

# Effects of Lewis number on conditional fluid velocity statistics in low Damköhler number turbulent premixed combustion: A direct numerical simulation analysis

Nilanjan Chakraborty<sup>1,a)</sup> and Andrei N. Lipatnikov<sup>2</sup>

<sup>1</sup>*School of Mechanical and Systems Engineering, Newcastle University, Claremont Road, Newcastle-Upon-Tyne NE1 7RU, United Kingdom*

<sup>2</sup>*Department of Applied Mechanics, Chalmers University of Technology, Gothenburg 412 96, Sweden*

(Received 13 October 2012; accepted 28 February 2013; published online 1 April 2013)

The effects of global Lewis number  $Le$  on the statistics of fluid velocity components conditional in unburned reactants and fully burned products in the context of Reynolds Averaged Navier Stokes simulations have been analysed using a Direct Numerical Simulations (DNS) database of statistically planar turbulent premixed flames with a low Damköhler number and Lewis number ranging from 0.34 to 1.2. The conditional velocity statistics extracted from DNS data have been analysed with respect to the well-known Bray-Moss-Libby (BML) expressions which were derived based on bi-modal probability density function of reaction progress variable for high Damköhler number flames. It has been shown that the Lewis number substantially affects the mean velocity and the velocity fluctuation correlation conditional in products, with the effect being particularly pronounced for low  $Le$ . As far as the mean velocity and the velocity fluctuation correlation conditional in reactants are concerned, the BML expressions agree reasonably well with the DNS data reported in the present work. Based on *a priori* analysis of present and previously reported DNS data, the BML expressions have been empirically modified here in order to account for Lewis number effects, and the non-bimodal distribution of reaction progress variable. Moreover, it has been demonstrated for the first time that surface averaged velocity components and Reynolds stresses conditional in unburned reactants can be modelled without invoking expressions involving the Lewis number, as these surface averaged conditional quantities remain approximately equal to their conditionally averaged counterparts in the unburned mixture. © 2013 American Institute of Physics. [<http://dx.doi.org/10.1063/1.4795548>]

## I. INTRODUCTION

Statistics of fluid velocity conditional in unburned reactants and fully burned products are of fundamental importance in turbulent premixed combustion.<sup>1–7</sup> The analysis of Bray *et al.*<sup>1</sup> relates the turbulent scalar flux  $\overline{\rho u_i'' c''}$  to the slip velocity  $\overline{(u_i)_P} - \overline{(u_i)_R}$ , where  $\rho$  is the fluid density,  $u_i$  is the  $i$ th component of fluid velocity,  $q'' = q - \tilde{q}$ ,  $\tilde{q} = \overline{\rho q} / \bar{\rho}$  are the Favre fluctuation and Favre mean of a general quantity  $q$ , with the overbar suggesting a suitable Reynolds averaging operation. The subscripts R and P are used to denote the conditional Reynolds averaged values in reactants and products, respectively. In addition to the conditional mean velocities (i.e.,  $\overline{(u_i)_R}$  and  $\overline{(u_i)_P}$ ), the surface-weighted mean velocities conditional in reactants and products (i.e.,  $\overline{(u_i)_{R_s}}$  and  $\overline{(u_i)_{P_s}}$ ), play a pivotal role in the modelling of turbulent premixed flames using Flame Surface Density (FSD)<sup>3,5,8,9</sup> and conditional mean equations<sup>6,7,10–13</sup> based methodologies. Moreover, conditional

<sup>a)</sup>Email: [nilanjan.chakraborty@newcastle.ac.uk](mailto:nilanjan.chakraborty@newcastle.ac.uk). Telephone: +44 0191 222 3570. Fax: +44 0191 222 8600.

velocity statistics are useful for modelling the pressure gradient related terms in the transport equations for turbulent kinetic energy and turbulent scalar fluxes, as demonstrated by Domingo and Bray.<sup>4</sup>

In conventional Reynolds Averaged Navier Stokes (RANS) simulations, the conditional mean velocities  $\overline{(u_i)}_R$  and  $\overline{(u_i)}_P$  are needed to evaluate turbulent scalar flux  $\overline{\rho u_i'' c''}$ , whereas Reynolds stresses conditional in reactants and products (i.e.,  $\overline{(u_i' u_j')}_R$  and  $\overline{(u_i' u_j')}_P$ ) are used for the closure of  $\overline{\rho u_i'' u_j''}$ . Alternatively, it is possible to obtain  $\overline{(u_i)}_R$  and  $\overline{(u_i)}_P$  ( $\overline{(u_i' u_j')}_R$  and  $\overline{(u_i' u_j')}_P$ ) from  $\tilde{u}_i$  and  $\overline{\rho u_i'' c''}$  ( $\overline{\rho u_i'' u_j''}$ ) using algebraic expressions. In either of these methodologies, the Bray-Moss-Libby<sup>1</sup> expressions are commonly invoked. They result straightforwardly from a hypothesis that the probability density function (pdf) of  $c$  (i.e.,  $P(c)$ ) is bi-modal in nature,<sup>1</sup> which is valid for high Damköhler number flames (i.e.,  $Da \gg 1$ ), but may be rendered invalid for small values of Damköhler number, i.e.,  $Da < 1$ . Recently, Chakraborty and Lipatnikov<sup>14</sup> assessed the performance of the BML expressions (the expressions which can be derived based on presumed bi-modal pdf of  $c$  are referred to as the BML expressions in this paper) for evaluating  $\overline{(u_i)}_R$ ,  $\overline{(u_i)}_P$ ,  $\overline{(u_i' u_j')}_R$ , and  $\overline{(u_i' u_j')}_P$  by *a priori* analysis of a Direct Numerical Simulation (DNS) database of freely propagating turbulent premixed flames characterised by a large Damköhler number associated with the corrugated flamelets regime combustion.<sup>15</sup> The obtained results have indicated that although the BML approach is capable for predicting the relations between  $\overline{(u_i)}_R$ ,  $\overline{(u_i)}_P$ ,  $\tilde{u}_i$ , and  $\overline{\rho u_i'' c''}$  under conditions of  $Da \gg 1$ , a slight departure from bi-modal distribution of  $P(c)$  has major influences on the predictions of conditional Reynolds stresses  $\overline{(u_i' u_j')}_R$  and  $\overline{(u_i' u_j')}_P$  even in high  $Da$  flames. Nevertheless, DNS data analysed in a subsequent paper by Chakraborty and Lipatnikov<sup>16</sup> implies that the BML expressions may be useful for evaluating  $\overline{(u_i)}_R$ ,  $\overline{(u_i)}_P$ ,  $\overline{(u_i' u_j')}_R$ , and  $\overline{(u_i' u_j')}_P$  even at low  $Da$  for unity Lewis number flames. However, this does not necessarily imply that BML expressions are valid for low  $Da$  combustion but some of the expressions derived based on presumed bi-modal pdf of  $c$  might perform reasonably well beyond the regime for which the BML methodology is strictly valid. It is worth noting that Damköhler number provides the ratio of large scale turbulent time scale to chemical time scale and thus small (large) values of  $Da$  are commonly associated with thick (thin) reaction zone. However, recent experimental<sup>17–21</sup> and DNS<sup>22–25</sup> data demonstrate that reaction zones remain thin even at very small (large) values of Damköhler (Karlovitz) number.

The state of the reacting mixture in premixed flames is often characterised by a single reaction progress variable, where the molecular diffusivities of all species are taken to be equal to the molecular thermal diffusivity.<sup>1–7,10–14,16</sup> In actual combustion processes, diffusion of different species and heat are characterised by their respective diffusivities. As a result, local mixture composition and temperature are affected by imbalance between local diffusion of main reactants and heat and such phenomena strongly affect turbulent burning rate, as reviewed in Ref. 26. Differential diffusion of heat and mass is commonly accounted for by characterizing the mixture composition by two scalar quantities, namely, the normalised mass fraction of the deficient reactant, and the non-dimensional temperature, as well as the ratio of the thermal diffusivity to molecular diffusivity of the deficient reactant, which is commonly known as the Lewis number  $Le$ . Such an approach is typical for both theoretical<sup>27–29</sup> and DNS<sup>30–37</sup> studies, which have addressed various effects associated with differential diffusion rates of heat and mass. However, to the best of our knowledge, the effects of non-unity Lewis number  $Le$  on the statistical behaviours of conditional mean and surface-weighted velocity components and Reynolds stresses are yet to be addressed in the literature. To date, there is no analysis in the open literature about the evaluation of conditional mean velocities in low  $Da$  non-unity Lewis number combustion where BML analysis is not strictly valid. In this study, this gap is filled by analysing the statistics of conditional mean velocities using a DNS database of low Damköhler number (i.e.,  $Da < 1$ ) turbulent premixed flames for different values of Lewis number  $Le$  ranging from 0.34 to 1.2.

In this respect, the main objectives of this study are as follows:

1. To analyse the statistical behaviours of the conditional mean velocity and their relation to the Favre mean velocity in the context of RANS for low Damköhler number non-unity Lewis number combustion.

2. To identify the expressions for extracting conditional mean velocities from Favre mean velocities, which are valid for a range of values of  $Le$ .

It is worth stressing that, to the best of our knowledge, the influences of  $Le$  on conditioned velocities and Reynolds stresses have not yet been addressed in the literature and therefore the present analysis attempts for the very first time to parameterize the conditional velocity statistics in low Damköhler number flames for a wide range of values of global Lewis number.

The rest of the paper will be organised as follows. The necessary mathematical background will be provided in Sec. II of the paper. This will be followed by a brief discussion on numerical implementation. Following this, results will be presented and subsequently discussed. Finally, main findings will be summarised and conclusions will be drawn.

## II. MATHEMATICAL BACKGROUND

In principle DNS of turbulent reacting flows should account for both three-dimensionality of turbulence and detailed chemical structure of the flame. However, the limitation of computer storage capacity until recently restricted DNS either to two dimensions with detailed chemistry or in three dimensions with simplified chemistry. As turbulent velocity field is inherently three-dimensional in nature and vortex stretching mechanism is absent in two dimensions, the second approach takes precedence in the present study, which is based on a single-step irreversible Arrhenius type chemistry. Although it is now possible to carry out three-dimensional DNS with detailed chemistry, the computational cost associated with them are much too high (e.g., several millions of CPU hours)<sup>38</sup> to carry out an extensive parametric analysis as done in this analysis. As the present paper deals with the effects of global Lewis number on the conditional fluid velocity statistics in turbulent premixed flames, three-dimensional simplified chemistry based DNS data with different values of  $Le$  is considered to be sufficient for the present analysis. In this analysis, the reaction progress variable  $c$  is defined in terms of the mass fraction of a suitable reactant  $Y_R$  (e.g., fuel mass fraction  $Y_F$ ) in the following manner:

$$c = (Y_{R0} - Y_R)/(Y_{R0} - Y_{R\alpha}), \quad (1)$$

where subscripts 0 and  $\alpha$  indicate values in pure reactants and in fully burned products, respectively.

The BML expressions are expected to work well for high values of Damköhler number (i.e.,  $Da > 1$ )<sup>1,2</sup> and it has been found that conditional velocity statistics in unity Lewis number flames under  $Da < 1$  combustion can reasonably be parameterised by incorporating moderate modifications to the conventional BML expressions in such a manner that they recover the correct limiting behaviour for  $Da \rightarrow \infty$  and  $Le \rightarrow 1$ . Thus, it is worth summarising the derivation and the assumptions pertinent to the BML expressions.

The pdf of reaction progress variable  $c$  and the joint pdf of velocity vector  $\vec{u}$  and  $c$  according to BML analysis are given by (Refs. 1 and 2)

$$P(c; \vec{x}) = \alpha_c(\vec{x})\delta(c) + \beta_c(\vec{x})\delta(1 - c) + \gamma_c(\vec{x})f_1(c; \vec{x})[H(c) - H(c - 1)], \quad (2a)$$

$$P(\vec{u}, c; \vec{x}) = \alpha_c(\vec{x})P_R(\vec{u}; 0; \vec{x})\delta(c) + \beta_c(\vec{x})P_P(\vec{u}; 1; \vec{x})\delta(1 - c) + \gamma_c(\vec{x})f_2(\vec{u}, c; \vec{x})[H(c) - H(c - 1)], \quad (2b)$$

where  $\alpha_c$ ,  $\beta_c$ , and  $\gamma_c$  are the coefficients for the progress variable pdf,  $P_R(\vec{u}; \vec{x})$  and  $P_P(\vec{u}; \vec{x})$  refer to pdfs of  $\vec{u}$  in reactants and products, respectively, and the functions  $f_1$  and  $f_2$  originate due to burning gases at the interior of the flame. It is assumed that  $P_R(\vec{u}; \vec{x})$ ,  $P_P(\vec{u}; \vec{x})$ , and  $f_2(\vec{u}, c; \vec{x})$  are normalised in such a manner that they individually integrate to unity.<sup>1,2</sup> The last term on the right hand side of Eqs. (2a) and (2b) refers to the contribution of burning fluid and scales with  $1/Da$  and thus this term might have non-negligible effects for  $Da < 1$ . Based on the presumed pdfs given by Eqs. (2a) and (2b), one obtains

$$\int_0^1 P(c)dc = \alpha_c + \beta_c + O(\gamma_c) = 1 \quad \text{and} \quad \bar{\rho} = \int_0^1 \rho_c P(c)dc = \alpha_c \rho_0 + \beta_c \bar{\rho}_b + O(\gamma_c), \quad (3)$$

where  $\bar{\rho}_b$  is the mean burned gas density,  $\rho_0$  is the unburned gas density, and  $\rho_c$  is the mean value of density conditional on  $c$ . For low Mach number adiabatic unity Lewis number flames  $\rho_c$  and  $\bar{\rho}_b$  are given by:  $\rho_c = 1/(1 + \tau c)$  and  $\bar{\rho}_b = 1/(1 + \tau)$ . If  $Le \neq 1$ , then the mean product density  $\bar{\rho}_b$  depends on the Lewis number. The contribution of  $O(\gamma_c)$  scales as  $O(\gamma_c) \sim O(1/Da)$  and thus for large values of Damköhler number (i.e.,  $Da \gg 1$ ) the contribution of  $O(\gamma_c)$  becomes negligible in Eq. (3) which yields the following expressions of  $\alpha_c$  and  $\beta_c$  for unity Lewis number flames:

$$\alpha_c = (1 - \tilde{c})/(1 + \tau \tilde{c}) \text{ and } \beta_c = (1 + \tau)\tilde{c}/(1 + \tau \tilde{c}). \quad (4)$$

Based on Eq. (2), one obtains the following relation for the Favre mean velocity components  $\tilde{u}_i$  (Refs. 1 and 2):

$$\tilde{u}_i = \int_{-\alpha}^{\alpha} \int_0^1 \rho u_i P(\tilde{u}, c) dc d\tilde{u} / \bar{\rho} = \overline{(u_i)_R} (1 - \tilde{c}) + \overline{(u_i)_P} \tilde{c} + O(\gamma_c). \quad (5)$$

The conditional mean values in unburned reactants and products (i.e.,  $\overline{(q)_R}$  and  $\overline{(q)_P}$ ) for a general quantity  $q$  which is dependent on  $\tilde{u}$ , are evaluated as

$$\begin{aligned} \overline{(q)_R} &= \int_0^{\varepsilon} \int_{-\alpha}^{\alpha} q P(c, \tilde{u}) d\tilde{u} dc \bigg/ \int_0^{\varepsilon} \int_{-\alpha}^{\alpha} P(c, \tilde{u}) d\tilde{u} dc \\ \text{and } \overline{(q)_P} &= \int_{1-\varepsilon}^1 \int_{-\alpha}^{\alpha} q P(c, \tilde{u}) d\tilde{u} dc \bigg/ \int_{1-\varepsilon}^1 \int_{-\alpha}^{\alpha} P(c, \tilde{u}) d\tilde{u} dc, \end{aligned} \quad (6)$$

where  $\varepsilon$  is a small number (i.e.,  $0 < \varepsilon \ll 1$ ). It is possible to obtain the following relation for turbulent scalar flux  $\overline{\rho u_i'' c''}$  using Eqs. (2b) and (5) (Refs. 1 and 2):

$$\overline{\rho u_i'' c''} = \int_{-\alpha}^{\alpha} \int_0^1 \rho (u_i - \tilde{u}_i)(c - \tilde{c}) P(\tilde{u}, c) dc d\tilde{u} = \bar{\rho} [\overline{(u_i)_P} - \overline{(u_i)_R}] \tilde{c} (1 - \tilde{c}) + O(\gamma_c). \quad (7)$$

Using Eqs. (5) and (7), one obtains the following relations for  $\overline{(u_i)_R}$  and  $\overline{(u_i)_P}$ :

$$\overline{(u_i)_R} = \tilde{u}_i - \overline{\rho u_i'' c''} / \bar{\rho} (1 - \tilde{c}), \quad (8a)$$

$$\overline{(u_i)_P} = \tilde{u}_i + \overline{\rho u_i'' c''} / \bar{\rho} \tilde{c}. \quad (8b)$$

Using Eq. (2b) it is possible to obtain the following expressions of  $\overline{\rho u_i'' u_j''}$  and  $\overline{\rho u_i'' u_j'' c''}$ :

$$\begin{aligned} \overline{\rho u_i'' u_j''} &= \int_{-\alpha}^{\alpha} \int_0^1 \rho (u_i - \tilde{u}_i)(u_j - \tilde{u}_j) P(\tilde{u}, c) dc d\tilde{u} \\ &= \bar{\rho} [\overline{(u_i)_P} - \overline{(u_i)_R}] [\overline{(u_j)_P} - \overline{(u_j)_R}] \tilde{c} (1 - \tilde{c}) + \bar{\rho} \overline{(u_i' u_j')_R} (1 - \tilde{c}) + \bar{\rho} \overline{(u_i' u_j')_P} \tilde{c} + O(\gamma_c), \end{aligned} \quad (9a)$$

$$\begin{aligned} \overline{\rho u_i'' u_j'' c''} &= \int_{-\alpha}^{\alpha} \int_0^1 \rho (u_i - \tilde{u}_i)(u_j - \tilde{u}_j)(c - \tilde{c}) P(\tilde{u}, c) dc d\tilde{u} \\ &= \bar{\rho} [\overline{(u_i)_P} - \overline{(u_i)_R}] [\overline{(u_j)_P} - \overline{(u_j)_R}] \tilde{c} (1 - \tilde{c}) (1 - 2\tilde{c}) - \bar{\rho} \overline{(u_i' u_j')_R} \tilde{c} (1 - \tilde{c}) + \bar{\rho} \overline{(u_i' u_j')_P} \tilde{c} (1 - \tilde{c}) + O(\gamma_c). \end{aligned} \quad (9b)$$

The expressions for Reynolds stresses conditional in reactants and products (i.e.,  $\overline{(u'_i u'_j)}_R$  and  $\overline{(u'_i u'_j)}_P$ ) can be obtained using Eqs. (7), (9a), and (9b) in the following manner:

$$\overline{(u'_i u'_j)}_R = \frac{\rho u''_i u''_j}{\bar{\rho}} - \frac{\rho u''_i u''_j c''}{\bar{\rho}(1 - \tilde{c})} - \frac{\rho u''_i c''}{\bar{\rho}^2} \frac{\rho u''_j c''}{(1 - \tilde{c})^2} \quad \text{and} \quad \overline{(u'_i u'_j)}_P = \frac{\rho u''_i u''_j}{\bar{\rho}} + \frac{\rho u''_i u''_j c''}{\bar{\rho}\tilde{c}} - \frac{\rho u''_i c''}{\bar{\rho}^2} \frac{\rho u''_j c''}{\tilde{c}^2}. \quad (10)$$

It is worth noting that Eqs. (8)–(10) are strictly valid for high Damköhler number (i.e.,  $Da \gg 1$ ) flames. It remains to be seen how these relations (Eqs. (8)–(10)) perform for low Damköhler number non-unity Lewis number flames and this will be addressed in Sec. IV of this paper.

The surface averaged value of fluid velocity component  $\overline{(u_i)}_s$  is expressed in the following manner:

$$\overline{(u_i)}_s = \overline{u_i} |\nabla c| / \Sigma_{gen}, \quad (11)$$

where  $\Sigma_{gen}$  is the generalised flame surface density (i.e.,  $\Sigma_{gen} = |\nabla c|$ ).<sup>9,39</sup> Conditional surface averaged quantities such as  $\overline{(u_i)}_{Rs}$  and  $\overline{(u_i u_j)}_{Rs}$  play a key role in the balance equations for conditional velocities and Reynolds stresses.<sup>10</sup> A simple model for  $\overline{(u_i)}_{Rs}$  is proposed in Ref. 10 based on the DNS data by Im *et al.*<sup>6</sup>

$$\overline{(u_i)}_{Rs} = \overline{(u_i)}_R. \quad (12)$$

For a hypothetical fully developed, constant-density, statistically planar, one-dimensional flame propagating from right to left  $\overline{(u_1)}_R \rightarrow \bar{u}_1 = S_T$  in the reference frame attached to the flame, whereas  $\overline{(u_1)}_{Rs} \rightarrow S_L < S_T$ , because the instantaneous propagation velocity of a flamelet ( $u_1 - S_L$ ) that reaches the leading edge should be equal to zero in the selected reference frame (otherwise the flamelet would cross the leading edge, that is impossible by the definition). Therefore, Eq. (12) yields wrong result at  $\tilde{c} \rightarrow 0$  in this simple case. For these reasons, the following linear interpolation has also been proposed in Ref. 10:

$$\overline{(u_i)}_{Rs} = \langle c \rangle \overline{(u_i)}_R + (1 - \langle c \rangle) \{ \overline{(u_i)}_P + (1/\sigma - 1) M_i M_j \overline{(u_j)}_P \}. \quad (13)$$

Here,  $\sigma = (1 + \tau)$  and  $M_i = \partial \langle c \rangle / \partial x_i / |\nabla \langle c \rangle|$  in which  $\langle c \rangle$  is either equal to  $\bar{c}$  or equal to  $\tilde{c}$ . This model effectively ensures that  $\overline{(u_i)}_{Rs} \rightarrow \overline{(u_i)}_P / \sigma$  when either  $\bar{c} \rightarrow 0$  or  $\tilde{c} \rightarrow 0$ . Similarly,  $\overline{(u_i)}_{Rs} \rightarrow \overline{(u_i)}_R$  when either  $\bar{c} \rightarrow 1$  or  $\tilde{c} \rightarrow 1$  according to Eq. (13). In deriving Eq. (13), it is assumed that, at the leading and trailing edges, (i) the flamelet is parallel to the flame brush (i.e.,  $M_i = N_i = \partial c / \partial x_i / |\nabla c|$ ); (ii) the velocity component tangential to the flamelet is assumed to be unaffected by the local heat release (i.e.,  $(u_i)_R - N_i N_j (u_j)_R = (u_i)_P - N_i N_j (u_j)_P$ ); (iii) the velocity component normal to the flamelet is taken to be equal to laminar burning velocity (i.e.,  $(u_i)_R N_i \rightarrow S_L$  and  $(u_i)_P N_i \rightarrow \sigma S_L$ ). The performance of the expressions given by Eqs. (12) and (13) for non-unity Lewis number flames with small values of Damköhler number (i.e.,  $Da < 1$ ) will be assessed in Sec. IV of this paper.

### III. NUMERICAL IMPLEMENTATION

The simulations have been carried out using a three-dimensional DNS code called SENGAs where mass, momentum, energy, and species transport equations are solved in non-dimensional form.<sup>40</sup> The simulation domain is taken to be a cube of size  $24.1\delta_{th} \times 24.1\delta_{th} \times 24.1\delta_{th}$  where the thermal flame thickness  $\delta_{th}$  is given by  $\delta_{th} = (T_{ad} - T_0) / \text{Max} |\nabla \hat{T}|_L$  where subscript L refers to the quantities in unstrained planar laminar flame. For the cubic domain, the boundaries in the direction of mean flame propagation (i.e.,  $x_1$  direction) are taken to be partially non-reflecting whereas the transverse boundaries are taken to be periodic. The partially non-reflecting boundaries are specified using the Navier Stokes Characteristic Boundary Conditions (NSCBC) formulation.<sup>41</sup> All the spatial derivatives for all the internal grid points are evaluated using a 10th order central difference scheme and the order of differentiation drops gradually to a 2nd order one-sided scheme near non-periodic boundaries. The time advancement is carried out using an explicit 3rd order low storage Runge-Kutta scheme.<sup>42</sup> For all the simulations, turbulent velocity field is initialised

TABLE I. Initial values of simulation parameters and non-dimensional numbers relevant to the DNS database.

Le	$u'/S_L$	$l/\delta_L$	$l/\delta_{th}$	$\tau$	$Re_t$	$Da$
0.34	7.5	1.13	2.45	4.5	47.0	0.33
0.6	7.5	1.76	2.45	4.5	47.0	0.33
0.8	7.5	2.13	2.45	4.5	47.0	0.33
1.0	7.5	2.45	2.45	4.5	47.0	0.33
1.2	7.5	2.72	2.45	4.5	47.0	0.33

with the help of a standard pseudo-spectral method<sup>43</sup> using Batchelor-Townsend<sup>44</sup> turbulent kinetic energy spectrum. The flame is initialised by an unstrained planar steady laminar flame solution. The grid resolution is determined by the resolution of flame and in all cases about 10 grid points are kept within  $Max(\delta_L, \delta_{th})$  where  $\delta_L = 1/Max|\nabla c|_L$  is an alternative flame thickness, which is greater (smaller) than  $\delta_{th}$  for the  $Le < 1$  ( $Le > 1$ ) flames. The thicknesses  $\delta_L$  and  $\delta_{th}$  are equal to each other for the unity Lewis number flames. The thermo-chemical parameters for the flames in the present database are chosen in such a manner that the normalised turbulent rms velocity fluctuation  $u'/S_L$ , integral length scale to thermal flame thickness ratio  $l/\delta_{th}$ , heat release parameter  $\tau = (T_{ad} - T_0)/T_0$ , the laminar burning velocity for unstrained planar flame  $S_L$ , and thermal flame thickness  $\delta_{th}$  remain identical for all the flames in this database. The dynamic viscosity, thermal conductivity, density-weighted diffusivity, and specific heats are taken to be constant and independent of temperature. The initial values of  $u'/S_L$  and  $l/\delta_{th}$  for all the flames are presented in Table I along with the values of  $\delta_L/\delta_{th}$ , Damköhler number  $Da = lS_L/u'\delta_{th}$ , and turbulent Reynolds number  $Re_t = \rho_0 u' l / \mu_0$  where  $\rho_0$  and  $\mu_0$  are unburned gas density and viscosity, respectively. Standard values are taken for Prandtl number ( $Pr = 0.7$ ), ratio of specific heats ( $\gamma = C_P/C_V = 1.4$ ), and the Zel'dovich number ( $\beta = T_{ac}(T_{ad} - T_0)/T_{ad}^2 = 6.0$ ) where  $T_{ac}$  is the activation temperature. Recent experimental investigations<sup>45,46</sup> on premixed turbulent combustion involving alternative fuels under conditions realised in gas turbines were performed for  $Da < 1$ , and therefore the initial simulation parameters listed in Table I are of interest in terms of the development of high fidelity models for low Damköhler number premixed combustion for gas turbine applications. Moreover,  $Da < 1$  conditions are common in fuel-lean turbulent premixed combustion in IC engines and gas turbine applications.<sup>47</sup> There have been several analyses<sup>48–55</sup> in the past where turbulent premixed flame modelling has been carried out for Damköhler numbers, which are either comparable to, or smaller than, the Damköhler number  $Da$  values considered in this analysis.

For all the flames considered here, the values of  $u'/S_L$  and  $l/\delta_{th}$  listed in Table I are associated with the thin reaction zones regime combustion according to the regime diagram by Peters.<sup>15</sup> In the thin reaction zones regime, the Kolmogorov length scale  $\eta$  is smaller than the flame thickness but larger than the reaction zone thickness  $\delta_r \sim \delta_{th}/10$ . As a result of this, turbulent eddies can penetrate into the preheat zone and perturb it while the reaction zone retains its quasi-laminar structure. According to Peters,<sup>15</sup> this regime is characterized by  $1 < Ka < 100$ , where  $Ka \sim \delta_{th}^2/\eta^2$  is the Karlovitz number, which can also be scaled as  $Ka \sim (u'/S_L)^{3/2}(l/\delta_{th})^{-1/2}$  using the Kolmogorov scaling. The Karlovitz number evaluated using  $Ka \sim (u'/S_L)^{3/2}(l/\delta_{th})^{-1/2}$  is equal to 13.2 for all cases considered here. It is worth noting that the applicability of the Kolmogorov scaling for moderate values of  $Re_t$  (see Table I), and thus the value of Karlovitz number based on this scaling, should be considered with care.

In all the cases, simulations have been carried out for about three initial eddy turn over times (i.e.,  $3.34t_f = 3.34l/u'$ ) which corresponds to about one chemical time scale  $t_c = \delta_{th}/S_L$ . It is admitted that the simulation time remains small but it is comparable to that used in several previous DNS studies.<sup>8,9,14,16,39,40,49–55</sup> By the time the statistics were extracted the value of  $u'/S_L$  in the unburned gas ahead of the flame decayed by about 50% of its initial value, whereas the value of  $l/\delta_{th}$  in the fresh gas increased by about 1.7 times. Interested readers are referred to Refs. 9,37,56–58 for further details on the flow conditions when the statistics were extracted.

In this analysis, all Reynolds or Favre averaged quantities were evaluated by averaging the relevant quantity over each  $x_2 - x_3$  plane at a given  $x_1$  location. In order to check the statistical

convergence, the averaged quantities were evaluated using half of the domain in the  $x_2 - x_3$  plane and were compared to the corresponding quantities using the full sample size available in the same plane. The qualitative and quantitative agreements between the results obtained based on full and half of the sample sizes have been found to be satisfactory (i.e., maximum difference in magnitude is of the order of 3%). Some results evaluated based on full and half of the sample sizes have been shown in Ref. 8 and thus will not be repeated here.

In the present study, the conditional mean quantities are evaluated using Eq. (6) where  $\varepsilon$  is taken to be 0.1 following the previous analysis by Domingo and Bray.<sup>4</sup> This essentially suggests that the mean quantities conditional in reactants are evaluated using the data corresponding to  $0 < c < 0.1$ . Similarly, the mean quantities conditional in products are evaluated using the data corresponding to  $0.9 < c < 1$ . A smaller value of  $\varepsilon$  yields qualitatively similar results as those obtained using  $\varepsilon = 0.1$  but the sample size for evaluating the conditional mean values decrease with decreasing  $\varepsilon$ . By contrast, increasing  $\varepsilon$  value (e.g.,  $0.15 \geq \varepsilon \geq 0.1$ ) gives rise to similar qualitative trends as obtained using  $\varepsilon = 0.1$  but increasing the value of  $\varepsilon$  by a large margin is likely to lead to  $\bar{q}_R$  and  $\bar{q}_P$  values which are not representative of conditional means in reactants and products, respectively. The quantitative agreement between the conditional velocity statistics obtained for  $0.05 \leq \varepsilon \leq 0.15$  is indeed found to be excellent. In Sec. IV, the presentation of conditional velocity statistics will be restricted to a range of  $\bar{c}$  where variations in  $\varepsilon$  between 0.05 and 0.15 and halving the sample size in transverse direction do not significantly ( $\sim < 5\%$ ) alter the quantitative variations.

#### IV. RESULTS AND DISCUSSION

The distributions of normalised vorticity magnitude (i.e.,  $\sqrt{\omega_i \omega_i} \times \delta_{th}/S_L$  where  $\omega_i$  is the  $i$ th component of vorticity vector) on  $x_1 - x_2$  mid-plane for cases A–E are shown in Figs. 1(a)–1(e) to provide an idea of the turbulent flow field for the cases considered here. The contours of  $c$  from 0.1 to 0.9 (left to right) in steps of 0.1 are also shown in Figs. 1(a)–1(e) by white lines. Figures 1(a)–1(e) indicate that the global Lewis number has significant influence on the distribution of vorticity in turbulent premixed flames. It is evident that the vorticity magnitude  $\sqrt{\omega_i \omega_i} \times \delta_{th}/S_L$  drops significantly towards the burned gas side of the flame brush for cases C–E due to thermal expansion, increase in the kinematic viscosity, and decay of turbulence. By contrast, vorticity magnitude  $\sqrt{\omega_i \omega_i} \times \delta_{th}/S_L$  in the burned gases assumes high values in case A and in some locations vorticity magnitude shows augmentation on the burned gas side of the flame brush in comparison to the values in the unburned gas. This behaviour can also be discerned for case B although the extent of vorticity magnitude augmentation in case B is much smaller than in case A. The increase in kinematic viscosity and thermal expansion act to decrease vorticity, whereas vorticity in flames are produced due to the baroclinic torque  $\nabla p \times \nabla \rho$ . The effects of baroclinic torque strengthen with decreasing  $Le$  because the magnitude of  $\nabla p$  assumes high values in case A due to high burning rate.<sup>56,57</sup> This can be substantiated from the values of normalised turbulent burning velocity  $S_T/S_L$  and normalised flame surface area  $A_T/A_L$  presented in Table II where  $S_T$  is evaluated in terms of volume-integrating the reaction rate of progress variable  $S_T = 1/(\rho_0 A_P) \int_V \dot{\omega} d\vartheta$  and the flame surface area  $A$  is evaluated using volume-integration of reaction progress variable gradient  $A = \int_V |\nabla c| d\vartheta$ , where  $d\vartheta$  is an infinitesimal volume element,  $A_P$  is the projected area in the direction of mean flame propagation, and the subscripts  $L$  and  $T$  refer to laminar and turbulent flame quantities. The thermo-diffusive imbalance in the  $Le < 1$  flames augments the rate of burning,<sup>26</sup> which in turn strengthens the local pressure gradient and flame normal acceleration.<sup>27–34,36,56–58</sup> It has been shown in Refs. 56–58 that strong flame normal acceleration for low Lewis number  $Le \ll 1$  flames (e.g., cases A and B) gives rise to considerable flame-generated velocity fluctuations which counters the decay of turbulence in the burned gases due to increase in kinematic viscosity with increasing temperature. Interested readers are referred to Ref. 58 for further information on flame generated velocity fluctuations for the flames considered in this analysis. The following analysis does not focus on the effects of  $Le$  on vorticity distribution and thus will not be elaborated here but it can be appreciated from Figs. 1(a)–1(e) that  $Le$  significantly affects the fluid velocity field in turbulent premixed flames and thus is likely have considerable influence on conditional velocity statistics.

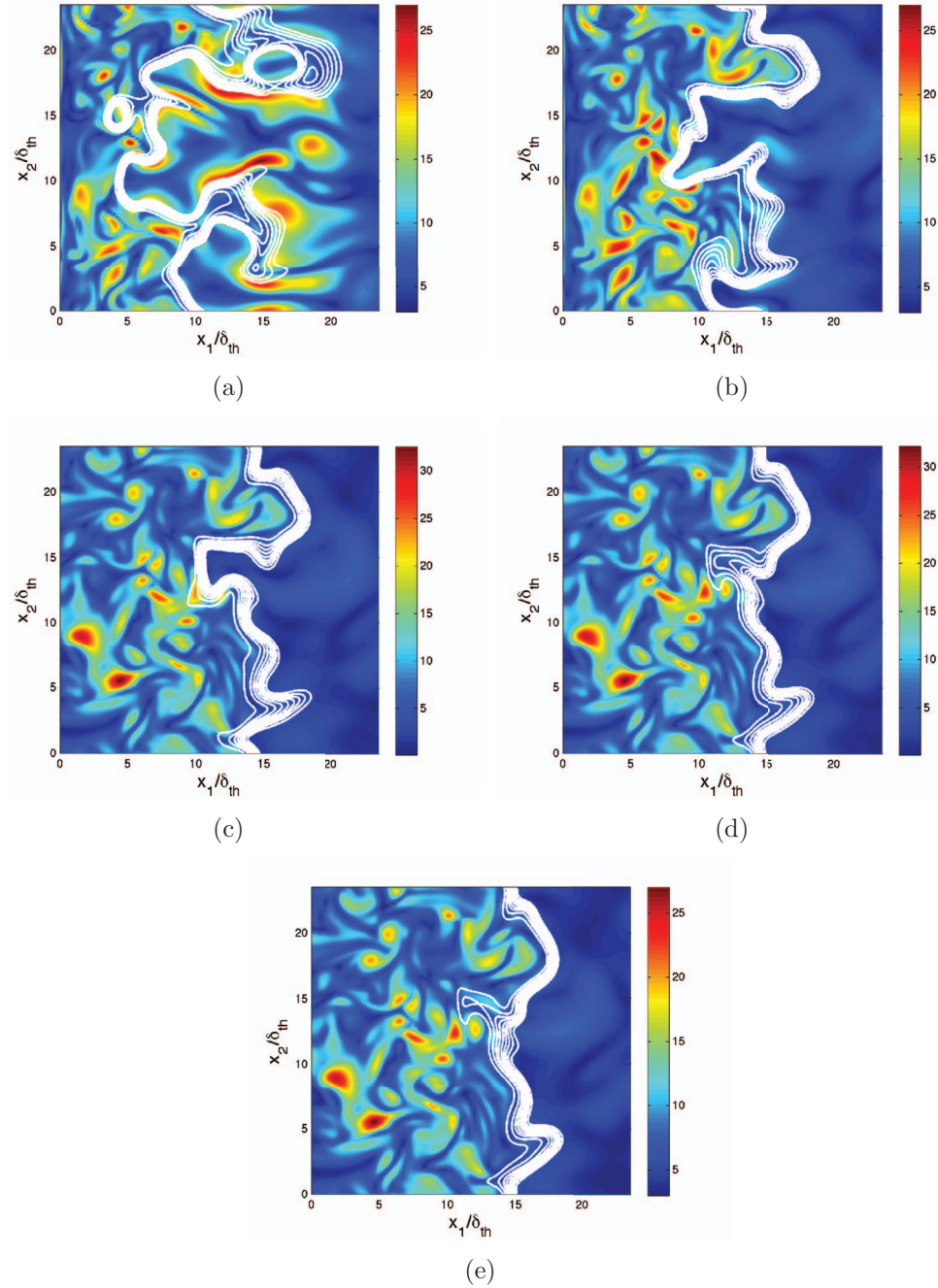


FIG. 1. Distribution of normalised vorticity magnitude  $\sqrt{\omega_i \omega_i} \times \delta_{th}/S_L$  in the central  $x_1 - x_2$  plane for cases (a)–(e) A–E at the time when the statistics were extracted. The white lines indicate reaction progress variable  $c$  contours from  $c = 0.1$  to  $0.9$  from left to right in steps of  $0.1$ .

The nature of pdf of  $c$  can be characterised in terms of the variance  $\widetilde{c''^2}$ . For a bi-modal distribution of  $c$ , the variance of reaction progress variable  $c''^2$  is given by

$$\widetilde{c''^2} = \tilde{c}(1 - \tilde{c}) + O(\gamma_c). \quad (14)$$

The variations of  $\widetilde{c''^2}$  with  $\tilde{c}$  for all the flames are shown in Fig. 2(a) which indicates that  $\widetilde{c''^2}$  remains smaller than  $\tilde{c}(1 - \tilde{c})$  for cases A–E. This indicates that the assumption of bi-modal distribution of  $c$ , as done in BML analysis<sup>1</sup> is likely to be rendered invalid in all cases considered here. It is important

TABLE II. The effects of Lewis number on normalised turbulent flame speed  $S_T/S_L$  and normalised flame surface area  $A_T/A_L$  after 3.34 initial eddy turn over times.

Le	$S_T/S_L$	$A_T/A_L$
0.34	13.70	3.93
0.6	4.58	2.66
0.8	2.53	2.11
1.0	1.83	1.84
1.2	1.50	1.76

to note that  $\tilde{c}(1 - \tilde{c})$  is the maximum possible value of  $\tilde{c}''^2$  which is obtained only when  $O(\gamma_c)$  remains negligible. Thus, the deviation of the pdf of  $c$  from bi-modal distribution can be quantified in terms of the segregation factor  $g = \tilde{c}''^2 / \tilde{c}(1 - \tilde{c})$ , which decreases from unity with the increasing deviation from the bi-modal distribution of  $c$ . The pdfs of  $c$  at the location corresponding to  $\tilde{c} = 0.5$  for all the cases are shown in Fig. 2(b), which indicates that there is a significant probability of finding  $0 \leq c \leq 1$  and the pdfs of  $c$  are not bi-modal in all cases considered here. This suggests that  $O(\gamma_c)$  contribution is likely to be non-negligible for cases A–E as  $Da$  is small in these cases. It is also worth noting that Fig. 2(b) does not reveal a notable influence of the Lewis number on the pdf shape at  $\tilde{c} = 0.5$ , whereas Fig. 2(a) indicates a decrease in the segregation factor at higher values of  $\tilde{c}$  when  $Le$  is decreased.

The variations of  $(u_1)_R/S_L$  with  $\tilde{c}$  for cases A–E are shown in Figs. 3(a)–3(e), respectively, which indicate that  $(u_1)_R/S_L$  increases from unburned gas side to the burned gas side of the flame brush for all cases due to thermal expansion and flame propagation. The variations of  $(u_2)_R/S_L$  and  $(u_3)_R/S_L$  are not shown because these components are identically equal to zero for statistically planar flames. Comparing Figs. 3(a)–3(e), it is evident that the global Lewis number  $Le$  has major influence on the magnitude of  $(u_1)_R/S_L$  and it is found to increase with decreasing  $Le$ . Moreover, due to increasing flame normal acceleration with decreasing  $Le$ , the slip velocity (i.e.,  $(u_i)_p - (u_i)_R$ ) assumes much greater value in the flames with low  $Le$ , which can be substantiated from Fig. 3(f). It is also worth noting that a positive (negative) value of  $(u_1)_p - (u_1)_R$  is associated with the counter-gradient (gradient) transport,<sup>1,56,57</sup> which can be substantiated from Fig. 3(g), where a positive (negative) value of  $\rho u_1'' c'' \cdot (\partial \tilde{c} / \partial x_1) \times \delta_{th} / \rho_0 S_L$  indicates a counter-gradient (gradient) type transport. Interested readers are referred to Refs. 56 and 57 for the effects of  $Le$  on turbulent scalar transport and this will not be discussed further in this paper.

It is evident from Fig. 3(d) that Eq. (8a) underpredicts the magnitude of  $(u_1)_R/S_L$  for the low Damköhler number unity Lewis number flame, which is consistent with earlier findings.<sup>16</sup> As the bi-modal distribution does not accurately describe the reaction progress variable distribution in cases C–E (see Fig. 2(b)), the expression given by Eq. (8a) does not adequately predict  $(u_1)_R/S_L$  in these cases.

As discussed in Ref. 16, the segregation factor  $g = \tilde{c}''^2 / \tilde{c}(1 - \tilde{c})$  plays a key role in determining the contribution of  $O(\gamma_c)$  in Eq. (7). As  $\tilde{c}''^2 \approx \tilde{c}(1 - \tilde{c})$  in high Damköhler number flames, Eq. (7) can be written as:  $\rho u_i'' c'' = \bar{\rho}[(u_i)_p - (u_i)_R] \tilde{c}''^2 + O(\gamma_c)$ , which in combination with  $\tilde{u}_i = (u_i)_R(1 - \tilde{c}) + \tilde{c}(u_i)_p + O(\gamma_c)$  yields the following expression for  $(u_i)_R$  for unity Lewis number flames (Ref. 16):

$$(u_i)_R = \tilde{u}_i - \bar{\rho} u_i'' c'' / [g \bar{\rho} (1 - \tilde{c})]. \quad (15)$$

The predictions of Eq. (15) are shown in Figs. 3(a)–3(e) which indicate that Eq. (15) satisfactorily captures the behaviour of  $(u_i)_R$  for flames with Lewis number close to unity (i.e., cases C–E). However, Eq. (15) significantly underpredicts  $(u_i)_R$  for the major portion of the flame brush in cases A and B. By contrast, the original BML Eq. (8a) satisfactorily captures the statistical behaviour of  $(u_1)_R/S_L$  for the  $Le = 0.34$  and 0.6 flames (i.e., cases A and B, see Figs. 3(a) and 3(b)) even for low Damköhler number. Based on this observation Eq. (15) has been modified here in the

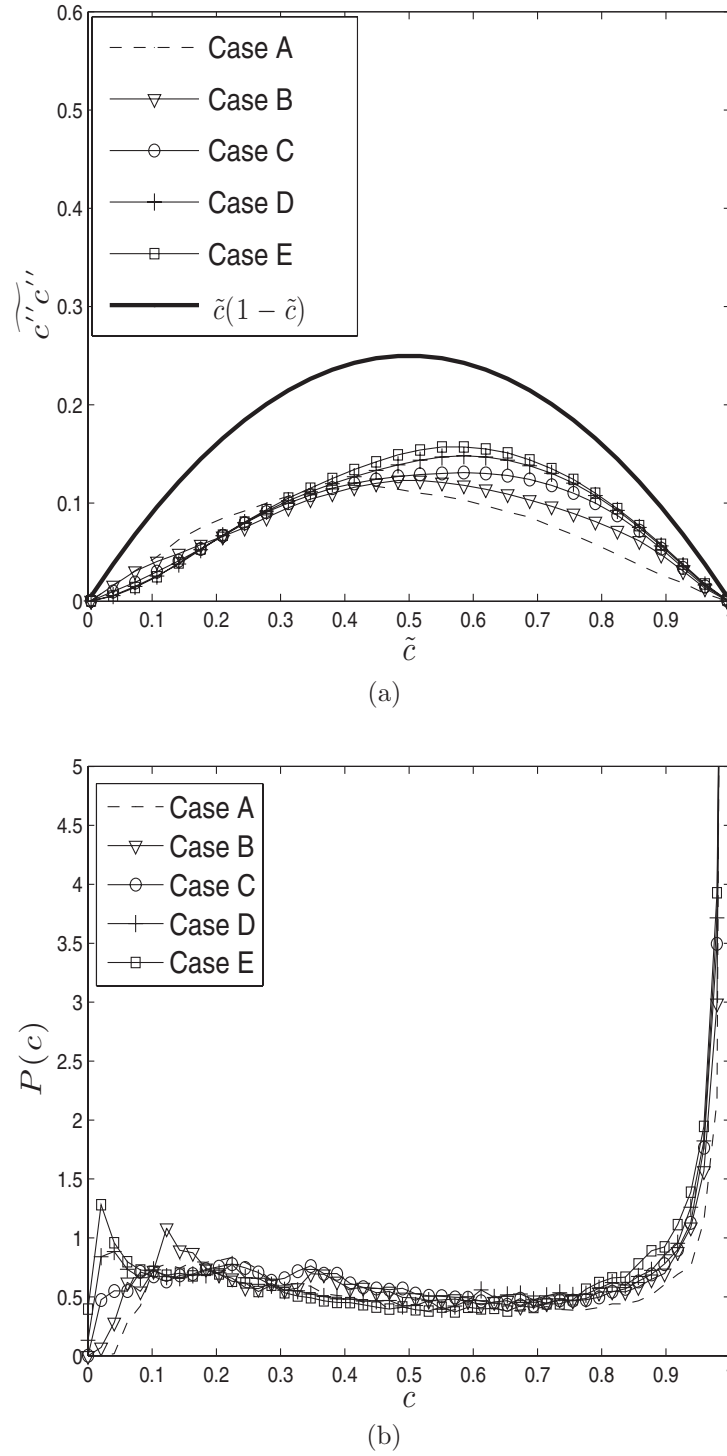


FIG. 2. (a) Variations of  $\overline{c''c''}$  with  $\tilde{c}$  across the flame brush for all cases considered here; (b) pdfs of  $c$  at the location corresponding to  $\tilde{c} = 0.5$  for all cases considered here.

following manner:

$$\overline{(u_i)_R} = \tilde{u}_i - \overline{\rho u_i'' c''} / [g^{Le^2} \tilde{\rho}(1 - \tilde{c})]. \quad (16)$$

Note that Eq. (16) becomes equivalent to Eq. (15) in the case of  $Le = 1$  and both Eqs. (15) and (16) reduce to the original BML Eq. (8a) in the case of  $g = 1$  associated with  $Da \rightarrow \infty$ . The predictions

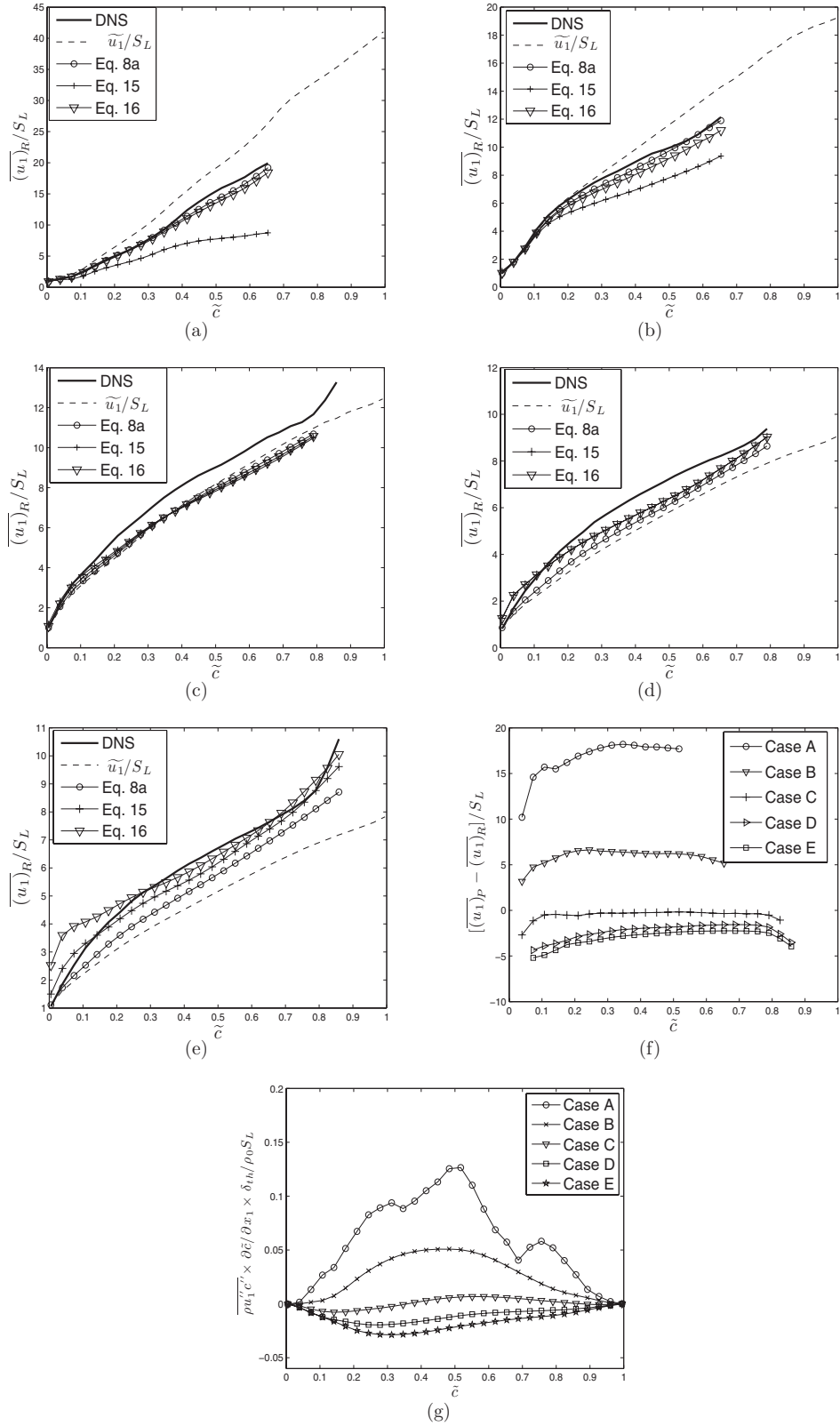


FIG. 3. Variations of  $(u_1)_R/S_L$  with  $\tilde{c}$  across the flame brush along with the predictions of Eqs. (8a), (15), and (16) for cases (a)–(e) A–E. Variations of (f)  $[(u_1)_P - (u_1)_R]/S_L$  and (g)  $\rho u_1' c'' \times \partial \tilde{c} / \partial x_1 \times \delta_{th} / \rho_0 S_L$  with  $\tilde{c}$  across the flame brush for all cases considered here.

of Eq. (16) are compared with  $\overline{(u_i)}_R$  obtained from DNS data in Figs. 3(a)–3(e), which indicate that Eq. (16) satisfactorily captures the behaviour of  $\overline{(u_i)}_R$  in the low  $Le$  flames (e.g., cases A and B) whereas the predictions of Eq. (16) remain comparable to those of Eq. (15) for the flames with  $Le \approx 1.0$  (e.g., cases C–E).

The predictions of Eq. (16) are better than Eq. (8a) for flame with  $Le = 1.0$  (see Fig. 3(d)), whereas the prediction of Eq. (16) remains comparable to that of Eq. (8a) for  $Le = 0.34, 0.6$ , and  $0.8$  flames. Reasonable agreement between Eq. (8a) and the DNS data in the low Lewis number cases could imply that the pdf of  $c$  is closer to a bi-modal pdf in these cases. However, Fig. 2(a) does not confirm such an assumption. Therefore, the agreement between Eq. (8a) and the DNS data is likely to be fortuitous, e.g., due to the cancellation of effects associated with a low Damköhler number by the effects associated with small values of Lewis number  $Le$ .

The variations  $\overline{(u_1)}_P/S_L$  with  $\tilde{c}$  for cases A–E are shown in Figs. 4(a)–4(e), respectively. The variations of  $\overline{(u_2)}_P/S_L$  and  $\overline{(u_3)}_P/S_L$  are not shown because these components are identically equal to zero for statistically planar flames. In all cases,  $\overline{(u_1)}_P/S_L$  increases from unburned gas side to the burned gas side of the flame brush due to flame propagation and thermal expansion. The predictions of Eq. (8b) are also shown in Figs. 4(a)–4(e) which indicate that Eq. (8b) significantly underpredicts the value of  $\overline{(u_1)}_P/S_L$  in cases A and B (low Lewis number), and slightly overpredicts it in cases C–E. Equation (8b) is derived based on the bi-modal distribution of  $c$  so it is not surprising that this relation does not perform well in the cases where the assumption related to bi-modal pdf is not satisfied.

Equation (7) can be written as:  $\overline{\rho u_i'' c''} = \bar{\rho}[\overline{(u_i)}_P - \overline{(u_i)}_R] \tilde{c}''^2 + O(\gamma_c)$  as  $\tilde{c}''^2 \approx \tilde{c}(1 - \tilde{c})$  in high Damköhler number flames, which in combination with  $\tilde{u}_i = \overline{(u_i)}_R(1 - \tilde{c}) + \tilde{c}\overline{(u_i)}_P + O(\gamma_c)$  yields the following expression for  $\overline{(u_i)}_P$ :

$$\overline{(u_i)}_P = \tilde{u}_i + \overline{\rho u_i'' c''} / [\bar{\rho} g \tilde{c}]. \quad (17a)$$

The philosophy behind the derivation of Eq. (17a) is similar to that of Eq. (15). However, contrary to  $\overline{(u_i)}_R$  prediction by Eq. (15), such a method does not work well for  $\overline{(u_i)}_P$  when Eq. (17a) is used, even if the Lewis number is close to unity. It can be seen from Fig. 4 that Eq. (17a) underpredicts the magnitude of  $\overline{(u_1)}_P/S_L$  towards the unburned gas side of the flame brush in cases A, B, D, and E. Chakraborty and Lipatnikov<sup>16</sup> reported the same trend in the case of  $Le = 1$  and  $Da < 1$ . To resolve the problem, they proposed an expression for  $\overline{(u_i)}_P$  by arithmetic averaging Eqs. (8b) and (17a)

$$\overline{(u_i)}_P = \tilde{u}_i + [(1 + g)/2g] \times \overline{\rho u_i'' c''} / \bar{\rho} \tilde{c}. \quad (17b)$$

Figures 4(c)–4(e) demonstrate that Eq. (17b) satisfactorily predicts the variation of  $\overline{(u_1)}_P$  throughout the flame brush for  $Le \approx 1.0$  (i.e., cases C–E). For high Damköhler number flames  $g \approx 1$  due to bi-modal pdf of  $c$  and under that condition Eq. (17b) becomes equivalent to Eqs. (8b) and (17a). However, Eq. (17b) significantly underpredicts  $\overline{(u_1)}_P$  for low  $Le$  cases, i.e., the use of the  $Le$ -independent factor  $(1 + g)/2g$  in the second term on the right hand side of Eq. (17b) is not sufficient to account for strengthening of reactive contribution  $[\overline{(u_1)}_P - \tilde{u}_1]$  due to decreasing Lewis number  $Le$  as a result of augmented burning rate (see Table II). In order to overcome this limitation, Eq. (17b) has been modified here in the following manner:

$$\overline{(u_i)}_P = \tilde{u}_i + [(f_1(Le) + g)/2g] \times \overline{\rho u_i'' c''} / \bar{\rho} \tilde{c}, \quad (17c)$$

where  $f_1(Le)$  is a function, which assumes a value equal to unity for the unity Lewis number flames (i.e.,  $f_1(Le = 1.0) = 1.0$ ) so that Eq. (17c) becomes identical to Eq. (17b) for  $Le = 1.0$ . Here, the function  $f_1(Le)$  is proposed in the following manner by analysing the DNS data so that  $f_1(Le = 1.0) = 1.0$ :

$$f_1(Le) = 1.5 + 0.5 \operatorname{erf}[14.29(0.65 - Le)]. \quad (17d)$$

The function given by Eq. (17d) increases with decreasing  $Le$ , thus, accounting for strengthening of the reactive contribution to  $\overline{(u_1)}_P$  for  $Le = 0.34$  and  $0.6$  flames. This function  $f_1$  reaches an asymptotic value of unity for  $Le \approx 1.0$  flames. Figures 4(a)–4(e) indicate that the prediction of Eq. (17c) remains comparable to that of Eq. (17b) for the flames with Lewis number close to unity

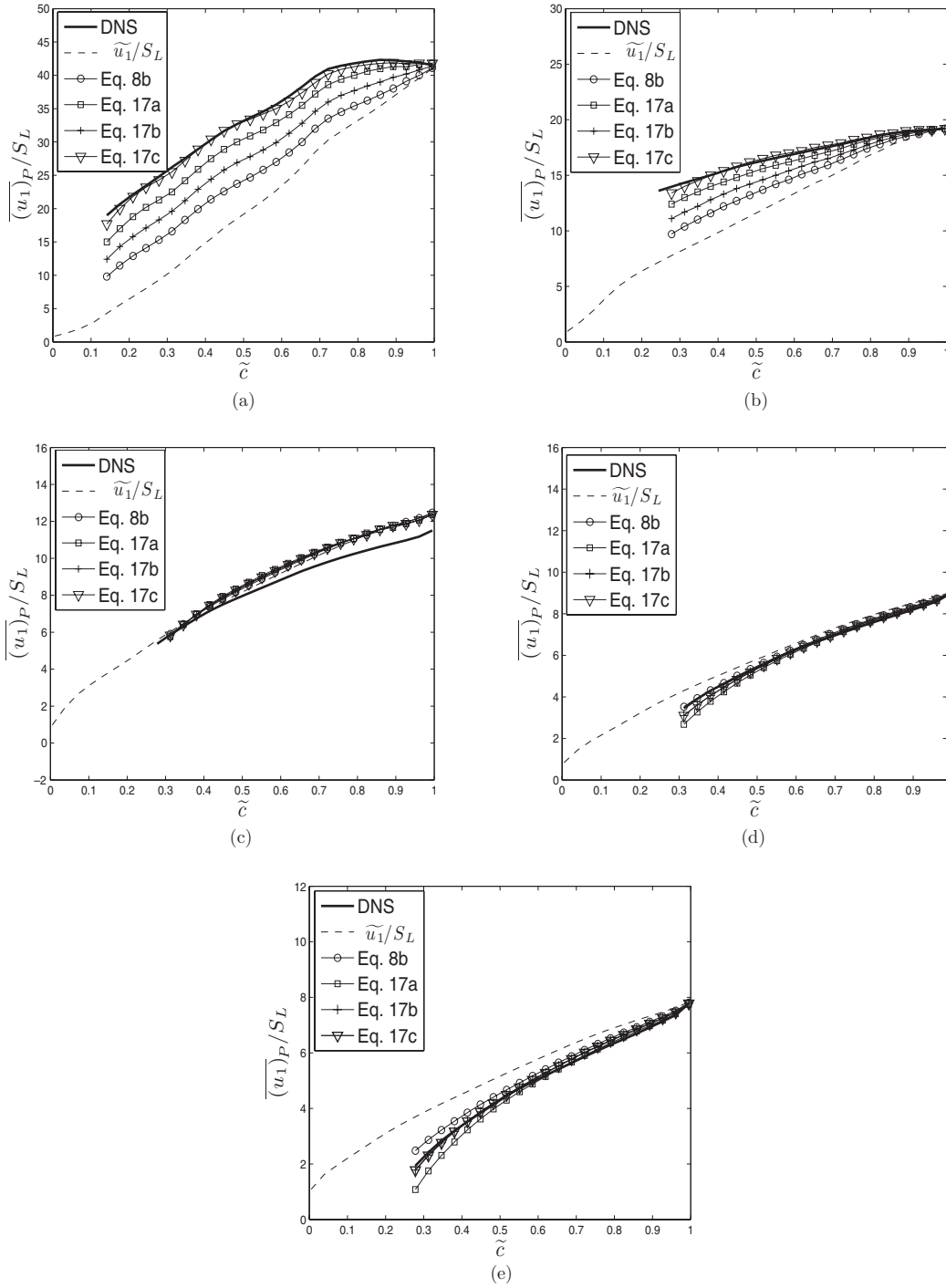


FIG. 4. Variations of  $(u_1)_P / S_L$  with  $\tilde{c}$  across the flame brush along with the predictions of Eqs. (8b) and (17a)–(17c) for cases (a)–(e) A–E.

(e.g., cases C–E) but Eq. (17c) captures the statistical behaviours of  $(u_1)_P$  in a better manner than Eqs. (8b), (17a), and (17b) for the low  $Le$  flames (e.g., cases A and B).

The findings based on Figs. 3 and 4 can be summarised as follows:

1. The theoretical BML expression (i.e., Eq. (8a)) slightly underpredicts  $(u_1)_R / S_L$  for all cases considered here, while Eq. (16) shows similar performance for low Lewis number flames, but

its prediction remains better in comparison to Eq. (8a) for  $Le \approx 1.0$  flames analysed here, and for both high and low Damköhler number combustion with unity Lewis number discussed in Ref. 16.

2. The theoretical BML expression (i.e., Eq. (8b)) predicts  $\overline{(u_1)_P}/S_L$  reasonably well for  $Le = 0.8 - 1.2$  flames considered here, while significantly underpredicts this conditional velocity when Lewis number is low (e.g.,  $Le = 0.34$  and  $0.6$  flames). A newly proposed empirical expression given by Eq. (17c) parameterizes the DNS data shown in Fig. 4, as well as DNS data analysed in Refs. 14 and 16.
3. For  $Da \rightarrow \infty$ , the segregation factor  $g$  approaches to unity (i.e.,  $g \rightarrow 1$ ) and Eqs. (16) and (17c) become identical to the theoretical Eqs. (8a) and (8b), respectively.

The influences of Lewis number on conditional velocities is more pronounced in the products than in the reactants. This could be explained by local variations in burning rate due to the imbalance of local heat and species diffusion fluxes, which affect the velocity components when a gas volume passes through the heat-release zone,<sup>56–58</sup> but weakly influence the velocity field ahead of the reaction zone.

The variations of  $\overline{(u'_1 u'_1)_R}/S_L^2$  with  $\tilde{c}$  for all the cases are shown in Fig. 5. It is evident that  $\overline{(u'_1 u'_1)_R}/S_L^2$  decays from unburned gas side to burned gas side for all the cases. For the flames with Lewis number close to unity (i.e., cases C–E) the variation of  $\overline{\rho u''_1 u''_1}/\bar{\rho} S_L^2$  approximates the distribution of  $\overline{(u'_1 u'_1)_R}/S_L^2$  for the major portion of the flame brush, but the difference between  $\overline{\rho u''_1 u''_1}/\bar{\rho} S_L^2$  and  $\overline{(u'_1 u'_1)_R}/S_L^2$  is significant for cases A and B. The difference between  $\overline{(u'_1 u'_1)_R}$  and  $\overline{\rho u''_1 u''_1}/\bar{\rho}$  arises due to chemical reaction. The effects of chemical reaction are particularly strong for the low  $Le$  flames due to augmented heat release (see Table II) even if the Damköhler number is low. As a result of this, the contribution of  $\overline{(u'_1 u'_1)_R} - \overline{\rho u''_1 u''_1}/\bar{\rho}$  plays an important role for cases A and B, which makes the distributions of  $\overline{(u'_1 u'_1)_R}/S_L^2$  and  $\overline{\rho u''_1 u''_1}/\bar{\rho} S_L^2$  significantly different from each other.

Figure 5 indicates that Eq. (10) predicts the magnitude of  $\overline{(u'_1 u'_1)_R}/S_L^2$  reasonably well in all the cases considered in the present paper. It is worth noting, however, that a previous DNS based analysis<sup>14</sup> for unity Lewis number and large Damköhler number combustion has revealed that Eq. (10) does not work well, and even a small deviation of the pdf of  $c$  from the presumed bi-modal distribution substantially affects the prediction of  $\overline{(u'_1 u'_1)_R}/S_L^2$ . A subsequent analysis<sup>16</sup> of DNS data obtained from unity Lewis number low Damköhler number flames has shown that, contrary to common expectations, a decrease in  $Da$  does not make the prediction of Eq. (10) worse, and its prediction agrees reasonably well with  $\overline{(u'_1 u'_1)_R}/S_L^2$  obtained from the DNS data of low  $Da$  flames with  $Le = 1.0$ . Figure 5 further supports this observation for different values of Lewis number  $Le$ . This trend is attributed to a decrease in the reactive contributions (see the second and third terms on the right hand side of Eq. (10)) to the conditional Reynolds stresses  $\overline{(u'_1 u'_1)_R}$  with decreasing Damköhler number so that  $\overline{(u'_1 u'_1)_R}$  remains close to  $\overline{\rho u''_1 u''_1}/\bar{\rho}$  (i.e.,  $\overline{(u'_1 u'_1)_R} \approx \overline{\rho u''_1 u''_1}/\bar{\rho}$ ) if  $Le \approx 1$  and  $Da < 1$ . The DNS data shown in Fig. 5 imply that the weakening of reactive contribution to the conditional Reynolds stresses  $\overline{(u'_1 u'_1)_R}$  with decreasing  $Da$  compensates the error due to the deviation from the presumed bimodal pdf of  $c$  when the difference  $[\overline{(u'_1 u'_1)_R} - \overline{\rho u''_1 u''_1}/\bar{\rho}]$  is evaluated using Eq. (10).

Despite the reasonable accuracy of Eq. (10) indicated by Fig. 5, it would be desirable to have an expression applicable to both low and high Damköhler number combustion. For this purpose, the following expression was proposed in Ref. 16 for unity Lewis number flames:

$$\overline{(u'_i u'_j)_R} = \overline{\rho u''_i u''_j}/\bar{\rho} - \overline{\rho u''_i u''_j c''}/\bar{\rho}(1 - \tilde{c}) - 0.5(1 + g^{-1})(\overline{\rho u''_i c''}/\bar{\rho})(\overline{\rho u''_j c''}/\bar{\rho})/(1 - \tilde{c})^2. \quad (18)$$

Equation (18) has been obtained by averaging Eq. (10) and the following expression  $\overline{(u'_i u'_j)_R} = \overline{\rho u''_i u''_j}/\bar{\rho} - \overline{\rho u''_i u''_j c''}/\bar{\rho}(1 - \tilde{c}) - g^{-1}(\overline{\rho u''_i c''}/\bar{\rho})(\overline{\rho u''_j c''}/\bar{\rho})/(1 - \tilde{c})^2$  which results from substitution of Eq. (7) and  $[(u_i)_P - (u_i)_R] = \overline{\rho u''_i c''}/\bar{\rho} \tilde{c}^{1/2}$  into Eqs. (9a) and (9b). For large values of Damköhler number (i.e.,  $Da \rightarrow \infty$ ), the segregation factor approaches unity (i.e.,  $g \rightarrow 1$ ), and as a result Eq. (18) becomes equivalent to Eq. (10).

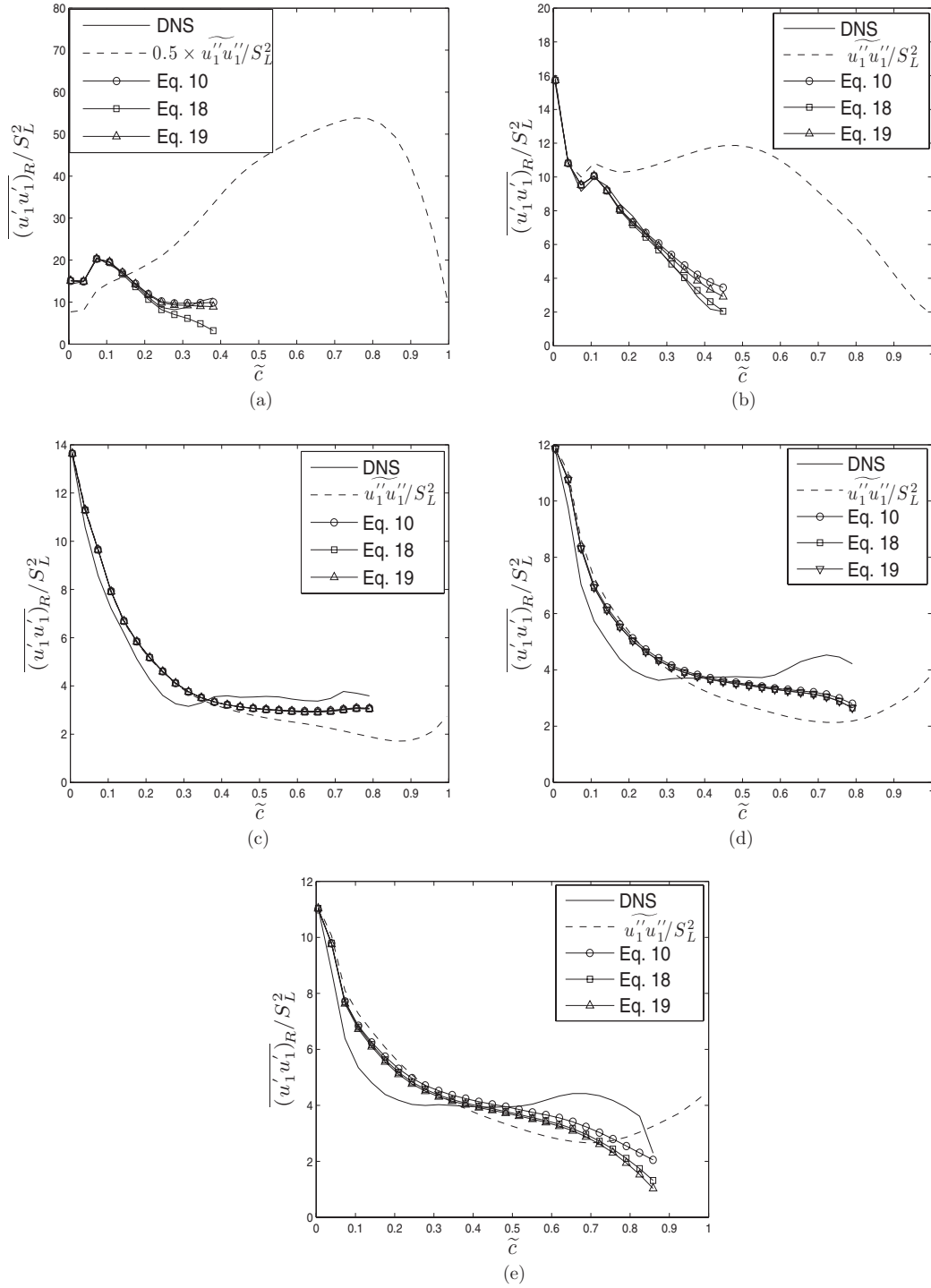


FIG. 5. Variations of  $\overline{(u_1' u_1')}_R / S_L^2$  and  $\overline{\rho u_1'' u_1''} / \bar{\rho} S_L^2$  with  $\tilde{c}$  across the flame brush along with the predictions of Eqs. (10), (18), and (19) for cases (a)–(e) A–E.

However, Fig. 5(a) shows that Eq. (18) underestimates  $\overline{(u_1' u_1')}_R$  for  $\tilde{c} > 0.2$  in case A, because  $0.5(1 + g^{-1})$  is substantially larger than unity in this case and the reactive contribution to  $\overline{(u_1' u_1')}_R$  is overestimated. To resolve the problem, Eq. (18) could be further modified

as follows:

$$\overline{(u'_i u'_j)}_R = \overline{\rho u''_i u''_j} / \bar{\rho} - \overline{\rho u''_i u''_j c''} / \bar{\rho} (1 - \tilde{c}) - 0.5(1 + g^{-Le^{1.5}})(\overline{\rho u''_i c''} / \bar{\rho})(\overline{\rho u''_j c''} / \bar{\rho}) / (1 - \tilde{c})^2. \quad (19)$$

Equation (19) is exactly equal to Eq. (18) if  $Le = 1.0$ , but the magnitude of the last term of Eq. (19) remains smaller than that in Eq. (18) for  $Le < 1$  flames if  $g$  is substantially smaller than unity. It can be seen from Fig. 5(a) that Eq. (19) provides improved (as compared to Eq. (18)) prediction of  $\overline{(u'_1 u'_1)}_R$  when  $Le = 0.34$ . Moreover, predictions of Eqs. (10) and (19) remain close to one another in all cases considered in the present paper, but Eq. (19) performs better than Eq. (10) in high Damköhler number flames analysed in previous studies.<sup>14,16</sup> For large values of Damköhler number (i.e.,  $Da \rightarrow \infty$ ), the segregation factor approaches unity (i.e.,  $g \rightarrow 1$ ), and thus Eq. (19) becomes equivalent to the BML expression given by Eq. (10).

Figure 6 indicates that  $\overline{(u'_2 u'_2)}_R / S_L^2$  and  $\overline{\rho u''_2 u''_2} / \bar{\rho} S_L^2$  remain close to each other for all cases considered here, i.e., the net reactive contribution  $[\overline{(u'_2 u'_2)}_R - \overline{\rho u''_2 u''_2} / \bar{\rho}]$  remains negligible. This is consistent with the previous findings for unity Lewis number low Damköhler number combustion by Chakraborty and Lipatnikov.<sup>16</sup> The predictions of Eqs. (10), (18), and (19) for  $\overline{(u'_2 u'_2)}_R$  remain identical to each other, because  $\overline{\rho u''_2 c''}$  is identically equal to zero for statistically planar flames. This also reduces the net reactive contributions to  $\overline{(u'_2 u'_2)}_R / S_L^2$ . As  $\overline{(u'_2 u'_2)}_R / S_L^2$  and  $\overline{\rho u''_2 u''_2} / \bar{\rho} S_L^2$  are statistically similar to  $\overline{(u'_3 u'_3)}_R / S_L^2$  and  $\overline{\rho u''_3 u''_3} / \bar{\rho} S_L^2$ , respectively, the variations of  $\overline{(u'_3 u'_3)}_R / S_L^2$  and  $\overline{\rho u''_3 u''_3} / \bar{\rho} S_L^2$  are not shown here for the sake of conciseness.

The variations of  $\overline{(u'_1 u'_1)}_P / S_L^2$  and  $\overline{\rho u''_1 u''_1} / \bar{\rho} S_L^2$  with  $\tilde{c}$  for all cases considered here are shown in Figs. 7(a)–7(e) along with the prediction of Eq. (10). As in the case of  $\overline{(u'_1 u'_1)}_R / S_L^2$ , the variation of  $\overline{(u'_1 u'_1)}_P / S_L^2$  remains close to  $\overline{\rho u''_1 u''_1} / \bar{\rho} S_L^2$ , and Eq. (10) predicts  $\overline{(u'_1 u'_1)}_P / S_L^2$  satisfactorily when Lewis number is close to unity (cases C–E). However, for the flames with low  $Le$  (cases A and B), Eq. (10) significantly overpredicts  $\overline{(u'_1 u'_1)}_P$ . The effects of chemical reaction are stronger in the flames with a low  $Le$ , and as a result of this, the contributions of  $[\overline{(u'_1 u'_1)}_P - \overline{\rho u''_1 u''_1} / \bar{\rho}]$  are of higher importance for cases A and B. As shown in previous analyses<sup>14,16</sup> for unity Lewis number flames, Eq. (10) does not work well for  $Da > 1$  flames even for a small deviation of the pdf of  $c$  from the presumed bi-modal distribution, which substantially affects the prediction of  $\overline{(u'_1 u'_1)}_P$ , though Eq. (10) predicts  $\overline{(u'_1 u'_1)}_P$  reasonably well for  $Da < 1$  due to weak reactive contributions. In Ref. 16, the BML expression given by Eq. (10), which was originally derived for high Damköhler number flames, was modified for low Damköhler number combustion as follows. Using Eq. (7) and  $[(u_i)_P - (u_i)_R] = \overline{\rho u''_i c''} / \bar{\rho} \tilde{c}^2$  in Eqs. (9a) and (9b) yields  $\overline{(u'_i u'_j)}_P = \overline{\rho u''_i u''_j} / \bar{\rho} + \overline{\rho u''_i u''_j c''} / \bar{\rho} \tilde{c} - g^{-1}(\overline{\rho u''_i c''} / \bar{\rho})(\overline{\rho u''_j c''} / \bar{\rho}) / \tilde{c}^2$ . Weighting this expression and Eq. (10) by  $g$  and  $(1 - g)$  gives rise to

$$\overline{(u'_i u'_j)}_P = \overline{\rho u''_i u''_j} / \bar{\rho} + \overline{\rho u''_i u''_j c''} / \bar{\rho} \tilde{c} - (2 - g)(\overline{\rho u''_i c''} / \bar{\rho})(\overline{\rho u''_j c''} / \bar{\rho}) / \tilde{c}^2. \quad (20)$$

The prediction of Eq. (20) provides a reasonable agreement with  $\overline{(u'_i u'_j)}_P$  obtained from DNS data for low Damköhler number unity Lewis number flames.<sup>16</sup> It is worth noting that for high values of Damköhler number (i.e.,  $Da \rightarrow \infty$ ), the segregation factor approaches unity (i.e.,  $g \rightarrow 1$ ), and thus Eq. (20) becomes identical to Eq. (10). It can be seen from Fig. 7 that Eq. (20) satisfactorily predicts  $\overline{(u'_1 u'_1)}_P$  for the flames with Lewis number close to unity (cases C–E), but it still overpredicts  $\overline{(u'_1 u'_1)}_P$  for low  $Le$  flames (cases A and B). In order to resolve this problem, Eq. (20) is modified here in the following manner:

$$\overline{(u'_i u'_j)}_P = \overline{\rho u''_i u''_j} / \bar{\rho} + \overline{\rho u''_i u''_j c''} / \bar{\rho} \tilde{c} - f_2(Le)(2 - g)(\overline{\rho u''_i c''} / \bar{\rho})(\overline{\rho u''_j c''} / \bar{\rho}) / \tilde{c}^2, \quad (21a)$$

$$\text{where } f_2(Le) = (1 - \tilde{c})^{-\zeta(Le)} \text{ with } \zeta(Le) = 0.5 + 0.5 \operatorname{erf}[14.29(0.65 - Le)]. \quad (21b)$$

The function  $f_2(Le)$  is proposed here in such a manner that Eqs. (21) becomes identical to Eq. (20) for  $Le = 1.0$ , whereas the magnitude of the reactive contribution to  $\overline{(u'_i u'_j)}_P$  strengthens with decreasing  $Le$  and towards the burned gas side of the flame brush. Figure 7 indicates that the predictions of

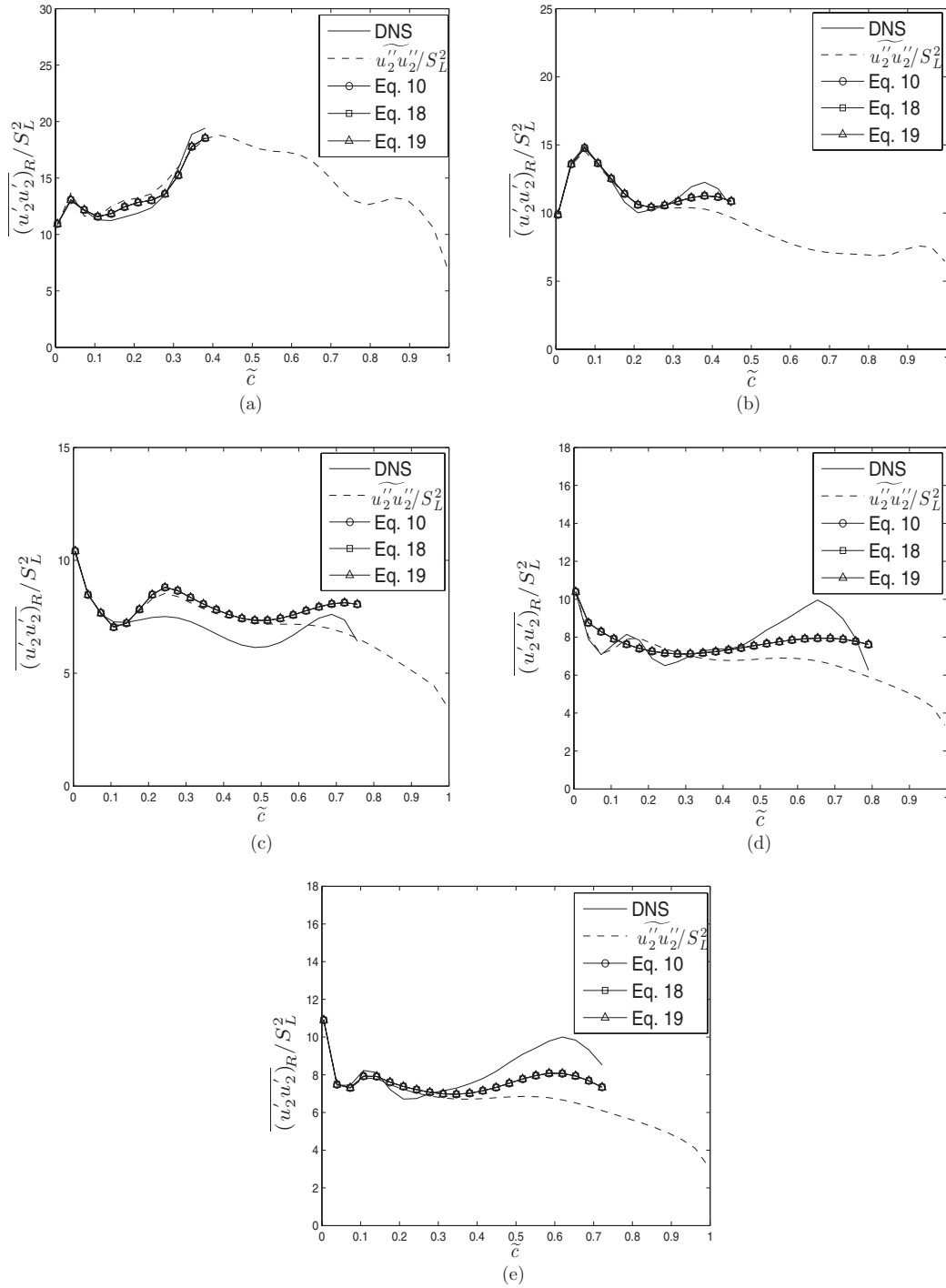


FIG. 6. Variations of  $\overline{(u'_2 u'_2)}_R / S_L^2$  and  $\overline{\rho u''_2 u''_2} / \bar{\rho} S_L^2$  with  $\tilde{c}$  across the flame brush along with the predictions of Eqs. (10), (18), and (19) for cases (a)–(e) A–E.

Eqs. (21) for  $\overline{(u'_1 u'_1)}_p$  remain comparable to that of Eq. (20) for the flames with Lewis number close to unity  $Le \approx 1.0$  (i.e., cases C–E) but Eqs. (21) capture  $\overline{(u'_1 u'_1)}_p$  more satisfactorily than Eqs. (10) and (20) in the flames with a low  $Le$  (e.g., cases A and B).

It is evident from Figs. 8(a)–8(e) that  $\overline{(u'_2 u'_2)}_p / S_L^2$  and  $\overline{\rho u''_2 u''_2} / \bar{\rho} S_L^2$  remain close to each other for all cases considered here. This suggests that the contribution arising from chemical reaction

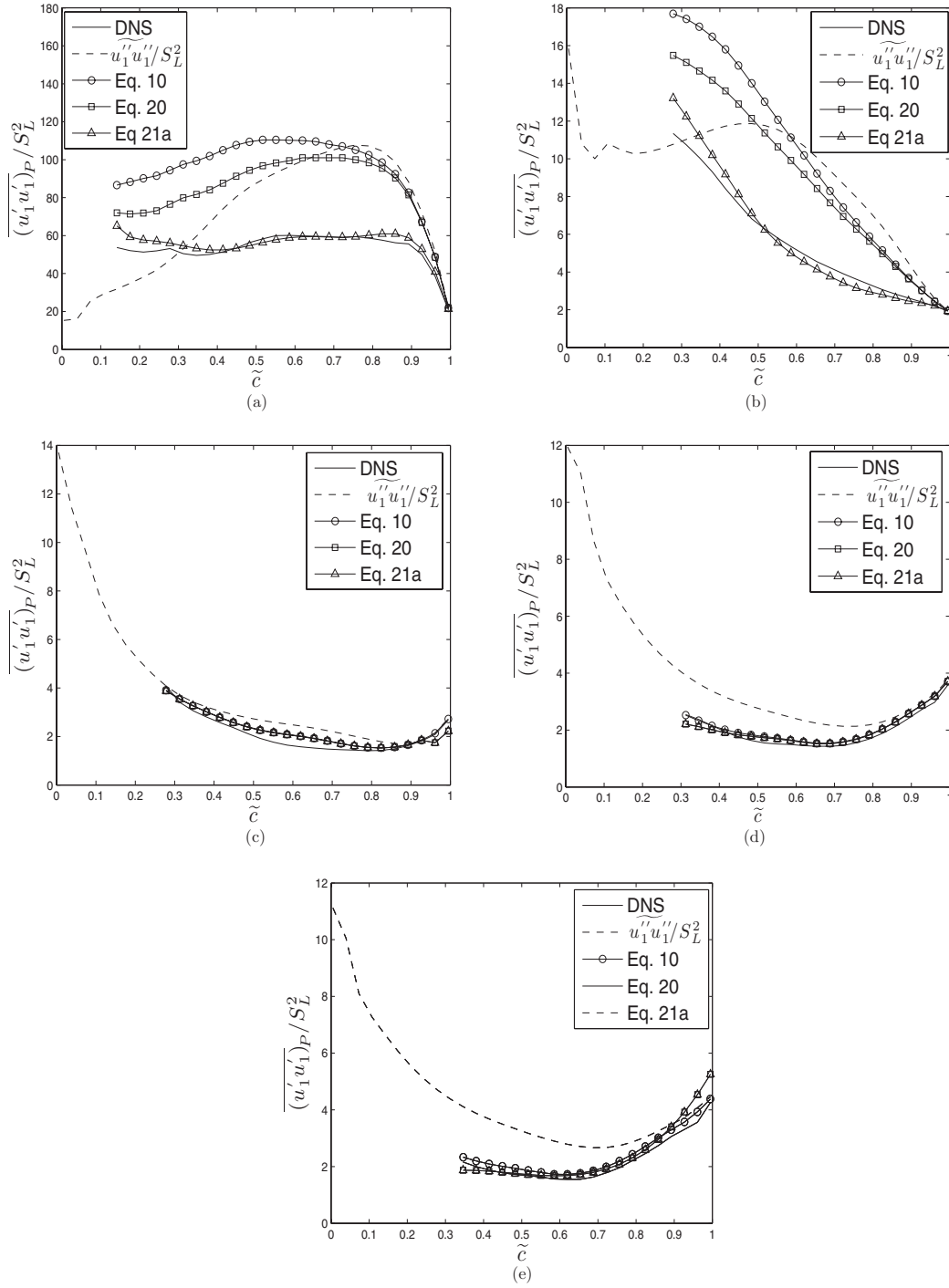


FIG. 7. Variations of  $(u'_1 u'_1)_P / S_L^2$  and  $\overline{\rho u''_1 u''_1} / \bar{\rho} S_L^2$  with  $\tilde{c}$  across the flame brush along with the predictions of Eqs. (10), (20), and (21a) for cases (a)–(e) A–E.

$[(u'_2 u'_2)_P - \overline{\rho u''_2 u''_2} / \bar{\rho}]$  does not play a major role for the low Damköhler number flames, which is consistent with the previous findings by Chakraborty and Lipatnikov.<sup>16</sup> As  $\overline{\rho u''_2 c''}$  remains identically zero (i.e.,  $\overline{\rho u''_2 c''} = 0$ ) for statistically planar flames, the predictions of Eqs. (10), (20), and (21) are identical for  $(u'_2 u'_2)_P$  (see Fig. 8). Moreover, the original BML expression given by Eq. (10)

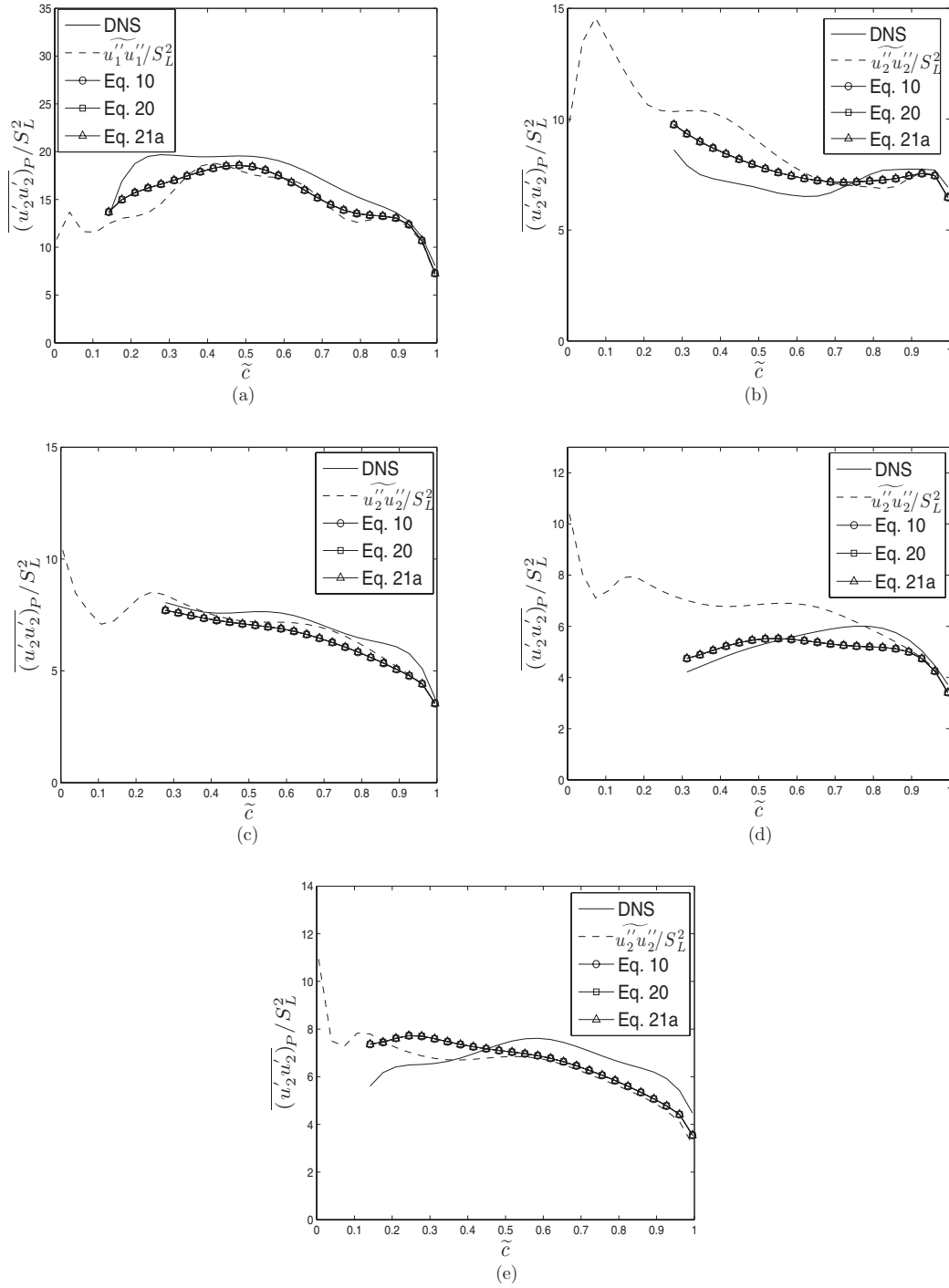


FIG. 8. Variations of  $\overline{(u'_2 u'_2)}_P / S_L^2$  and  $\overline{\rho u''_2 u''_2} / \bar{\rho} S_L^2$  with  $\tilde{c}$  across the flame brush along with the predictions of Eqs. (10), (20), and (21a) for cases (a)–(e) A–E.

reasonably predicts not only  $\overline{(u'_2 u'_2)}_R$  (see Fig. 6), but also  $\overline{(u'_2 u'_2)}_P$  (see Fig. 8) for all cases considered here. As  $\overline{(u'_2 u'_2)}_P / S_L^2$  and  $\overline{\rho u''_2 u''_2} / \bar{\rho} S_L^2$  are statistically similar to  $\overline{(u'_3 u'_3)}_P / S_L^2$  and  $\overline{\rho u''_3 u''_3} / \bar{\rho} S_L^2$ , respectively, the variations of  $\overline{(u'_3 u'_3)}_P / S_L^2$  and  $\overline{\rho u''_3 u''_3} / \bar{\rho} S_L^2$  are not shown here for the sake of conciseness.

The findings based on Figs. 5–8 can be summarised as follows:

1. The theoretical BML expression given by Eq. (10) predicts  $\overline{(u'_1 u'_1)}_R$ ,  $\overline{(u'_2 u'_2)}_R$ , and  $\overline{(u'_2 u'_2)}_P$  satisfactorily for cases A–E, with  $\overline{(u'_2 u'_2)}_R$  and  $\overline{(u'_2 u'_2)}_P$  being close to  $\overline{\rho u''_2 u''_2}$ . Moreover, Eq. (10) predicts  $\overline{(u'_1 u'_1)}_P$  satisfactorily for cases C–E, but overestimates this correlation for cases A and B.
2. The empirical expression given by Eq. (19) not only parameterizes  $\overline{(u'_1 u'_1)}_R$  obtained from DNS data shown in Figs. 5 and 6 (Eq. (10) is also capable for doing so), but also for  $Da > 1$  flames with  $Le = 1.0$  (Refs. 14 and 16), where the prediction of Eq. (10) remains worse than Eq. (19).
3. Equation (20) empirically parameterizes  $\overline{(u'_1 u'_1)}_P$  not only for  $Le = 0.8 - 1.2$ , but also for  $Le = 0.34$  and  $0.6$ .
4. For  $Da \rightarrow \infty$ , the segregation factor  $g$  approaches to unity (i.e.,  $g \rightarrow 1$ ) and Eqs. (19) and (20) become identical to the theoretical Eq. (10).

Stronger influences of the Lewis number on conditional Reynolds stresses in the products (than in reactants) may be explained in terms of the local variations in burning rate due to the imbalance of local heat and species diffusion fluxes, which in turn affect the velocity statistics when a gas volume passes through the heat-release zone,<sup>56–58</sup> even though the velocity field ahead of the reaction zone gets marginally influenced.

It is worth noting that in an actual RANS simulation, the quantities  $\overline{\rho u''_i c''}$  and  $\overline{\rho u''_i u''_j c''}$  are modelled and the accuracy of their modelling are also likely to affect the performance of Eqs. (8), (10) and (15)–(21). Modelling of  $\overline{\rho u''_i c''}$  and  $\overline{\rho u''_i u''_j c''}$  have been discussed in Refs. 1, 49, 56, 57, 59–61 and thus will not be repeated here for the sake of brevity. Moreover,  $\tilde{c}''^2$  needs to be evaluated in order to obtain the segregation factor  $g = \tilde{c}''^2 / \tilde{c}(1 - \tilde{c})$ . The modelling of  $\tilde{c}''^2$  for low Damköhler number non-unity Lewis number flames has been discussed in Ref. 62 and will not be taken up here. Interested readers are referred to Refs. 56–62 for further details on the modelling of  $\tilde{c}''^2$ ,  $\overline{\rho u''_i c''}$ ,  $\overline{\rho u''_i u''_j c''}$ , and  $\overline{\rho u''_i u''_j}$ .

The variations of  $\overline{(u_1)}_{Rs}/S_L$  and  $\overline{(u_1)}_R/S_L$  with  $\tilde{c}$  along with the predictions of Eq. (13) according to  $\langle c \rangle = \tilde{c}$  and  $\langle c \rangle = \tilde{c}$  are shown in Figs. 9(a)–9(e) for cases A–E, respectively. It is worth stressing that these velocities were evaluated in the coordinate framework selected, so that the mean velocity of unburned gas upstream of the flame brush is equal to  $S_L$ . It is evident from Figs. 9(a)–9(e) that the simple expression given by Eq. (12) captures the behaviour of  $\overline{(u_1)}_{Rs}/S_L$  throughout the flame brush,<sup>10</sup> which is in agreement with earlier DNS results.<sup>6, 7, 14, 16</sup> Figures 9(a)–9(e) show that the performance of Eq. (13) is comparable for  $\langle c \rangle = \tilde{c}$  and  $\langle c \rangle = \tilde{c}$  and the model given by Eq. (13) underpredicts  $\overline{(u_1)}_{Rs}/S_L$  for all cases considered here. It is worth reminding that Eq. (13) is a linear interpolation between two limiting cases, i.e.,  $\overline{(u_1)}_P/\sigma$  at  $\tilde{c} = 0$  (or  $\tilde{c} = 0$ ) and  $\overline{(u_1)}_R$  at  $\tilde{c} = 1$  (or  $\tilde{c} = 1$ ). As shown in Ref. 14, Eq. (13) performs well at the leading edge of a unity Lewis number premixed turbulent flame characterized by  $Da > 1$ .

Lee and Huh<sup>7</sup> proposed a model for  $\overline{(u_1)}_{Rs}$  as

$$\overline{(u_1)}_{Rs} = \overline{(u_1)}_R - K_1(\partial^2 \tilde{c} / \partial x_1^2) / (\partial \tilde{c} / \partial x_1), \quad (22)$$

where  $K_1$  is a tuning parameter that is proportional to but significantly larger than the kinematic eddy viscosity  $C_\mu(\tilde{k}^2/\tilde{\epsilon})_R$  conditional in unburned gas,<sup>7</sup> where  $C_\mu = 0.09$  is a model constant. The prediction of Eq. (22) for  $K_1 = 2C_\mu(\tilde{k}^2/\tilde{\epsilon})_R$  is also shown in Figs. 9(a)–9(e), which demonstrates that  $K_1(\partial^2 \tilde{c} / \partial x_1^2) / (\partial \tilde{c} / \partial x_1)$  remains much smaller than  $\overline{(u_1)}_R$  and  $\overline{(u_1)}_{Rs}$  and the prediction of Eq. (22) remains comparable to Eq. (12) for the major part of turbulent flame brush for all the flames considered here. The variations of  $[\overline{(u_1)}_R - \overline{(u_1)}_{Rs}]/S_L$  and  $K_1(\partial^2 \tilde{c} / \partial x_1^2) / [(\partial \tilde{c} / \partial x_1)S_L] = 2C_\mu(\tilde{k}^2/\tilde{\epsilon})_R(\partial^2 \tilde{c} / \partial x_1^2) / [(\partial \tilde{c} / \partial x_1)S_L]$  with  $\tilde{c}$  are shown in Figs. 10(a)–10(e). Equation (22) overpredicts  $[\overline{(u_1)}_R - \overline{(u_1)}_{Rs}]/S_L$  for a major portion of the flame brush for all cases considered here. Moreover,  $K_1(\partial^2 \tilde{c} / \partial x_1^2) / (\partial \tilde{c} / \partial x_1)$  becomes negative in a region towards the burned gas side of the flame brush where  $[\overline{(u_1)}_R - \overline{(u_1)}_{Rs}]/S_L$  remains positive (see Figs. 10(a)–10(e)).

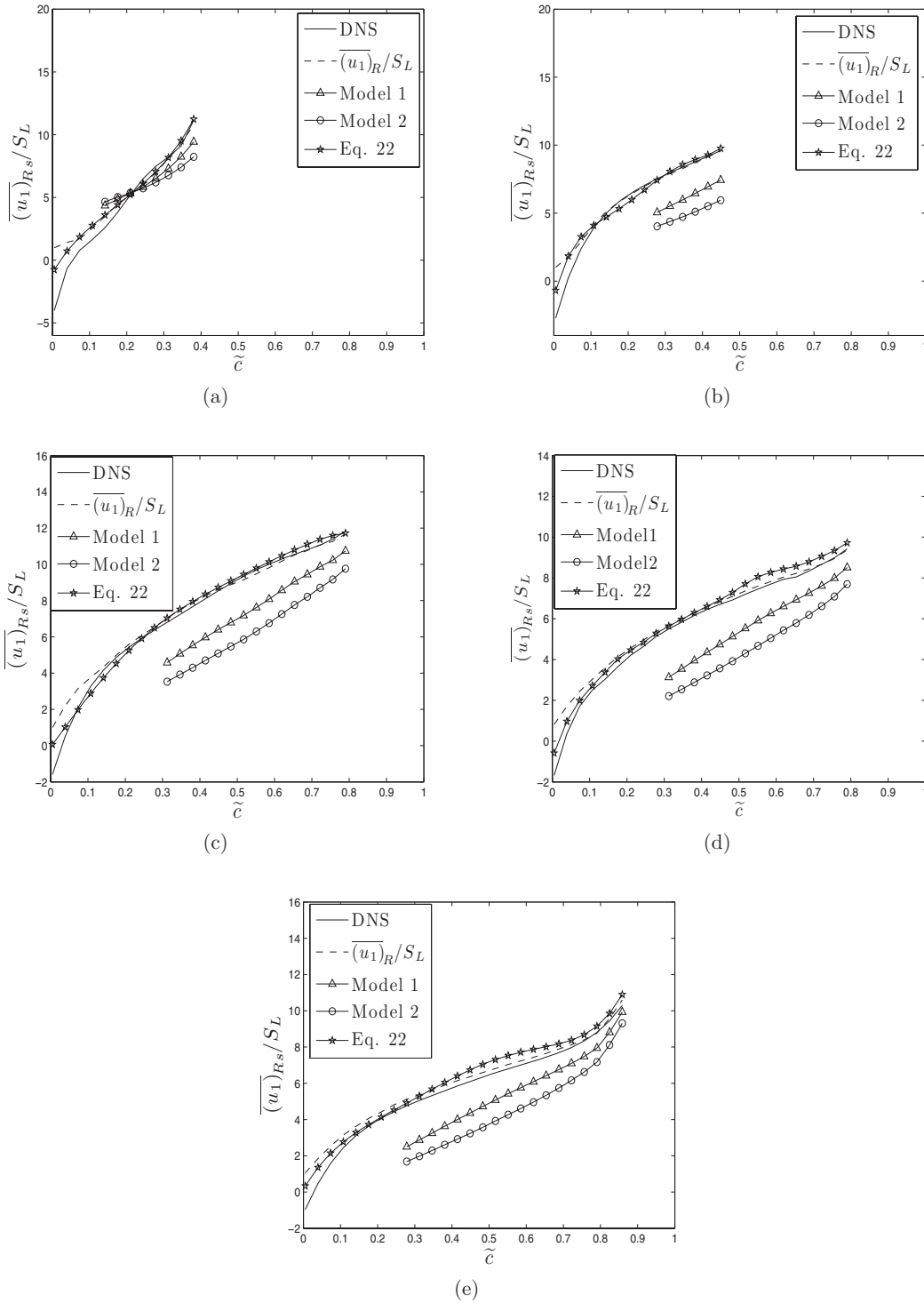


FIG. 9. Variations of  $(u_1)_{Rs}/S_L$  and  $(u_1)_R/S_L$  with  $\tilde{c}$  across the flame brush along with the predictions of Eqs. (12) and (13) according to  $\langle c \rangle = \bar{c}$  (shown as model 1 in the legend) and  $\langle c \rangle = \tilde{c}$  (shown as model 2 in the legend) and Eq. (22) for cases (a)–(e) A–E.

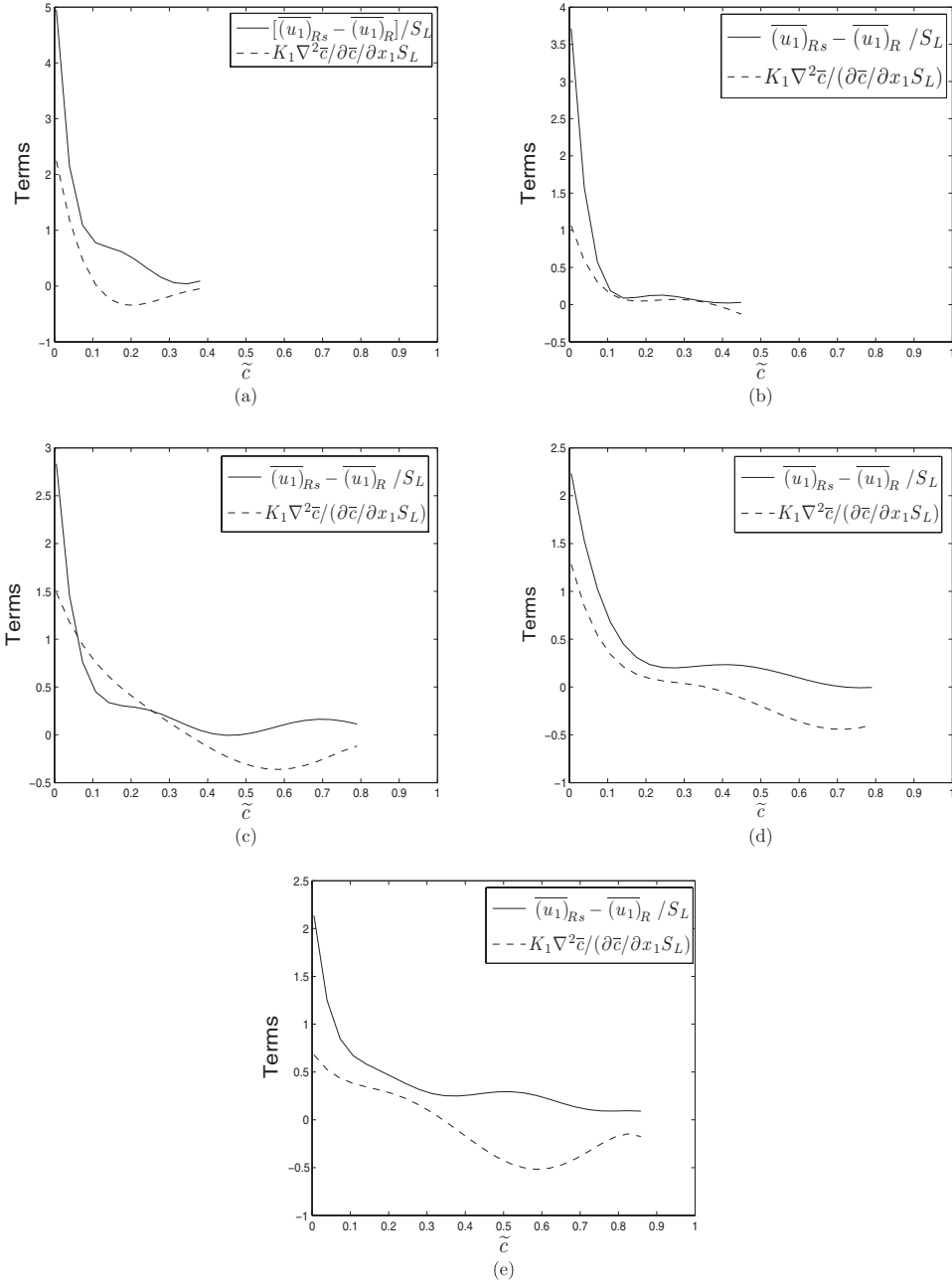


FIG. 10. Variations of  $[(\overline{u_1})_R - (\overline{u_1})_{Rs}]/S_L$  and  $K_1(\nabla^2 \tilde{c})/[(\partial \tilde{c}/\partial x_1)S_L] = 2C_\mu(\tilde{k}^2/\varepsilon)_R(\nabla^2 \tilde{c})/[(\partial \tilde{c}/\partial x_1)S_L]$  with  $\tilde{c}$  for cases (a)–(e) A–E.

The simplest possible model for the conditional surface-weighted Reynolds stresses (i.e.,  $\overline{(u_i u_j)_{Rs}}$ ) can be proposed as

$$\overline{(u_i u_j)_{Rs}} = \overline{(u_i u_j)_R}, \quad (23a)$$

whereas the following linear interpolation<sup>10</sup> ensures the correct behaviour of  $\overline{(u_i u_j)_{Rs}} \rightarrow \overline{(u_i u_j)_P}$  at  $\tilde{c} \rightarrow 0$  for a constant density “flame”:

$$\overline{(u_i u_j)_{Rs}} = (1 - \langle c \rangle) \overline{(u_i u_j)_P} + \langle c \rangle \overline{(u_i u_j)_R}. \quad (23b)$$

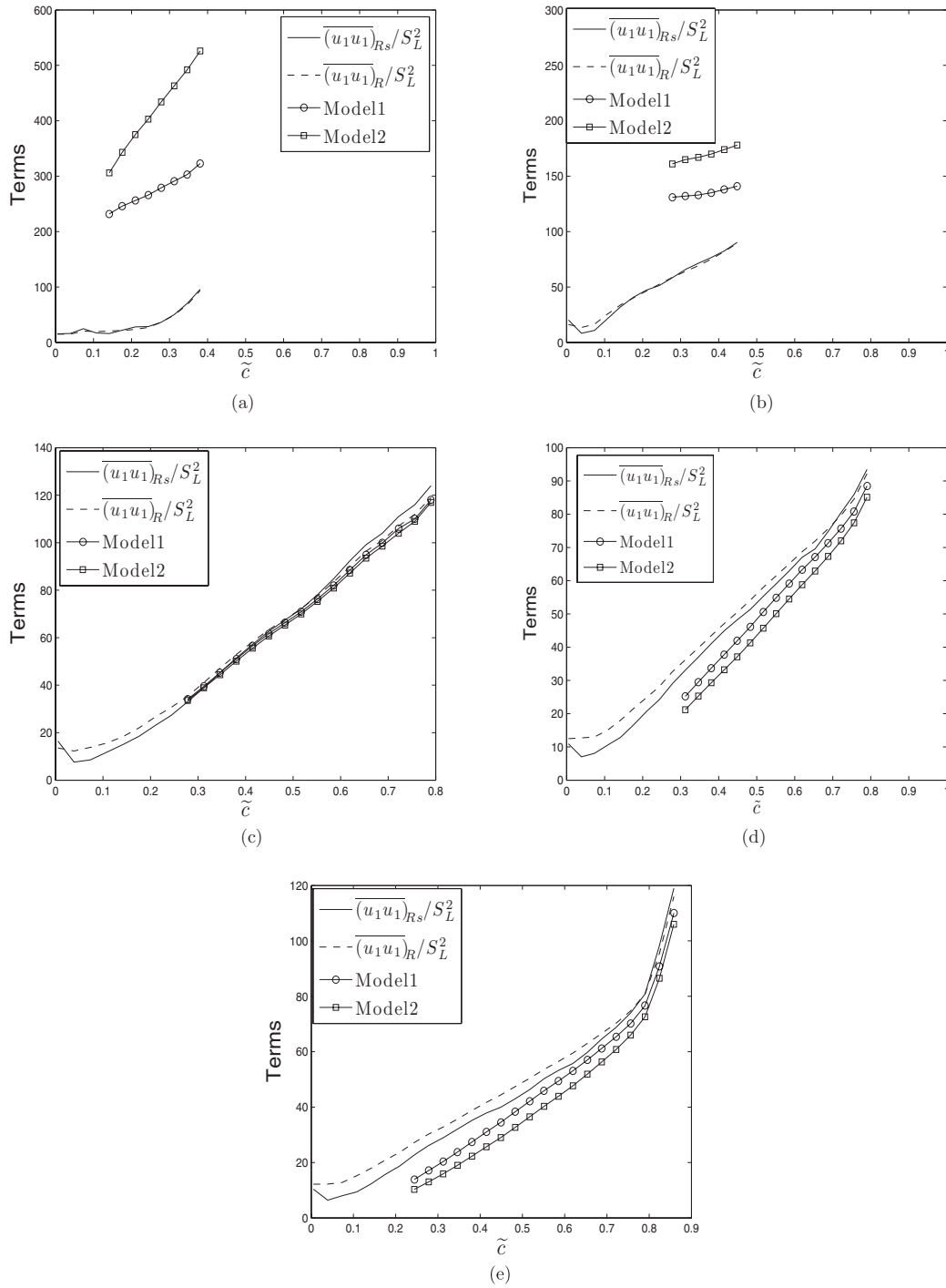


FIG. 11. Variations of  $\overline{(u_1 u_1)}_{Rs} / S_L^2$  with  $\tilde{c}$  across the flame brush along with the predictions of Eqs. (23a) (i.e.,  $\overline{(u_1 u_1)}_{Rs} / S_L^2 = \overline{(u_1 u_1)}_R / S_L^2$ ) and (23b) for cases (a)–(e) A–E. The model given by Eq. (23b) with  $\langle c \rangle = \tilde{c}$  and  $\langle c \rangle = \tilde{c}$  are shown as model 1 and model 2, respectively, in the legend.

The variations of  $\overline{(u_1 u_1)}_{Rs} / S_L^2$  and  $\overline{(u_1 u_1)}_R / S_L^2$  with  $\tilde{c}$  are shown in Figs. 11(a)–11(e) for cases A–E, respectively, along with the predictions of Eqs. (23a) and (23b) (for  $\langle c \rangle = \tilde{c}$  and  $\langle c \rangle = \tilde{c}$ ). The corresponding variations for  $\overline{(u_2 u_2)}_{Rs} / S_L^2$  and  $\overline{(u_2 u_2)}_R / S_L^2$  with  $\tilde{c}$  are shown in Figs. 12(a)–12(e). It is evident from Figs. 11 and 12 that  $\overline{(u_1 u_1)}_{Rs}$  and  $\overline{(u_2 u_2)}_{Rs}$  are appropriately captured by  $\overline{(u_1 u_1)}_R$  and  $\overline{(u_2 u_2)}_R$ , respectively.

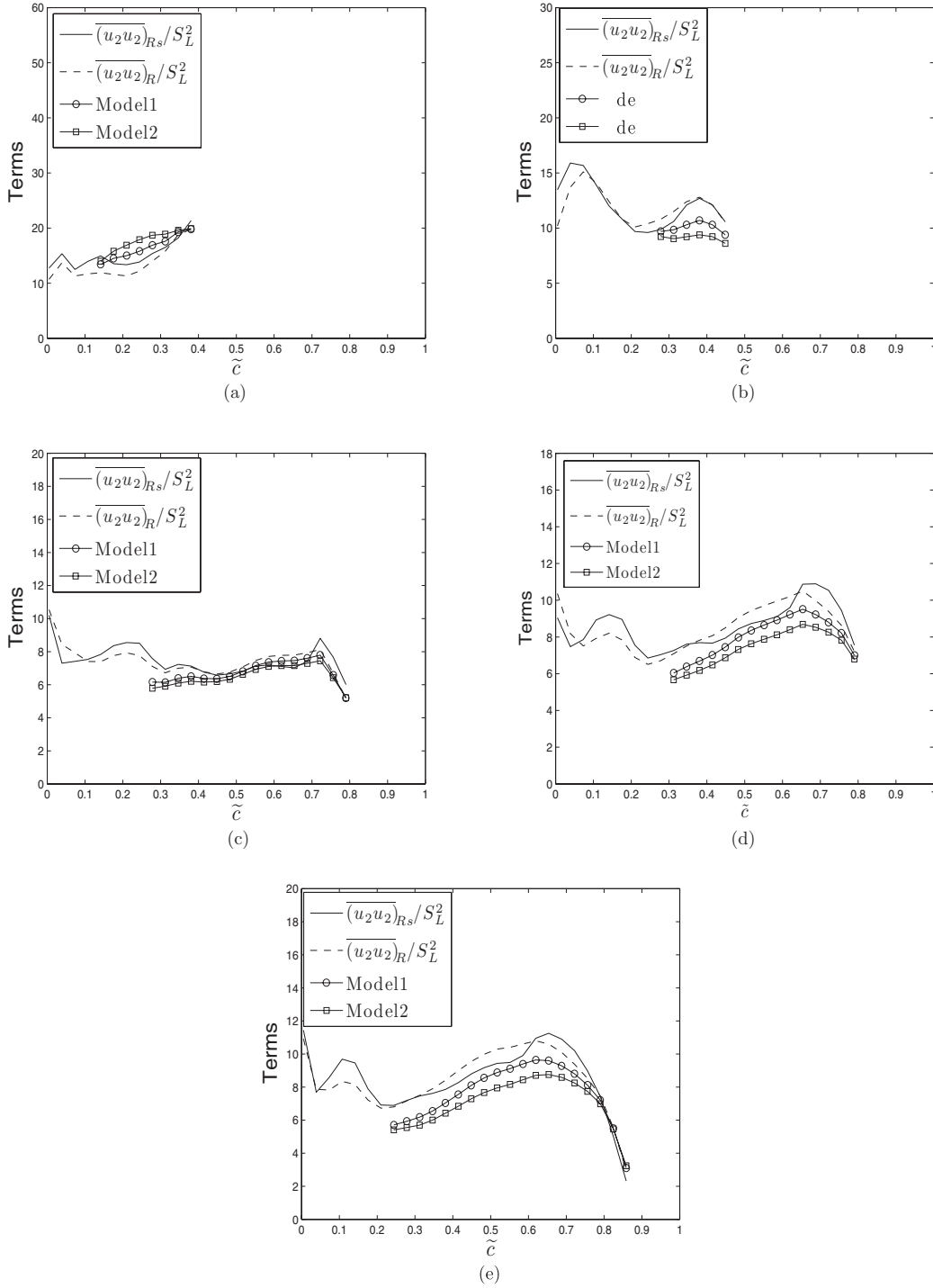


FIG. 12. Variations of  $\overline{(u_2 u_2)}_{Rs} / S_L^2$  with  $\tilde{c}$  across the flame brush along with the predictions of Eqs. (23a) (i.e.,  $\overline{(u_2 u_2)}_{Rs} / S_L^2 = \overline{(u_2 u_2)}_R / S_L^2$ ) and (23b) for cases (d)–(f) A–C. The model given by Eq. (23b) with  $\langle c \rangle = \tilde{c}$  and  $\langle c \rangle = \bar{c}$  are shown as model 1 and model 2, respectively, in the legend.

According to Eq. (23b) the quantity  $\overline{(u_1 u_1)}_{Rs}$  is bound between  $\overline{(u_1 u_1)}_P$  at  $\tilde{c} = 0$  (or  $\bar{c} = 0$ ) to  $\overline{(u_1 u_1)}_R$  at  $\tilde{c} = 1$  (or  $\bar{c} = 1$ ) and as  $\overline{(u_1)}_P$  and  $\overline{(u'_1 u'_1)}_P$  are greater than  $\overline{(u_1)}_R$  and  $\overline{(u'_1 u'_1)}_R$ , respectively, in cases A and B (see Figs. 2–5 and 7), the model given by Eq. (23b) overpredicts the magnitude of  $\overline{(u_1 u_1)}_{Rs}$  for the major portion of the flame brush. Moreover, in cases A and B  $\overline{(u'_2 u'_2)}_P$  remains

greater than  $\overline{(u'_2 u'_2)}_R$  (see Figs. 6 and 8), which leads to an overprediction for the model given by Eq. (23b), whereas Eq. (23a) satisfactorily predicts  $\overline{(u_2 u_2)}_{Rs}$  for the major part of the flame brush. In cases C–E, the magnitudes of  $\overline{(u_1 u_1)}_P$  and  $\overline{(u_1 u_1)}_R$  ( $\overline{(u_2 u_2)}_P$  and  $\overline{(u_2 u_2)}_R$ ) remain comparable and thus the predictions of Eq. (23b) are found to be in better agreement with  $\overline{(u_1 u_1)}_{Rs}$  ( $\overline{(u_2 u_2)}_{Rs}$ ) extracted from DNS data than in cases A and B.

The above results suggest that the relations between surface-weighted velocity components and velocity correlations conditional on reactants (i.e.,  $\overline{(u_i)}_{Rs}$  and  $\overline{(u_i u_j)}_{Rs}$ ) with un-weighted conditional averages (i.e.,  $\overline{(u_i)}_R$  and  $\overline{(u_i u_j)}_R$ ) are not directly affected by  $Le$ , and the surface-weighted conditional quantities are well approximated by un-weighted conditional quantities.

## V. CONCLUSIONS

The effects of global Lewis number  $Le$  on the statistics of fluid velocities conditional in reactants and products have been analysed in the context of RANS simulations using a database of statistically planar turbulent premixed flames with Lewis number ranging from 0.34 to 1.2 for small values of Damköhler number. It has been shown that the non-unity Lewis number substantially affects the mean velocity  $\overline{(u_1)}_P$  and the velocity fluctuation correlation  $\overline{(u'_1 u'_1)}_P$  conditional in products, with the effect being particularly pronounced for low  $Le$ . However, the BML expressions for the mean velocity  $\overline{(u_1)}_R$  and the velocity fluctuation correlation  $\overline{(u'_1 u'_1)}_R$  conditional in reactants agree reasonably well with the DNS data reported in the present work, even though the cases considered here represent low Damköhler number  $Da$  combustion, and the BML expressions are expected to be strictly valid for high values of  $Da$ . Accordingly, in order to parameterize both the present and the earlier<sup>14,16</sup> DNS data, the BML expressions have been modified here by introducing empirical functions  $f_k(g, Le)$  of the segregation factor  $g = c''^2 / \tilde{c}(1 - \tilde{c})$  and the Lewis number  $Le$  so that the original theoretical expressions are recovered in the case of high Damköhler and unity Lewis number, i.e.,  $f_k(g \rightarrow 1, Le \rightarrow 1) \rightarrow 1$ . The newly proposed expressions (see Eqs. (16), (17c), (19), and (21a)) have been demonstrated to capture the behaviours of  $\overline{(u_i)}_R$ ,  $\overline{(u_i)}_P$ ,  $\overline{(u'_i u'_j)}_R$ , and  $\overline{(u'_i u'_j)}_P$  satisfactory for a large range of values of  $Le$ . Moreover, the newly proposed expressions reduce to the expressions proposed earlier by the present authors<sup>16</sup> based on previous DNS based analyses of high<sup>14</sup> and low<sup>16</sup> Damköhler number unity Lewis number flames. Thus, these new expressions could be used either as DNS-derived parameterisations for the assessment of future models, or as semi-empirical models for investigating conditioned characteristics of velocity field in premixed turbulent flames. It is worth noting that the newly proposed expressions are not meant to extend the validity of BML methodology for low Damköhler number combustion and more analysis is needed to assess the extent to which the BML methodology can be applied beyond high Damköhler number conditions.

It has been demonstrated for the first time that the conditional surface averaged velocities  $\overline{(u_i)}_{Rs}$  and velocity correlations  $\overline{(u_i u_j)}_{Rs}$  can be effectively modelled by  $\overline{(u_i)}_R$  and  $\overline{(u_i u_j)}_R$ , respectively, for a wide range of values of global Lewis numbers. This suggests that the surface averaged quantities can be modelled without invoking expressions that involve explicit Lewis number dependence.

The present modelling has been carried out for moderate values of turbulent Reynolds number  $Re_t$  and simplified chemistry. Although no assumption has been made in this analysis which could have a significant  $Re_t$  dependence, both experimental and detailed chemistry based DNS data for higher values of  $Re_t$  are necessary for more comprehensive assessment of expressions proposed in the present study. Some of these issues will form the basis of future investigations.

## ACKNOWLEDGMENTS

N.C. gratefully acknowledges the financial support provided by the Engineering and Physical Sciences Research Council (U.K.) EPSRC(GB). A.L. gratefully acknowledges the financial support provided by Swedish Energy Agency and by the Chalmers Combustion Engine Research Centre (CERC).

- <sup>1</sup> K. N. C. Bray, P. A. Libby, and J. B. Moss, "Unified modelling approach for premixed turbulent combustion – Part I: General formulation," *Combust. Flame* **61**, 87 (1985).
- <sup>2</sup> P. A. Libby and K. N. C. Bray, "Implications of the laminar flamelet model in premixed turbulent combustion," *Combust. Flame* **39**, 33 (1980).
- <sup>3</sup> R. S. Cant, S. B. Pope, and K. N. C. Bray, "Modelling of flamelet surface to volume ratio in turbulent premixed combustion," *Proc. Combust. Inst.* **23**, 809–815 (1991).
- <sup>4</sup> P. Domingo and K. N. C. Bray, "Laminar flamelet expressions for pressure fluctuation terms in second moment models of premixed turbulent combustion," *Combust. Flame* **121**, 555 (2000).
- <sup>5</sup> D. Veynante and L. Vervisch, "Turbulent combustion modelling," *Prog. Energy Combust. Sci.* **28**, 193 (2002).
- <sup>6</sup> Y.-H. Im, K. Y. Huh, S. Nishiki, and T. Hasegawa, "Zone conditional assessment of flame-generated turbulence with DNS database of a turbulent premixed flame," *Combust. Flame* **137**, 478 (2004).
- <sup>7</sup> E. Lee and K. Y. Huh, "Zone conditional modeling of premixed turbulent flames at a high Damköhler number," *Combust. Flame* **138**, 211 (2004).
- <sup>8</sup> A. Trouvé and T. J. Poinso, "The evolution equation for flame surface density in turbulent premixed combustion," *J. Fluid Mech.* **278**, 1 (1994).
- <sup>9</sup> N. Chakraborty and R. S. Cant, "Effects of Lewis number on flame surface density transport in turbulent premixed combustion," *Combust. Flame* **158**, 1768 (2011).
- <sup>10</sup> A. N. Lipatnikov, "Conditionally averaged balance equations for modeling premixed turbulent combustion in flamelet regime," *Combust. Flame* **152**, 529 (2008).
- <sup>11</sup> A. N. Lipatnikov, "A test of conditioned balance equation approach," *Proc. Combust. Inst.* **33**, 1497 (2011).
- <sup>12</sup> A. N. Lipatnikov, "Conditioned moments in premixed turbulent reacting flows," *Proc. Combust. Inst.* **33**, 1489 (2011).
- <sup>13</sup> V. A. Sabel'nikov and A. N. Lipatnikov, "A simple model for evaluating conditioned velocities in premixed turbulent flames," *Combust. Sci. Technol.* **183**, 588 (2011).
- <sup>14</sup> N. Chakraborty and A. Lipatnikov, "Statistics of conditional fluid velocity in the corrugated flamelets regime of turbulent premixed combustion: A direct numerical simulation study," *J. Combust.* **2011**, 628208 (2011).
- <sup>15</sup> N. Peters, *Turbulent Combustion* (Cambridge University Press, Cambridge, UK, 2000).
- <sup>16</sup> N. Chakraborty and A. Lipatnikov, "Conditional velocity statistics for high and low Damköhler number turbulent premixed combustion in the context of Reynolds averaged Navier Stokes simulations," *Proc. Combust. Inst.* **34**, 1333 (2013).
- <sup>17</sup> M. J. Dunn, A. R. Masri, and R. W. Bilger, "A new piloted premixed jet burner to study strong finite-rate chemistry effects," *Combust. Flame* **151**, 46 (2007).
- <sup>18</sup> M. J. Dunn, A. R. Masri, R. W. Bilger, R. S. Barlow, and G.-H. Wang, "The compositional structure of highly turbulent piloted premixed flames issuing into a hot coflow," *Proc. Combust. Inst.* **32**, 1779 (2009).
- <sup>19</sup> M. J. Dunn, A. R. Masri, R. W. Bilger, and R. S. Barlow, "Finite rate chemistry effects in highly sheared turbulent premixed flames," *Flow, Turbul. Combust.* **85**, 621 (2010).
- <sup>20</sup> Z. S. Li, B. Li, Z. W. Sun, X.-S. Bai, and M. Aldén, "Turbulence and combustion interaction: High resolution local flame front structure visualization with simultaneous single-shot PLIF of CH and CH<sub>2</sub>O in a piloted premixed jet flame spectroscopic," *Combust. Flame* **157**, 1087 (2010).
- <sup>21</sup> J. Sjöholm, J. Rosell, B. Li, M. Richter, Z. Li, X.-S. Bai, and M. Aldén, "Simultaneous visualization of OH, CH, CH<sub>2</sub>O and toluene PLIF in a methane jet flame with varying degrees of turbulence," *Proc. Combust. Inst.* **34**, 1475 (2013).
- <sup>22</sup> A. Y. Poludnenko and E. S. Oran, "The interaction of high-speed turbulence with flames: Global properties and internal flame structure," *Combust. Flame* **157**, 995 (2010).
- <sup>23</sup> A. Y. Poludnenko and E. S. Oran, "The interaction of high-speed turbulence with flames: Turbulent flame speed," *Combust. Flame* **158**, 301 (2011).
- <sup>24</sup> A. J. Aspden, M. S. Day, and J. B. Bell, "Lewis number effects in distributed flames," *Proc. Combust. Inst.* **33**, 1473 (2011).
- <sup>25</sup> A. J. Aspden, M. S. Day, and J. B. Bell, "Turbulence-flame interactions in lean premixed hydrogen: Transition to the distributed burning regime," *J. Fluid Mech.* **680**, 287 (2011).
- <sup>26</sup> A. N. Lipatnikov and J. Chomiak, "Molecular transport effects on turbulent flame propagation and structure," *Prog. Energy Combust. Sci.* **31**, 1 (2005).
- <sup>27</sup> G. I. Sivashinsky, "Instabilities, pattern formation and turbulence in flames," *Annu. Rev. Fluid Mech.* **15**, 179 (1983).
- <sup>28</sup> P. Clavin and F. A. Williams, "Effects of Lewis number on propagation of wrinkled flames in turbulent flow," *Prog. Astronaut. Aeronaut.* **76**, 403 (1981).
- <sup>29</sup> P. A. Libby, A. Linan, and F. A. Williams, "Strained premixed laminar flames with non-unity Lewis numbers," *Combust. Sci. Technol.* **34**, 257 (1983).
- <sup>30</sup> W. T. Ashurst, N. Peters, and M. D. Smooke, "Numerical simulation of turbulent flame structure with non-unity Lewis number," *Combust. Sci. Technol.* **53**, 339 (1987).
- <sup>31</sup> D. C. Haworth and T. J. Poinso, "Numerical simulations of Lewis number effects in turbulent premixed flames," *J. Fluid Mech.* **244**, 405 (1992).
- <sup>32</sup> C. J. Rutland and A. Trouvé, "Direct simulations of premixed turbulent flames with nonunity Lewis numbers," *Combust. Flame* **94**, 41 (1993).
- <sup>33</sup> H. G. Im and J. H. Chen, "Preferential diffusion effects on the burning rate of interacting turbulent premixed hydrogen-air flames," *Combust. Flame* **131**, 246 (2002).
- <sup>34</sup> N. Chakraborty and R. S. Cant, "Influence of Lewis number on curvature effects in turbulent premixed flame propagation in the thin reaction zones regime," *Phys. Fluids* **17**, 105105 (2005).
- <sup>35</sup> N. Chakraborty and R. S. Cant, "Influence of Lewis number on strain rate effects in turbulent premixed flame propagation in the thin reaction zones regime," *Int. J. Heat Mass Transfer* **49**, 2158 (2006).
- <sup>36</sup> J. Yuan, Y. Ju, and C. K. Law, "Coupled hydrodynamic and diffusional-thermal instabilities in flame propagation at small Lewis numbers," *Phys. Fluids* **17**, 074106 (2005).

- <sup>37</sup> N. Chakraborty, M. Klein, and N. Swaminathan, "Effects of Lewis number on reactive scalar gradient alignment with local strain rate in turbulent premixed flames," *Proc. Combust. Inst.* **32**, 1409 (2009).
- <sup>38</sup> J. H. Chen, A. Choudhary, B. de Supinski, M. DeVries, E. R. Hawkes, S. Klasky, W. K. Liao, K. L. Ma, J. Mellor-Crummey, N. Podhowski, R. Sankaran, S. Shende, and C. S. Yoo, "Terascale direct numerical simulations of turbulent combustion using S3D," *Comput. Sci. Discovery* **2**, 015001 (2009).
- <sup>39</sup> M. Boger, D. Veynante, H. Boughanem, and A. Trouvé, "Direct numerical simulation analysis of flame surface density concept for large eddy simulation of turbulent premixed combustion," *Proc. Combust. Inst.* **27**, 917 (1998).
- <sup>40</sup> K. W. Jenkins and R. S. Cant, "DNS of turbulent flame kernels," in *Proceedings of the 2nd AFOSR Conference on DNS and LES* (Kluwer Academic Publishers, Dordrecht, 1999), p. 192.
- <sup>41</sup> T. Poinso and S. K. Lele, "Boundary conditions for direct simulation of compressible viscous flows," *J. Comput. Phys.* **101**, 104 (1992).
- <sup>42</sup> A. A. Wray, "Minimal storage time advancement schemes for spectral methods," Report No. MS 202 A-1 (NASA Ames Research Center, California, 1990).
- <sup>43</sup> R. S. Rogallo, "Numerical experiments in homogeneous turbulence," NASA Technical Memorandum 91416 (NASA Ames Research Center, California, 1981).
- <sup>44</sup> G. K. Batchelor and A. A. Townsend, "Decay of turbulence in the final period," *Proc. R. Soc. A* **194**, 527 (1948).
- <sup>45</sup> S. Danielle, P. Jansohn, J. Mantzaras, and K. Boulouchos, "Turbulent flame speed for syngas at gas turbine relevant conditions," *Proc. Combust. Inst.* **33**, 2937 (2011).
- <sup>46</sup> P. Venkateswaran, A. Marshall, D. Shin, D. Noble, J. Seitzman, and T. Lieuwen, "Measurements and analysis of turbulent consumption speeds of H<sub>2</sub>/CO mixtures," *Combust. Flame* **158**, 1602 (2011).
- <sup>47</sup> T. J. Poinso and D. Veynante, *Theoretical and Numerical Combustion* (R. T. Edwards, Inc., Philadelphia, 2001).
- <sup>48</sup> E. R. Hawkes, O. Chatakonda, H. Kolla, A. R. Kerstein, and J. H. Chen, "A petascale direct numerical simulation study of the modelling of flame wrinkling for large-eddy simulations in intense turbulence," *Combust. Flame* **159**, 2690 (2012).
- <sup>49</sup> D. Veynante, A. Trouvé, K. N. C. Bray, and T. Mantel, "Gradient and counter-gradient turbulent scalar transport in turbulent premixed flames," *J. Fluid Mech.* **332**, 263 (1997).
- <sup>50</sup> F. Charlette, C. Meneveau, and D. Veynante, "A power-law flame wrinkling model for LES of premixed turbulent combustion. Part I: Nondynamic formulation and initial tests," *Combust. Flame* **131**, 181 (2002).
- <sup>51</sup> N. Swaminathan and K. N. C. Bray, "Effect of dilatation on scalar dissipation in turbulent premixed flames," *Combust. Flame* **143**, 549 (2005).
- <sup>52</sup> N. Swaminathan and R. Grout, "Interaction of turbulence and scalar fields in premixed flames," *Phys. Fluids* **18**, 045102 (2006).
- <sup>53</sup> R. Grout, "An age extended progress variable for conditioned reaction rates," *Phys. Fluids* **19**, 105107 (2007).
- <sup>54</sup> I. Han and K. H. Huh, "Roles of displacement speed on evolution of flame surface density for different turbulent intensities and Lewis numbers for turbulent premixed combustion," *Combust. Flame* **152**, 194 (2008).
- <sup>55</sup> I. Han and K. H. Huh, "Effects of Karlovitz number on the evolution of the flame surface density in turbulent premixed flames," *Proc. Combust. Inst.* **32**, 1419 (2009).
- <sup>56</sup> N. Chakraborty and R. S. Cant, "Effects of Lewis number on scalar transport in turbulent premixed flames," *Phys. Fluids* **21**, 035110 (2009).
- <sup>57</sup> N. Chakraborty and R. S. Cant, "Effects of Lewis number on turbulent scalar transport and its modelling in turbulent premixed flames," *Combust. Flame* **156**, 1427 (2009).
- <sup>58</sup> N. Chakraborty, M. Katragadda, and R. S. Cant, "Effects of Lewis number on turbulent kinetic energy transport in turbulent premixed combustion," *Phys. Fluids* **23**, 075109 (2011).
- <sup>59</sup> A. N. Lipatnikov and J. Chomiak, "Effects of premixed flames on turbulence and turbulent scalar transport," *Prog. Energy Combust. Sci.* **36**, 1–102 (2010).
- <sup>60</sup> B. J. Daly and F. H. Harlow, "Transport equations of turbulence," *Phys. Fluids* **13**, 2634 (1970).
- <sup>61</sup> P. A. Durbin and B. A. Pettersson-Reif, *Statistical Theory and Modelling of Turbulent Flows*, 1st ed. (John Wiley & Sons, 2001).
- <sup>62</sup> N. Chakraborty and N. Swaminathan, "Effects of Lewis number on scalar variance transport in turbulent premixed flames," *Flow, Turbul. Combust.* **87**, 261 (2011).