3 ; 1 \right),$$

$$F_{42}, F_{46}, F_{47} \simeq \mathcal{O} \left(\rho_u \left(\frac{u_L^0}{\delta_L^0} \right)^3 ; \left(\frac{u' Da}{u_{ref}} \right)^{-1} \right),$$

$$F_{43} \simeq \mathcal{O} \left(\rho_u \left(\frac{u_L^0}{\delta_L^0} \right)^3 ; (Re_t Da)^{-1/2} \right),$$

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Fig. 1 Computational domain for the V-flame DNS

u'_{in}/u_L^0	$\bar{u}_{in}/u_L^0$	$Re_{l,in}$	$l_{t,in}/\delta_L^0$	Ka_{in}	Da_{in}
2.0	16.6	37	12.82	0.79	6.41

Table 1 DNS database parameters at inlet plane

Sampling location	u' / u_L^0	Re_{l_t}	l_t / δ_L^0	Ka	Da
Region a	1.51	22.16	10.0	0.50	9.94
Region b	1.48	17.56	8.6	0.49	9.09
Region c	1.41	22.16	9.8	0.46	10.31

Table 2 DNS database parameters at the sampling locations

Sampling location	$Re_{l_t} \times Da$	n_e	n_g	$2(1+\tau)^{0.7} \left(\frac{N_x}{n_g} n_e \right)^2$
Region a	220.3	1.48	28	889
Region b	159.62	1.72	30	1047
Region c	228.47	1.51	29	863

Table 3 The numerical resolution criterion of Poinot et al [29]

Fig. 2 Favre averaged progress variable $\tilde{c}$ contours 0.1 – 0.9. The dashed lines represent the sampling locations, and the solid line represents the flame centre line.

Fig. 3 Spatial variation of instantaneous progress variable at different times compared with the Favre averaged progress variable. The symbols represent exact grid points inside the domain.

Fig. 4 Convergence of D_f in time for different realisations of the flow field. The values are normalised using the respective ρ_u, u_L^0 and δ_L^0 .

Fig. 5 Pdfs of the direction cosines and the associated angles at $y^+ \approx 23$

Fig. 6 Pdfs of the direction cosines and the associated angles at $y^+ \approx 25$

Fig. 7 Pdfs of the direction cosines and the associated angles at $y^+ \approx 27$

Fig. 8 Normalised dilatation in the V-flame DNS

Fig. 9 Leading order terms. The values are normalised using the respective ρ_u, u_L^0 and δ_L^0 .

Fig. 10 Leading order terms without the diffusion/dissipation and source terms. The values are normalised using the respective ρ_u, u_L^0 and δ_L^0 .

Fig. 11 Comparisons of F_{TS} model predictions and the DNS results. The values are normalised using the respective ρ_u, u_L^0 and δ_L^0 .

Fig. 12 Comparisons of F_D model predictions and the DNS results. The values are normalised using the respective ρ_u, u_L^0 and δ_L^0 .

Fig. 13 Comparisons of $(D_f + F_1)$ model predictions and the DNS results. The values are normalised using the respective ρ_u, u_L^0 and δ_L^0 .