ABSTRACT
Algebraic and transport equation-based closures of Favre-filtered scalar dissipation rate (SDR) $N_c$ of the reaction progress variable, in the context of large eddy simulations, have been assessed using detailed chemistry direct numerical simulation (DNS) data of a stoichiometric H$_2$-air turbulent V flame. The Favre-filtered SDR $N_c$ and the unclosed terms of its transport equation have been extracted by explicitly filtering the DNS data for different choices of the reaction progress variable. An algebraic closure of SDR, which was proposed previously using simple chemistry DNS data, has been found to predict the Favre-filtered SDR $N_c$ satisfactorily for detailed chemistry DNS data for different choices of the reaction progress variable. Similarly, the models of the unclosed sub-grid convection, density variation, scalar-turbulence interaction, reaction rate gradient, molecular dissipation, and diffusivity gradient terms of the Favre-filtered SDR $N_c$ transport equation, which have previously been proposed based on simple chemistry DNS data, have been found to satisfactorily predict both the qualitative and quantitative behaviors of these unclosed terms for a range of filter widths $\Delta$, for two different choices of reaction progress variable in the case of the detailed chemistry DNS dataset considered in this analysis.

Introduction
The rate of micro-mixing plays a key role in the fundamental physical understanding and modeling of turbulent reacting flows (Bilger, 2004). The quantity that characterizes the rate of micro-mixing is the scalar dissipation rate (SDR), which is often used for the probability density function (PDF) (Dopazo, 1994; O’Brien, 1980) and conditional moment closure (CMC) (Bilger, 2004; Klimenko and Bilger, 1999) methodologies especially in the context of non-premixed combustion modeling. Bray (1980) demonstrated that the Favre-averaged SDR in the context of Reynolds averaged Navier Stokes (RANS) plays a key role in the closure of mean reaction rate for infinitely fast chemistry (i.e., for
large values of Damköhler number). It was subsequently demonstrated by Chakraborty and Cant (2011) using scaling arguments and direct numerical simulation (DNS) data that the SDR-based reaction rate closure derived by Bray (1980) also remains valid for low Damköhler number combustion as long as the flamelet assumption remains valid. A number of recent analyses (Butz et al., 2015; Dunstan et al., 2013; Gao et al., 2014a, 2014b; Langella et al., 2015; Ma et al., 2014a, 2014b) demonstrated that the SDR-based closure for RANS proposed by Bray (1980) can also be used for large eddy simulations (LES) when the filter size $\Delta$ is much greater than the thermal flame thickness $\delta_{th}$.

$$\delta_{th} = \frac{(T_{ad} - T_0)}{Max[\nabla \hat{T}]}_L,$$

where $T_{ad}$, $T_0$, and $\hat{T}$ are the adiabatic flame, unburned gas, and instantaneous temperatures, respectively. The SDR-based filtered reaction rate closure $\tilde{w}$ of reaction progress variable $c$ for large filter widths (i.e., $\Delta >\delta_{th}$) takes the following form (Butz et al., 2015; Dunstan et al., 2013; Gao et al., 2014a, 2014b; Ma et al., 2014a):

$$\tilde{w} = \frac{2\rho \hat{N}_c}{(2\epsilon_m - 1)} \left[ \frac{\int_0^1 [\hat{w}]_f f_b(c) dc}{\int_0^1 [\tilde{w}]_f f_b(c) dc} \right]$$

(1)

where $\rho$ is the density, $N_c = D \nabla c \cdot \nabla c$ is the instantaneous SDR, $\hat{Q} = \rho \bar{Q} / \rho$ is the Favre-filtered value of a quantity $Q$ with the over-bar indicating an LES filtering operation, and $D$ is the diffusivity of reaction progress variable $c$. In Eq. (1), $f_b(c)$ is the reacting mode probability density function (pdf) of $c$ and the subscript ‘L’ refers to the planar laminar flame conditions. The numerical value of $\epsilon_m$ remains within a range of 0.7–0.9 for typical hydrocarbon-air mixtures when $f_b(c)$ is chosen to be a smooth function, regardless of its exact form (Bray, 1980). There are other alternative approaches of LES premixed combustion modeling, such as the level-set (Freitag, 2007; Peters, 2000; Pitsch and Duchamp-de-Lageneste, 2002), flame surface density (FSD) (Chakraborty and Cant, 2009a; Chakraborty and Klein, 2008; Hawkes and Cant, 2000, 2001; Hernandez-Perez et al., 2011; Ma et al., 2013, 2014b; Reddy and Abraham, 2012), and the artificially thickened flame (ATF) (Charlette et al., 2002a, 2002b; Kuenne et al., 2011; Veynante and Poinset, 1997) methods, which also depend on flamelet assumption similar to the SDR-based reaction rate closure. There are other approaches [e.g., Eulerian stochastic field method (Jones et al., 2012)], which could be used for both flamelet and non-flamelet-type combustion but at the expense of higher computational cost than the SDR, level-set, and ATF approaches. The inter-relation between the temperature field and the flame surface is not straightforward and often empirically formulated in the level-set approach, whereas the temperature and species fields are inherently linked by combustion thermo-chemistry in the FSD, SDR, and ATF methodologies. Most wrinkling factor models used in the ATF methodology were proposed for unity Lewis number combustion but they do not adequately perform for non-unity Lewis number flames (Katragadda et al., 2012). It has been found that (Chakraborty and Cant, 2011; Gao et al., 2014a) that the SDR-based reaction rate closure remains valid for a range of different Lewis numbers $Le$, whereas the reaction rate closure by FSD needs a correction factor, which is a function of Lewis number (Chakraborty and
Cant, 2011). This makes the SDR-based closure a promising computationally inexpensive methodology for reaction rate closure in turbulent premixed combustion.

A number of analyses concentrated on SDR closures for premixed turbulent combustion in the context of RANS (Ahmed and Swaminathan, 2013; Chakraborty et al., 2008a; 2010, 2011; Chakraborty and Swaminathan, 2010, 2011, 2013; Dong et al., 2013; Kolla et al., 2009; Kolla and Swaminathan, 2010a, 2010b; Mantel and Borghi, 1994; Mura and Borghi, 2003; Mura et al., 2008, 2009; Sadasivuni et al., 2012) but limited effort has been directed to the closure of SDR for LES (Butz et al., 2015; Dunstan et al., 2013; Gao et al., 2014a, 2014b, 2015a, 2015b; Gao and Chakraborty, 2016; Langella et al., 2015; Ma et al., 2014a). Recently, Gao et al. (2014a, 2014b, 2015a) proposed algebraic closures of $\tilde{N}_c$ for both static and dynamic model coefficients and assessed their validity by extracting the relevant quantities from explicitly filtered DNS data (i.e., a priori assessment). These closures have subsequently been implemented in actual LES simulations for a number of configurations (Butz et al., 2015; Langella et al., 2015; Ma et al., 2014a) for the purpose of model validation (i.e., a-posteriori analysis), and a satisfactory level of agreement has been obtained with experimental measurements. However, all of the aforementioned analyses have been carried out in the context of simple single-step chemistry and thus it is important to compare the statistical behaviors of the SDR and its transport obtained from simple chemistry DNS data with corresponding statistics extracted from detailed chemistry DNS, to ascertain whether the modeling assumptions used for simple chemistry remain valid for predicting the dissipation rates of major species (i.e., SDRs of major reactants and products) in the context of detailed chemistry and transport. Moreover, it is possible to define $\dot{c}$ based on different species mass fractions in the context of detailed chemistry, and thus it is important to analyze if the choice of $\dot{c}$ affects the statistics of SDR transport. Furthermore, most existing SDR closures have been proposed for unity Lewis number $Le$ flames, but $Le$ is known to have significant influences on the statistical behavior of the unclosed terms of the Favre-averaged SDR transport equation in the context of RANS (Chakraborty and Swaminathan, 2010). Similar qualitative behavior has been observed for LES (Gao et al., 2014b; Gao and Chakraborty, 2016), and the submodels proposed by Gao et al. (2015b) for the unclosed terms of $\tilde{N}_c$ transport equations for the thermo-diffusively neutral flames needed modification to account for the non-unity Lewis number effects. Different chemical species have different Lewis numbers; thus, it remains to be assessed if the models for the SDR transport equation, which were previously proposed based on simple chemistry DNS data, are also valid in the context of detailed chemistry DNS data. In this respect the main objectives of the current analysis are:

(a) To indicate the influences of the definition of reaction progress variable $c$ on the SDR statistics.

(b) To assess if the closures of SDR and its transport, which were proposed previously based on simple chemistry DNS data, remain valid for a detailed chemistry DNS data.

In order to meet these objectives, the Favre-filtered SDR $\tilde{N}_c$ statistics obtained from a DNS dataset of a turbulent stoichiometric $H_2$-air V-shaped oblique premixed flame (Minamoto et al., 2011) has been considered.
The rest of the article is organized as follows. The information related to mathematical background and numerical implementation is provided in the next two sections. This is followed by the presentation of results and its subsequent discussion. Finally, the main findings are summarized and conclusions are drawn.

**Mathematical background**

For single step chemistry $c$ can be uniquely defined but in the context of detailed chemistry one can obtain different distributions of $c$ depending on its definition. For the detailed chemistry turbulent H$_2$-air V-flame dataset, two alternative definitions of reaction progress variable have been considered based on H$_2$ and H$_2$O mass fractions in the following manner:

\[
c_{H_2} = \frac{(Y_{H_2})_0 - (Y_{H_2})}{(Y_{H_2})_0 - (Y_{H_2})_\infty} \quad \text{and} \quad c_{H_2O} = \frac{(Y_{H_2O}) - (Y_{H_2O})_0}{(Y_{H_2O})_\infty - (Y_{H_2})_0}
\]  

(1)

where the subscripts 0 and $\infty$ indicate the values in unburned reactants and fully burned products, respectively. Thus, one gets $(Y_{H_2})_0 = 0.028$, $(Y_{H_2O})_0 = 0.0$, $(Y_{H_2})_\infty = 0.0$, and $(Y_{H_2O})_\infty = 0.255$ for stoichiometric H$_2$-air premixed flame. Equation (1) is valid not only for stoichiometric flames but for all equivalence ratios provided correct values of $(Y_{H_2})_0$, $(Y_{H_2O})_0$, $(Y_{H_2})_\infty$, and $(Y_{H_2O})_\infty$ corresponding to the equivalence ratio in question are used. The reaction progress variable is required to increase monotonically from 0 in unburned reactants to 1.0 in fully burned products and that is why the reaction progress variable in Eq. (1) is defined based on the mass fraction of either a major reactant or a major product species, which is consistent with several previous analyses (Chakraborty et al., 2008b; Hawkes and Chen, 2005, 2006; Kolla et al., 2009; Kolla and Swaminathan, 2010a, 2010b; Rogerson and Swaminathan, 2007).

It is worth noting that it will be improper to use the mass fraction of an intermediate species in Eq. (1), because in this particular case the reaction progress variable does not monotonically increase from 0 to 1 from the unburned to burned gases. Equation (1) reduces to $c_{H_2} = 1 - (Y_{H_2})/(Y_{H_2})_0$ when the value of $(Y_{H_2})_\infty$ is equal to zero, which is only true when either a fuel-lean or a stoichiometric flame is considered. Similarly, $c_{H_2O}$ becomes $c_{H_2O} = (Y_{H_2O})/(Y_{H_2O})_\infty$ when the product species is absent in the unburned gas [i.e., $(Y_{H_2O})_0 = 0.0$]. The non-dimensional temperature $c_\tau = (\bar{T} - T_0)/(T_{ad} - T_0)$ is often used as the reaction progress variable but instantaneous dimensional temperature $\bar{T}$ may assume super-adiabatic values (i.e., $\bar{T} > T_{ad}$) even under a globally adiabatic condition in the presence of significant differential diffusion of heat and species. This yields an unphysical value of reaction progress variable, which is greater than unity. In this respect, Eq. (1) is valid for all values of global Lewis number and equivalence ratio. However, most combustion models have been proposed for thermo-diffusively neutral conditions so it might be advantageous to define the reaction progress variable based on a major reactant/product species, which has a Lewis number close to unity. In this respect, $c_{H_2O}$ is likely to be more advantageous than $c_{H_2}$.

Recently, Gao et al. (2014a) proposed an algebraic closure for the Favre-filtered SDR $\bar{N}_c$ in the following manner:
\[
\tilde{N}_c = \frac{\partial \tilde{\rho}_i \tilde{\rho}_i}{\partial t} + (1-f) \left[ \frac{2K_\varepsilon S_L}{Le^{1.88} \delta_{th}} + \left( C_3^* - \tau Da_{\Delta} C_4^* \right) \frac{2u'_\Delta}{3\Delta} \right] \frac{\tilde{\epsilon}(1-\tilde{\epsilon})}{\beta_c} \tag{2}
\]

where \( S_L \) is the unstrained laminar burning velocity, \( \delta_{th} \) is the thermal flame thickness, \( \tau = (T_{ad} - T_0) / T_0 \) is the heat release parameter, \( Le \) is the Lewis number of the species based on which the reaction progress variable is defined, and \( f = \exp[-0.7(\Delta / \delta_{th})^{1.7}] \) is a bridging function, with \( \Delta \) being the LES filter width. In Eq. (2), \( C_3^*, C_4^*, \) and \( \beta_c \) are the model parameters and Gao et al. (2014a) suggested the following expressions of these parameters:

\[
C_3^* = \frac{2.0\sqrt{Ka_{\Delta}}}{(1.0 + \sqrt{Ka_{\Delta}})}; \quad C_4^* = \frac{1.2(1.0 - \tilde{\epsilon})^{0.2+1.5|1-Le|}}{[Le^{2.57}(1 + Ka_{\Delta})^{0.4}]^2} \quad \text{and} \quad \beta_c = \max \left( \frac{2}{2c_m - 1}, \left[ 1.1 - \frac{\tau}{\tau + 1} + 0.41 \right]^{4.9} \right) \tag{3}
\]

where \( Da_{\Delta} = \Delta S_L / u'_\Delta \delta_{th} \) and \( Ka_{\Delta} = (u'_\Delta / S_L)^{3/2}(\Delta / \delta_{th})^{-1/2} \) are the local sub-grid Damköhler and Karlovitz numbers, respectively, with \( u'_\Delta = \sqrt{\langle \rho \tilde{u}_i \tilde{u}_i \rangle - \langle \tilde{\rho} \tilde{u}_i \tilde{u}_i \rangle / \tilde{\rho}} \) being the sub-grid level velocity fluctuation. Moreover, \( K_i^* \) is a thermo-chemical parameter, which is expressed as (Kolla et al., 2009; Rogerson and Swaminathan, 2007):

\[
K_i^* = \frac{\delta_{th}}{S_L} \int_0^1 \left[ \rho N_c \tilde{\rho}_i \tilde{\rho}_i \right] f(c) dc / \int_0^1 \rho N_c f(c) dc \tag{4}
\]

Interested readers are referred to Gao et al. (2014a, 2014b, 2015a), Ma et al. (2014a), and Butz et al. (2015) for the theoretical justification of the model expression given by Eq. (2). It was shown in previous analyses (Gao et al., 2014a, 2014b; Ma et al., 2014a) that Eq. (2) satisfactorily captures both volume-averaged and local behaviors of Favre-filtered SDR \( \tilde{N}_c \) for different values of \( \tau \) and \( Le \) based on simple chemistry DNS data in the conventional canonical configuration. The performance of the model given by Eq. (2) for a detailed chemistry DNS data for turbulent H₂-air V-shaped premixed flame will be assessed in the Results and Discussion section for Favre-filtered SDRs of reaction progress variables based on H₂ and H₂O mass fractions (i.e., \( c_{H_2} \) and \( c_{H_2O} \)).

The transport equation of Favre-filtered SDR \( \tilde{N}_c \) takes the following form (Gao et al., 2014a, 2014b, 2015b; Gao and Chakraborty, 2016):

\[
\frac{\partial (\tilde{\rho}_i \tilde{\rho}_i \tilde{N}_c)}{\partial t} + \frac{\partial (\tilde{\rho}_i \tilde{u}_i \tilde{N}_c)}{\partial x_i} = \frac{\partial}{\partial x_i} \left( \rho D_i \frac{\partial \tilde{N}_c}{\partial x_i} \right) + T_1 + T_2 + T_3 + T_4 - D_2 + f(D) \tag{5}
\]

where \( u_i \) is the \( i \)th component of velocity vector. On the left-hand side of Eq. (5) the terms denote the transient effects and resolved advection of \( \tilde{N}_c \), respectively. The term \( D_1 \) depicts the molecular diffusion of \( \tilde{N}_c \), and the terms \( T_1, T_2, T_3, T_4, (-D_2) \), and \( f(D) \) are expressed as:
\[ T_1 = -\frac{\partial}{\partial x_j} [\rho u_j N_c - \rho \bar{u}_j \bar{N}_c] \]  
(6a)

\[ T_2 = -\frac{2D}{\rho} \left[ \dot{\bar{w}} + \frac{\partial}{\partial x_j} \left( \rho D \frac{\partial c}{\partial x_j} \right) \right] \frac{\partial c}{\partial x_i} \frac{\partial \rho}{\partial x_i} \]  
\]  
(6b)

\[ T_3 = -2 \rho D \frac{\partial c}{\partial x_i} \frac{\partial u_i}{\partial x_j} \frac{\partial c}{\partial x_j} \]  
\]  
(6c)

\[ T_4 = 2D \frac{\partial \dot{\bar{w}}}{\partial x_i} \frac{\partial c}{\partial x_i} \]  
\]  
(6d)

\[ (-D_2) = -2 \rho D^2 \frac{\partial^2 c}{\partial x_i \partial x_j} \frac{\partial^2 c}{\partial x_i \partial x_j} \]  
(6e)

\[ f(D) = \overline{f_1(D)} = 2 \frac{\partial c}{\partial x_k} \frac{\partial (\rho D)}{\partial x_j} \frac{\partial c}{\partial x_j} + 2 \frac{\partial c}{\partial x_k} \frac{\partial^2 (\rho D)}{\partial x_j \partial x_j} \frac{\partial c}{\partial x_j} - \frac{\partial}{\partial x_j} \left( \rho N_c \frac{\partial D}{\partial x_j} \right) \]  
\]  
(6f)

The term \( T_1 \) denotes sub-grid convection, whereas \( T_2 \) denotes the effects of density variation due to heat release. The term \( T_3 \) is governed by the alignment of \( \nabla c \) with local strain rate \( e_{ij} = 0.5(\partial u_i/\partial x_j + \partial u_j/\partial x_i) \), and this term is commonly referred to as the scalar-turbulence interaction term. The term \( T_4 \) arises due to the correlation between \( \bar{\nabla} \dot{\bar{w}} \) and \( \nabla c \), whereas \( (-D_2) \) denotes the molecular dissipation of SDR and these terms will henceforth be referred to as the reaction rate gradient term and dissipation term, respectively. The term \( f(D) \) represents the effects of \( D \) variation. The terms \( T_1, T_2, T_3, T_4, (-D_2), \) and \( f(D) \) are unclosed and need modeling. Furthermore, the modeling of \( T_1 \) depends on the modeling of sub-grid SDR flux \( (\rho u_j N_c - \rho \bar{u}_j \bar{N}_c) \). Gao et al. (2014b, 2015b) recently analyzed the statistical behaviors of these unclosed terms (i.e., \( T_1, T_2, T_3, T_4, (-D_2), \) and \( f(D) \)) and proposed scaling estimates of these terms. These scaling estimates are summarized in Table 1 and these relations have subsequently been utilized to propose closures for \( (\rho u_j N_c - \rho \bar{u}_j \bar{N}_c), T_2, T_3, \) and \( (T_4 - D_2 + f(D)) \) in the context of LES by Gao et al. (2015b) based on the assessment of model performance with respect to the corresponding quantities extracted from explicitly filtered simple chemistry DNS data of turbulent premixed flames with \( Le = 1.0 \). These models have subsequently been modified to account for non-unity Lewis number effects by Gao and Chakraborty (2016). The models of \( (\rho u_j N_c - \rho \bar{u}_j \bar{N}_c), T_2, T_3, \) and \( (T_4 - D_2 + f(D)) \), as proposed by Gao and Chakraborty (2016), are summarized in Table 2. In Tables 1 and 2, \( (T_2)_{res}, (T_3)_{res}, (T_4)_{res}, (-D_2)_{res}, \) and \( \{f(D)\}_{res} \) are the resolved components of \( T_2, T_3, T_4, (-D_2), \) and \( f(D) \), which are given by:

\[ (T_2)_{res} = -\frac{2D}{\rho} \left[ \dot{\bar{w}} + \frac{\partial}{\partial x_j} \left( \rho D \frac{\partial c}{\partial x_j} \right) - \frac{\partial}{\partial x_j} \left( \rho u_j \right) \frac{\partial c}{\partial x_j} \right] \frac{\partial c}{\partial x_i} \frac{\partial \rho}{\partial x_i} \]  
\]  
(7a)
The performance of the models listed in Table 2 will be assessed in the Results and Discussion section for detailed chemistry DNS data of a stoichiometric turbulent H₂-air V-shaped premixed flame for reaction progress variables based on H₂ and H₂O mass fractions (i.e., $c_{H_2}$ and $c_{H_2O}$).
Table 2. Summary of the models for the unclosed terms of the SDR $\bar{N}_i$ transport equation as proposed by Gao and Chakraborty (2016).

| Term | Model expressions |
|------|-------------------|
| $[\bar{p}u_i\bar{N}_i - \bar{p}\bar{u}_i\bar{N}_i]$ | Model expression (FLUXG): $\frac{[\bar{p}u_i\bar{N}_i - \bar{p}\bar{u}_i\bar{N}_i]}{\bar{p} \bar{u}_i} = (\Phi' - \tilde{c}) \frac{[\bar{p}u_i\bar{N}_i - \bar{p}\bar{u}_i\bar{N}_i]}{\bar{p}\bar{u}_i}$, where $\gamma_1 = 1.8$, $\gamma_2 = 4.9 - 3.2\text{erf}(0.15\text{Re}_{\text{e},D})$, $\text{Re}_{\text{e},D} = \rho_0 u_{\text{e}}^3/\mu_0$, $\Phi' = 0.7 + 0.3(1 - \text{Le})$, and $\text{C}_f = 0.11$. |
| $T_2$ | Model expression (T2G): $T_2 = -\frac{2\bar{D}}{\bar{p}} \left[ \frac{\bar{w}}{\bar{N}_j} + \frac{\partial}{\partial x_j} \left( \frac{\bar{p}\bar{D}}{\bar{x}} \frac{\partial \bar{c}}{\partial x_j} \right) - \frac{\partial \bar{p}\bar{D}}{\partial x_j} \right] \frac{\partial \bar{c}}{\partial x_j} \frac{\partial \bar{p}}{\partial x_j}$, where $K_{\text{S,h}} = \left( u_{\text{h}}^3/\text{Le}_0 \right)^{3/2} \left( \text{Le}/\text{Le}_0 \right)^{-1/2}$ is the sub-grid Karlovitz number and $f_{T_2}(\text{Le}) = 3.3\text{Le}^{-2.57} \{\text{erf}[4(1.0 - \text{Le})] + 1.4\}^{-1}$. |
| $T_3$ | Model expression (T3G): $T_3 = -\frac{2\bar{D}}{\bar{p}} \frac{\partial}{\partial x_j} \left( \frac{\bar{p}\bar{D}}{\partial x_j} \right) \left( (1 - f_{T_3}) \left[ C_3 - \Gamma(\text{Le}) C_4 D_{\alpha,\text{h}}^2 \right] \frac{\partial \bar{p}}{\partial x_j} \right) \bar{N}_i$, where $C_3 = 7.5$, $C_4 = 0.75(1 + K_{\text{S,h}})^{-0.4}$, $f_{T_3} = \exp[-1.05(\text{Le}/\text{Le}_0)^{2}]$, $\Gamma(\text{Le}) = \frac{1}{\text{Le}_0^{1.5}} \left( \frac{\text{Le}_0}{\text{Le}} \right)^{1.3}$, $p = 0.2 + 1.5(1.0 - \text{Le})$, and $D_{\alpha,\text{h}}^2 = \text{S}_L\rho_0 \Delta/\mu_0\rho_{\text{d,h}}$ is the density-weighted sub-grid Damköhler number. |

[T4 - D2 + f(D)] Model expression (T4D2FG): $[T_4 - D_2 + f(D)]_{res} = (T_4)_{res} - (D_2)_{res} + \{f(D)\}_{res} - (1 - f_{T_4}) [\bar{N}_i - \bar{D} \bar{V} \bar{c} \bar{V} c \bar{e}]$ where $(T_4)_{res} = 2\bar{D} \frac{\partial\bar{c}}{\partial x_j} \bar{D} \frac{\partial\bar{c}}{\partial x_j}$, $(-D_2)_{res} = -2\bar{p}\bar{D} \frac{\partial\bar{c}}{\partial x_j} \bar{D} \frac{\partial\bar{c}}{\partial x_j}$, $\{f(D)\}_{res} = 2\bar{D} \frac{\partial\bar{c}}{\partial x_j} \frac{\partial\bar{c}}{\partial x_j} \bar{V} \bar{c} \bar{V} c \bar{e} + 2\bar{D} \frac{\partial\bar{c}}{\partial x_j} \frac{\partial\bar{c}}{\partial x_j} \bar{D} \frac{\partial\bar{c}}{\partial x_j} - \frac{\partial \bar{D} \bar{V} \bar{c} \bar{V} \bar{c} \bar{e}}{\partial x_j}$, $f_{T_4} = \exp[-0.27(\Delta/\delta_e)^{1.7}]$, $c^* = 1.0 - 0.83\text{erf}(0.5\Delta/\delta_e - 2.3)$, and $\beta_3 = 5.7\text{Le}^{-0.2}$. |

Numerical implementation

In the present study, a three-dimensional (3D) detailed H$_2$-air chemistry DNS data of a turbulent stoichiometric V-flame (Minamoto et al., 2011) has been considered. The V-flame case considers a stoichiometric premixed H$_2$-air mixture supplied at a temperature of 700 K and pressure 0.1 MPa with a mean inlet velocity 10$\text{S}_L$ (i.e., $U_{\text{inlet}} = 10\text{S}_L$). A detailed chemical kinetic mechanism involving 12 species and 27 reactions (Gutheil et al., 1993) has been used for the V-flame simulation and the temperature dependence of thermo-physical properties are considered according to the CHEMKIN database (Kee et al., 1986, 1989).

For V-flame simulation a rod of diameter $\delta_{\text{d,h}}$ is placed at a distance of 5 mm from the inlet boundary for the purpose of flame stabilization. The temperature, velocity, and species mass fraction within the rod is taken to be 2000 K, 0, and $Y_{a,b}$ (where the subscript $a, b$ refers to the fully burned gas value of the species $a$). A Gaussian function of the following form has been used to smoothly blend the values at the rod with the corresponding freestream values (Minamoto et al., 2011):
\[ Q(r; t = 0) = (Q_{\text{rod}} - Q_{\text{freestream}}) \exp \left[ -\frac{(r - r_w)^2}{2r_w^2} \right] + Q_{\text{freestream}} \]  

where \( Q \) is a general primitive variable, \( r \) is the radial co-ordinate from the center of the flame holder, and \( r_w \) is the radius of the flame holder. The fluid velocity at the inlet boundary is specified as the summation of mean inlet velocity and velocity fluctuations. The velocity fluctuations at the inlet are obtained by scanning a plane through a frozen field of incompressible turbulent velocity field. The simulation domain is taken to be a rectangle of 10 mm \( \times \) 5 mm \( \times \) 5 mm (29.7 \( \delta_{th} \) \( \times \) 14.85 \( \delta_{th} \) \( \times \) 14.85 \( \delta_{th} \)), which is discretized using a uniform Cartesian grid of \( 513 \times 257 \times 257 \). This grid ensures about 20 points within \( \delta_{th} \) and sufficient resolution of the boundary layer formed over the flame holder. It has been found that the values of \( l_c/dl \) and \( l_c'/dl \) remain about 4 and 7, where 

\[ l_c = 1/|\nabla c|_{\text{max}}, \quad l_c' = 1/|\nabla c'|, \quad \text{and} \quad dl = \sqrt{(\Delta x_1)^2 + (\Delta x_2)^2 + (\Delta x_3)^2}, \]  

with \( \Delta x_1, \Delta x_2, \) and \( \Delta x_3 \) being the grid spacing in \( x_1, x_2, \) and \( x_3 \) directions, respectively. Fourth-order finite-difference and third-order Runge–Kutta methods are used for spatial differentiation and explicit time-advancement, respectively. Turbulent inflow and non-reflecting outflow boundaries are specified in the stream-wise (i.e., \( x_1 \)-direction) directions whereas the transverse (\( x_2 \)) and span-wise (\( x_3 \)) boundaries are considered to be non-reflecting outflow and periodic, respectively. All of the non-periodic boundaries are specified using the Navier Stokes characteristics boundary conditions (NSBC) technique (Poinsot and Lele, 1992). The inlet values of normalized mean inlet velocity, normalized rms turbulent velocity fluctuation, integral length scale to thermal flame thickness ratio \( l/\delta_{th} \), turbulent Reynolds number \( Re_t = \rho_0 u' l / \mu_0 \), Damköhler number \( Da = l S_l/ u' \delta_{th} \), and Karlovitz number \( Ka = (u'/S_l)^{3/2} (l/\delta_{th})^{-1/2} \) are summarized in Table 3 along with the value of heat release parameter \( \tau = (T_{ad} - T_0) / T_0 \), where \( \rho_0 \) and \( \mu_0 \) are the unburned gas density and viscosity, respectively. The thermo-chemical parameter \( \kappa' / \tau \) is taken to be 0.78 following previous analysis (Minamoto et al., 2011). The flamelet assumption remains valid for the simulation parameters considered in this analysis (Peters, 2000). The simulation has been continued for 3 through-pass time (i.e., \( 3L_x / U_{inlet} \)), which corresponds to 8.91 chemical time scale (i.e., 8.91 \( \delta_{th} / S_l \)).

The Favre-filtered SDR \( \tilde{N}_c \) and the unclosed terms of its transport equation of \( \tilde{N}_c \) have been evaluated by explicitly filtering DNS data using a standard 3D Gaussian filter: 

\[ G(\tilde{r}) = (6 / \pi \Delta^2)^{3/2} \exp \left( -6 \tilde{r}^2 / \Delta^2 \right) \]  

(Boger et al., 1998; Charlette et al., 2002a, 2002b; Dunstan et al., 2013; Gao et al., 2014a, 2014b, 2015a, 2015b) and the filtered values of a general quantity \( Q \) is given by the following integral: 

\[ \tilde{Q}(\tilde{x}) = \int Q(\tilde{x} - \tilde{r})G(\tilde{r})d\tilde{r} \]  

For this analysis, results will be presented for \( \Delta \) ranging from \( \Delta \approx 0.5 \delta_{th} \) to \( \Delta \approx 3.0 \delta_{th} \). This range of filter widths is comparable to the range of \( \Delta \) used in several previous analyses (Boger et al., 1998; Charlette et al., 2002a, 2002b; Dunstan et al., 2013; Gao and Chakraborty, 2016; Gao

| \((u_{mean}/S_l)_{fl}\) | \((u'/S_l)_{fl}\) | \((l/\delta_{th})_{fl}\) | \(\tau\) | \((Re_t)_{fl}\) | \((Da)_{fl}\) | \((Ka)_{fl}\) |
|-----------------|-----------------|-----------------|------|-------------|-------------|-------------|
| 10.0            | 2.2             | 1.6             | 1.86 | 200         | 0.73        | 1.30        |

Table 3. List of the non-dimensional parameters at the inlet for the V flame case, which are shown with a subscript ‘fl’.
et al., 2014a, 2014b, 2015a, 2015b), and cover a range of different length scales from \( \Delta \) comparable to \( \delta_{th} \) up to \( 3.0\delta_{th} \), where \( \Delta \) is comparable to the integral length scale \( l \).

**Results and discussion**

*Flame turbulence interaction*

The distributions of reaction progress variables based on H\(_2\) and H\(_2\)O mass fractions (i.e., \( c_{H_2} \) and \( c_{H_2O} \)) at the central \( x_1 - x_2 \) mid-plane at when the statistics are extracted are shown in Figures 1a and 1b, respectively. It is evident from the reaction progress variable distributions in Figures 1a and 1b that the chemical reaction takes place in a continuous (i.e., unbroken) thin region separating unburned and burned gases, indicating flamelet regime of combustion (Peters, 2000), where the SDR closures discussed in this article are meant to be valid.

![Figure 1](image-url)

**Figure 1.** Distributions of \( c \) on \( x_1 - x_2 \) mid-plane for (a) \( c_{H_2} \) and (b) \( c_{H_2O} \) when the statistics were extracted.
**Algebraic closure of SDR $\tilde{N}_c$**

The performance of the algebraic SDR closure based on simple chemistry has been shown elsewhere (Gao et al., 2014a, 2014b; Ma et al., 2014a) and thus are not repeated here. A wrinkling factor $\Xi_D$ can be defined in the following manner in order to assess the volume-integrated behavior of the SDR closure (Dunstan et al., 2013; Gao et al., 2014a, 2014b, 2015a):

$$
\Xi_D = \frac{\langle \rho \tilde{N}_c \rangle_V}{\langle \rho D \nabla \tilde{c} \cdot \nabla \tilde{c} \rangle_V}
$$

The variation of $\Xi_D$ with $\Delta/\delta_{th}$ for SDRs for different reaction progress variable definitions based on $H_2$ and $H_2O$ mass fractions (i.e., $c_{H_2}$ and $c_{H_2O}$) is shown in Figure 2. It can be seen from Figure 2 that $\Xi_D$ increases with increasing $\Delta/\delta_{th}$, indicating that the sub-grid contribution to SDR increases with an increase in LES filter width. It can further be seen from Figure 2 that $\Xi_D$ for the SDR based on $c_{H_2}$ assumes greater values than the SDR of $c_{H_2O}$. This is consistent with previous findings (Gao et al., 2014a, 2014b, 2015a), which indicated that $\Xi_D$ assumes high values for small values of $Le$ (e.g., $Le_{H_2} = 0.3$ and $Le_{H_2O} = 1.18$). The slope $\alpha$ of the best-fit straight line, which approximates the variation of $\Xi_D$ with $\Delta/\delta_{th}$ for large filter widths (i.e., $\Delta \gg \delta_{th}$), provides an indication that $\Xi_D$ can, in principle, be expressed in terms of a power law as: $\Xi_D = (\Delta/\eta_i)^\alpha$, where $\eta_i/\delta_{th}$ is the normalized inner cut-off scale, which can be obtained from the abscissa of the intersection point of the best-fit straight line with $\Xi_D = 1.0$. It can be seen from Figure 2 that $\eta_i$ remains of the order of $\delta_{th}$ for $\Xi_D$ variations based on both $c_{H_2}$ and $c_{H_2O}$. Thus, a higher

![Figure 2](image-url)
value of $\alpha$ bears the signature of greater value of $\Xi_D$ and accordingly $\alpha$ for $\Xi_D$ based on $c_{H_2}$ is greater than that based on $c_{H_2O}$ (i.e., $\alpha = 1.39$ and 1.166 for $\Xi_D$ based on $c_{H_2}$ and $c_{H_2O}$, respectively). The increase in $\alpha$ with decreasing $Le$ is consistent with previous findings (Gao et al., 2014a, 2014b). Although the power law $(\Delta/\eta_i)^\alpha$ can be used to mimic the variation of $\Xi_D$ with $\Delta/\delta_{th}$, it cannot adequately capture the local behavior of Favre-filtered SDR $\tilde{N}_c$ due to multi-fractal nature of SDR, and interested readers are referred to Dunstan et al. (2013), Gao et al. (2014a, 2015a), and Langella et al. (2015) for further discussion on this behavior. The power law will not be discussed further in this article. From the foregoing, it is evident that an algebraic closure of SDR is ideally required to capture the correct variation of $\Xi_D$ with $\Delta/\delta_{th}$ irrespective of the definition of reaction progress variable along with capturing the local variation of $\tilde{N}_c$.

Figure 2 shows that Eq. (2) satisfactorily captures the behavior of the wrinkling factor $\Xi_D$ for both reaction progress variable definitions based on $H_2$ and $H_2O$ mass fractions. The variation of mean value of normalized Favre-filtered SDR (i.e., $\tilde{N}_c \times \delta_z/S_L$, where $\delta_z = D_0/S_L$ is the Zel’dovich flame thickness with $D_0$ being the unburned gas diffusivity for reaction progress variable) conditional on $\tilde{c}$ shown in Figure 3 for $\Delta = 0.5\delta_{th}, 1.7\delta_{th}$ and $\Delta = 3.0\delta_{th}$ for both reaction progress variable definitions based on $H_2$ and $H_2O$ mass fractions (i.e., $c_{H_2}$ and $c_{H_2O}$). It can be seen from Figure 3 that Eq. (2) satisfactorily predicts both the qualitative and quantitative behaviors of SDR across the flame brush for both choices of reaction progress variable. The observations based on Figures 2 and 3 reveal that the algebraic closure given by Eq. (2) satisfactorily predicts both volume-averaged and local behaviors of Favre-filtered SDR $\tilde{N}_c$ for a range of different filter widths for different choices of reaction progress variable in the context of detailed chemistry-based DNS data. It was shown earlier (Gao et al., 2014a, 2014b, 2015a) that the model given by Eq. (2) satisfactorily captures both the local and volume-averaged behaviors of Favre-filtered SDR $\tilde{N}_c$ in the context of simple chemistry DNS. Thus, the evidence suggests that the algebraic model given by Eq. (2) provides a robust closure for Favre-filtered SDR $\tilde{N}_c$ for both simple and detailed chemistry, and this inference was also supported by actual LES simulations (Butz et al., 2015; Ma et al., 2014a).

**Statistical behavior of the terms of the SDR transport equation**

The satisfactory performance of Eq. (2) can be justified in terms of statistical behaviors of the unclosed terms of the SDR transport equation [i.e., Eq. (5)]. The variation of the mean values of $T_1, T_2, T_3, T_4, (−D_2)$, and $f(D)$ conditional on $\tilde{c}$ is shown in Figure 4 for $\Delta \approx 0.5\delta_{th}, 1.7\delta_{th}$, and $3.0\delta_{th}$. It can be seen that the magnitude of $T_1$ remains smaller than that of the other terms in all cases for all filter widths irrespective of the choice of the definition of reaction progress variable. This tendency strengthens further with increasing $\Delta$, which is consistent with the scaling estimates presented in Table 1, because both $Da_\Delta$ and $Re_\Delta Da_\Delta = (\Delta/\delta_{th})^2$ increase with increasing $\Delta$ (Dunstan et al., 2013; Gao et al., 2014a; Ma et al., 2014a). The molecular dissipation term $−D_2$ remains the major sink term, whereas the density variation term $T_2$ acts as a source term for all cases for all filter widths irrespective of the choice of the definition of reaction progress variable. For thermo-diffusively neutral (i.e., $Le = 1.0$) globally adiabatic flames, $\rho$ can be expressed as $\rho = \rho_0/(1 + \tau \epsilon)$, which yields $T_2 = 2\rho(\partial u_i/\partial x_i)\tilde{N}_c$. As dilatation rate $(\partial u_i/\partial x_i)$ remains
predominantly positive in premixed flames, the contributions of $T_2$ remain positive for the cases with reaction progress variable Lewis number close to unity (i.e., $Le \approx 1.0$). Although the relation $T_2 = 2\rho(\partial u_i/\partial x_i)N_c$ does not strictly hold for $Le \neq 1.0$, the qualitative behavior of $T_2$ is expected to be similar to $2\rho(\partial u_i/\partial x_i)N_c$ and, thus, $T_2$ continues to behave as a source term even for the choices of $c$ for which $Le \neq 1.0$. According to the scaling analyses by Swaminathan and Bray (2005) and Gao et al. (2014b), the order of magnitude of $T_2$ is expected to be comparable to $T_3$, $T_4$, and $(-D_2)$ (see Table 1), which was previously confirmed previously using simple chemistry DNS data (Chakraborty et al.,

Figure 3. Variation of mean values of normalized SDR $\bar{N}_c \times \delta_z/S_L$ (—) conditional on $\bar{c}$ across the flame brush along with the predictions of Eq. (2) (——) for $\Delta = 0.5\delta_{th}$ (1st row), $1.7\delta_{th}$ (2nd row), and $3.0\delta_{th}$ (3rd row) for $c_{H_2}$ (1st column) and $c_{H_2O}$ (2nd column).
For both choices of reaction progress variable the magnitude of $T_2$ remains about 20% of the magnitudes of $T_4$ and $\sigma_0 D$ for all filter widths shown in Figure 4. The magnitude of $T_2$ depends on the correlations between $\nabla (\ln \rho)$, $\nabla c$, and $[\dot{\rho} + \nabla \cdot (\rho D \nabla c)]$ [see Eq. (6b)] and in the context of detailed chemistry these correlations are likely to be weaker than in the case of simple chemistry because the locations of high heat release (i.e., the locations of high $\nabla (\ln \rho)$) are not necessarily coincident with the locations of high values of $\nabla c$ for detailed chemistry cases (unlike simplified chemistry cases) when $c$ is defined based on major
reactants/products mass fractions especially in the presence of differential diffusion as in the case of H2-air flames. This along with small values of heat release parameter \( \tau \) (i.e., \( \tau = 1.86 \)) acts to reduce the magnitude of \( T_2 \) in comparison to the magnitudes of \( T_4 \) and \((-D_2)\) in the case considered here.

The mean value of the scalar-turbulence interaction term \( T_3 \) conditional on \( c \) acts as a leading order source term for both H2 and H2O based reaction progress variables (i.e., \( c_{H_2} \) and \( c_{H_2O} \)). The contribution of \( T_3 \) can be expressed as (Chakraborty and Swaminathan, 2007; Chakraborty et al., 2009; Swaminathan and Grout, 2006):

\[
T_3 = -2\rho(e_a \cos^2\alpha + e_\beta \cos^2\beta + e_\gamma \cos^2\gamma)\n
\]

where \( e_a \), \( e_\beta \), and \( e_\gamma \) are the most extensive, intermediate, and the most compressive principal strain rates; the angles between the corresponding eigenvectors with \( \nabla c \) are given by \( \alpha, \beta, \) and \( \gamma \), respectively. The scalar gradient \( \nabla c \) aligns with \( e_a \) when the strain rate induced by flame normal acceleration \( a_{chem} \) overcomes turbulent straining \( a_{turb} \), and vice versa (Chakraborty and Swaminathan, 2007; Chakraborty et al., 2009). The strain rate scales as \( a_{turb} \approx \tau f(Le) S_L/\delta_{th} \), where \( f(Le) \) is expected to decrease with increasing \( Le \) (Chakraborty et al., 2009). Scaling \( a_{turb} \) as \( a_{chem} \) \approx \tau f(Le) \) \( D_a \) and \( a_{chem} \approx \tau f(Le) \) \( D_a/Re_i^{1/2} \), respectively. Turbulent straining \( a_{turb} \) dominates over the strain rate due to flame normal acceleration \( a_{chem} \) throughout the flame brush in this V-flame case due to the small value of \( \tau \), which leads to a predominant alignment of \( \nabla c \) with \( e_\gamma \) leading to positive values of \( T_3 \) throughout the flame brush for both definitions of reaction progress variable (i.e., \( c_{H_2} \) and \( c_{H_2O} \)). It can be seen from Figure 4 that the relative magnitude of \( T_3 \) is greater in the case of H2O mass fraction based progress variable (i.e., \( c_{H_2O} \)) than in the case of H2 mass fraction based progress variable (i.e., \( c_{H_2} \)). The magnitude of conditional mean value of \( T_3 \) is comparable to that of \((-D_2)\) for H2O mass fraction based progress variable (i.e., \( c_{H_2O} \)), whereas conditional mean value of \( T_3 \) is smaller than that of \((-D_2)\) in the case of H2 mass fraction-based progress variable (i.e., \( c_{H_2} \)). As the Lewis number of H2 is smaller than H2O, the extent of alignment of \( \nabla c \) with \( e_\gamma \) is stronger for \( c_{H_2O} \) than in the case of \( c_{H_2} \). This leads to a stronger positive contribution of \( T_3 \) in the case of H2O mass fraction based progress variable (i.e., \( c_{H_2O} \)) than in the case of H2 mass fraction based progress variable (i.e., \( c_{H_2} \)).

The reaction rate contribution \( T_4 \) exhibits positive values for the major part of the flame brush before assuming negative values towards the burned gas side for small values of \( \Delta/\delta_{th} \) characterized by \( \Delta/\delta_{th} < 1 \) (e.g., \( \Delta \approx 0.5\delta_{th} \)). However, \( T_4 \) acts as a leading order source term throughout the flame brush for large filter widths characterized by \( \Delta/\delta_{th} < 1 \) (e.g., \( \Delta \approx 1.7\delta_{th} \) and \( 3.0\delta_{th} \)) irrespective of the choice of reaction progress variable. The term \( T_4 = 2\bar{D}\nabla \bar{w} \cdot \nabla c \) can alternatively be expressed as \( T_4 = -2\bar{D}(\partial \bar{w}/\partial n)|\nabla c| \), where \( n \) is the flame normal direction and \( \bar{N} = -\nabla c/|\nabla c| \) is the flame normal vector (Gao et al., 2014b). The quantity \( (\partial \bar{w}/\partial n) \) assumes negative values for the major part of the flame brush except the burned gas side where \( (\partial \bar{w}/\partial n) \) is positive. As flamelet assumption remains valid for the flames considered here (Peters, 2000), \( T_4 \) can be expressed as

\[
T_4 \approx -\int_0^\infty \int_0^1 [2\bar{D}(\partial \bar{w}/\partial n)|\nabla c|] \mathcal{L}p(c, |\nabla c|; \bar{x}; \Delta) dc dc |\nabla c|,
\]

where \( p \) is the sub-filter probability density function. The negative (positive) values of \( (\partial \bar{w}/\partial n) \) lead to positive (negative)
values of $T_4$ when the flame is partially resolved (i.e., $\Delta < \delta_{th}$, for example $\Delta \approx 0.5\delta_{th}$), which can be confirmed by Figure 4. For $\Delta > \delta_{th}$, the flame is completely unresolved and thus the sub-filter volume includes more positive samples with high magnitudes of $(-2D(\partial w/\partial n)|\nabla c|)$ than the negative samples, which are confined only in a small region within the flame front (i.e., only towards the trailing edge of the flame). This leads to predominantly positive values of $T_4$ throughout the flame brush for $\Delta > \delta_{th}$ (e.g., $\Delta \approx 1.7\delta_{th}$ and $3.0\delta_{th}$; see Figure 4).

The mean contribution of the diffusivity gradient term $f(D)$ conditional on $\tilde{c}$ assumes negative values towards the unburned gas side but exhibits positive values towards the burned gas side when the flame is partially resolved (i.e., $\Delta/\delta_{th}<1$, for example $\Delta \approx 0.5\delta_{th}$) and the reaction progress variable is defined based on $\text{H}_2\text{O}$ mass fraction. However, the mean value of $f(D)$ conditional on $\tilde{c}$ assumes positive (negative) values towards the unburned (burned) gas side of the flame brush for $\Delta \approx 0.5\delta_{th}$ when the reaction progress variable is defined based on $\text{H}_2$ mass fraction. The mass diffusivities of $\text{H}_2$ and $\text{H}_2\text{O}$ and their temperature dependences are different and thus the distributions of $f(D)$ with $\tilde{c}$ are different for different choices of the reaction progress variable. Figure 4 shows that mean value of $f(D)$ conditional on $\tilde{c}$ remains positive and its magnitude remains comparable to that of $T_2$ for $c_{\text{H}_2,\text{O}}$ in this V-flame case for large filter widths where the flame is completely unresolved (e.g., $\Delta \approx 1.7\delta_{th}$ and $3.0\delta_{th}$). However, the mean value of $f(D)$ conditional on $\tilde{c}$ remains negligible in comparison to the magnitudes of $T_2$, $T_3$, $T_4$, and $(-D_2)$ for reaction progress variable based on $\text{H}_2$ mass fraction.

It can further be seen from Figure 4 that the magnitudes of the terms $T_2$, $T_3$, $T_4$, $(-D_2)$, and $f(D)$ decrease with increasing $\Delta$. This is due to the convolution operation associated with LES filtering. The weighted averaging process associated with LES filtering includes an increasingly large number of samples with negligible magnitudes arising from the unburned and fully burned regions with increasing $\Delta$ and thus the magnitudes of $T_2$, $T_3$, $T_4$, $(-D_2)$, and $f(D)$ decrease with an increase in $\Delta$. Furthermore, the magnitudes of terms $T_2$, $T_3$, $T_4$, $(-D_2)$, and $f(D)$ remain consistent with the scaling estimates presented in Table 1.

The variations of the normalized mean values of $[T_2 + T_3 + T_4 + f(D)]$ and $(-D_2)$ are shown in Figure 5 for $\Delta \approx 0.5\delta_{th}$, $1.7\delta_{th}$, and $3.0\delta_{th}$. It is evident from Figure 5 that an approximate equilibrium is maintained between $[T_2 + T_3 + T_4 + f(D)]$ and $(-D_2)$ for $\Delta > \delta_{th}$ (e.g., $\Delta \approx 1.7\delta_{th}$ and $3.0\delta_{th}$). However, such equilibrium is not so prominent for the filter widths where the flame is partially resolved (e.g., $\Delta = 0.5\delta_{th}$). It is worth noting that the expression for $N_2$ in Eq. (2) is derived based on the assumption that an approximate equilibrium is maintained between the terms $[T_2 + T_3 + T_4 + f(D)]$ and $(-D_2)$ (Chakraborty and Swaminathan, 2011; Gao et al., 2014a, 2014b, 2015a). Figure 5 indicates that this assumption holds true for $\Delta > \delta_{th}$ (e.g., $\Delta \approx 1.7\delta_{th}$ and $3.0\delta_{th}$) and thus Eq. (2) satisfactorily predicts SDR $\tilde{N}_c$. Although the equilibrium between the terms $[T_2 + T_3 + T_4 + f(D)]$ and $(-D_2)$ is not maintained for $\Delta < \delta_{th}$, where the flame is partially resolved (e.g., $\Delta = 0.5\delta_{th}$), the resolved part $N_1$ remains the major contributor to the SDR $\tilde{N}_c$, and $(1 - f)$ in Eq. (2) attains a value close to zero when the flame is partially resolved and thus the inaccuracy incurred by evaluating the sub-grid part of SDR (i.e., $N_2 = \tilde{N}_c - N_1$) does not have any major implication on the performance of the model given by Eq. (2) for $\Delta < \delta_{th}$, which can be substantiated from Figures 2 and 3.
Transport equation-based SDR closure

It can be seen from Eq. 6a that the sub-grid flux of SDR (i.e., $\bar{pu}_iN_c - \bar{\rho}u_i\bar{N}_c$) needs to be properly modeled to close the turbulent transport term $T_1$. The sub-grid flux of SDR ($\bar{pu}_iN_c - \bar{\rho}u_i\bar{N}_c$) is often modeled using a gradient hypothesis as (Jones and Musogne, 1988):

**Figure 5.** Variations of $[T_2 + T_3 + T_4 + f(D)]$ and $(-D_2)$ conditionally averaged in bins of $\tilde{c}$ for $\Delta = 0.5\delta_{th}$ (1st row), $1.7\delta_{th}$ (2nd row), and $3.0\delta_{th}$ (3rd row) for $c_{H_2}$ (1st column) and $c_{H_2O}$ (2nd column). All of the terms are normalized with respect to the corresponding value of $\rho_0S^2_L/\delta_z^2$. 
where $D_t$ is the sub-grid scale eddy diffusivity. Several previous analyses (Chakraborty and Cant, 2009b; Chakraborty and Swaminathan, 2010; Veynante et al., 1997) indicated that turbulent flux of scalar gradients (e.g., FSD and SDR) exhibits counter-gradient (gradient) transport for the flames, where counter-gradient (gradient) transport is observed for $(\overline{\rho u_i N_c} - \overline{\rho \hat{u}_i \hat{N}_c})$. Furthermore, a previous analysis (Gao et al., 2014b) indicated that the turbulent transport term $T_1$ can be scaled as $T_1 \sim (\overline{\rho u_i N_c} - \overline{\rho \hat{u}_i \hat{N}_c})/\Delta$ and the flux $(\overline{\rho u_i N_c} - \overline{\rho \hat{u}_i \hat{N}_c})$ can be taken to scale with $(\overline{\rho u_i c} - \overline{\rho \hat{u}_i \hat{c}})\hat{N}_c$ (i.e., $(\overline{\rho u_i N_c} - \overline{\rho \hat{u}_i \hat{N}_c}) \sim (\overline{\rho u_i c} - \overline{\rho \hat{u}_i \hat{c}})\hat{N}_c$) for $\Delta \gg \delta_{th}$. Gao et al. (2015b) and Gao and Chakraborty (2016) have recently extended a RANS model proposed by Chakraborty and Swaminathan (2013) for the purpose of modeling $(\overline{\rho u_i N_c} - \overline{\rho \hat{u}_i \hat{N}_c})$ in the context of LES, which is referred to as the FLUXG model in Table 2. In the FLUXG model, $M_i = - (\partial \hat{c}/\partial x_i)/\|\nabla \hat{c}\|$ is the $i$th component of the resolved flame normal vector for LES; $\Phi' = 0.3(1 - Le) + 0.7$, $\gamma_1 = 1.8$, $\gamma_2 = 4.9 - 3.2erf(0.15\text{Re}_A)$, and $C_F = 0.11$ are the model parameters. This parameterization of $\gamma_2$ assumes an asymptotic value for large values of $\text{Re}_A$ (i.e., $\text{Re}_A \rightarrow \infty$). For non-unity Lewis number flames, the non-dimensional temperature $T^+ = (T - T_0)/(T_{ad} - T_0)$ becomes significantly different from the reaction progress variable $c$, which alters the distribution of heat release and thermal expansion within the flame brush in comparison to the $Le \approx 1.0$ flames. This behavior is mimicked here by introducing $Le$ dependence of the model parameter $\Phi'$ (Gao and Chakraborty, 2016). In the expression of FLUXG model, the first term on the right-hand side is primarily responsible for the effects of flame normal acceleration due to heat release, whereas the last term on the right-hand side of the FLUXG model represents turbulent transport according to conventional gradient hypothesis. Moreover, the first and second terms on the right-hand side of the FLUXG model satisfy the scaling estimates of $(\overline{\rho u_i N_c} - \overline{\rho \hat{u}_i \hat{N}_c})$ provided in Table 1.

The predictions of $I_{sg}^+ = (\overline{\rho u_i N_c} - \overline{\rho \hat{u}_i \hat{N}_c})M_i \times \delta_e/\rho_0 S_i^2$ according to the FLUXG model are compared to the corresponding quantity extracted from DNS data for $\Delta \approx 0.5\delta_{th}$ and $3.0\delta_{th}$ in Figure 6 for different progress variable definitions. It can be seen from Figure 6 that the FLUXG model reasonably captures both qualitative and quantitative behaviors of $I_{sg}^+$ when $Le_{H_2}$ and $Le_{H_2O}$ are used in $\Phi' = 0.3(1 - Le) + 0.7$ for $H_2$ and $H_2O$ mass fraction based reaction progress variables (i.e., $c_{H_2}$ and $c_{H_2O}$, respectively).

It is worth noting that the sub-grid flux of (i.e., $\overline{\rho u_i \hat{c}} - \overline{\rho \hat{u}_i \hat{c}}$) itself needs modeling in LES, and thus the modeling of $(\overline{\rho u_i N_c} - \overline{\rho \hat{u}_i \hat{N}_c})$ and $T_1$ depends on the closure of $(\overline{\rho u_i \hat{c}} - \overline{\rho \hat{u}_i \hat{c}})$. The modeling of $(\overline{\rho u_i \hat{c}} - \overline{\rho \hat{u}_i \hat{c}})$ is beyond the scope of current analysis and interested readers are referred to recent investigations by Gao et al. (2015c, 2015d) for further discussion on the closure of $(\overline{\rho u_i \hat{c}} - \overline{\rho \hat{u}_i \hat{c}})$.

Gao et al. (2015b) and Gao and Chakraborty (2016) recently proposed a model for $T_2$ and validated it with the help of simple chemistry DNS data, which is referred to as the T2G model in Table 2. It can be seen from Table 1 that the magnitude of $T_2$ is expected to increase with decreasing $Le$ due to the strengthening of heat release effects as a result of enhanced burning rate for small values of Lewis number and this effect is accounted for by $f_{T_2}(Le)$ in the T2G model (Gao and Chakraborty, 2016), which is consistent with the
scaling estimates presented in Table 1. The predictions of the T2G model for H₂ and H₂O mass fraction based reaction progress variables (i.e., $c_{H_2}$ and $c_{H_2O}$) are shown in Figure 7 for $\Delta \approx 0.5\delta_{th}$ and $3.0\delta_{th}$. Figure 7 shows that the T2G model reasonably captures both qualitative and quantitative behaviors of $T_2$ when $L_e_{H_2}$ and $L_e_{H_2O}$ are used in $f_{T_2}(L_e)$ (see Table 2) for H₂ and H₂O mass fraction based reaction progress variables, respectively.

The variations of the mean values of $T_3$ conditional on $\bar{c}$ are shown in Figure 8 for $\Delta \approx 0.5\delta_{th}$ and $3.0\delta_{th}$. The scaling estimates of the resolved and sub-grid part of $T_3$ have been provided in Table 1 (Gao et al., 2014b), which reveals that these scaling estimates are dependent of the Lewis number. Interested readers are referred to previous analyses (Chakraborty et al., 2009; Chakraborty and Swaminathan, 2010; Gao et al., 2014b) for further discussion on $Le$ effects on $T_3$. Gao et al. (2015b) and Gao and Chakraborty (2016) utilized the scaling estimates presented in Table 1 to propose a model for $T_3$, which is referred to as the T3G model in Table 2, where $C_3$ and $C_4$ are the model parameters and $Da_L^* = S_L\rho_0\delta_{th}/u_\alpha^*/\rho_0^*_N$ is the density-weighted local sub-grid Damköhler number. It is worth noting that the terms $C_3\bar{\rho}(u_\Delta^*/\Delta)\bar{N}_c$ and $-C_4\rho_0^*\tau(S_L^*/\delta_{th})\bar{N}_c$ in the T3G model are consistent with scaling estimates T3S1 and T3S2 presented in Table 1. The term $-C_4\rho_0^*\tau(S_L^*/\delta_{th})\bar{N}_c$ represents the alignment of $\nabla c$ with $e_\alpha$ under the action of flame normal acceleration, whereas $C_3\bar{\rho}(u_\Delta^*/\Delta)\bar{N}_c$ accounts for the alignment of $\nabla c$ with $e_\gamma$ under...
turbulent straining. The sub-grid Karlovitz number $K_a \Delta$ dependence of $C_4$ accounts for the weakening of the effects of flame normal acceleration with increasing Karlovitz number as the reacting flow field exhibits some attributes of passive scalar mixing for large values of Karlovitz number (Peters, 2000). The symbol $f_T$ in the T3G model is a bridging function in terms of $\Delta = \delta z$, which ensures that $(T_3)^{\text{res}}$ for $\Delta >> \delta_{th}$ and $T_3$ approaches to $(T_3)^{\text{res}}$ when the flow is fully resolved:

$$\lim_{\Delta \to 0} T_3 = \lim_{\Delta \to 0} \left(-2\rho D \frac{\partial c}{\partial x_i} \frac{\partial u_i}{\partial x_j} \frac{\partial c}{\partial x_j} \right) = -2\rho D \frac{\partial c}{\partial x_i} \frac{\partial u_i}{\partial x_j} \frac{\partial c}{\partial x_j}$$  \hspace{1cm} (11)$$

In the T3G model, $\Gamma(Le)$ addresses the strengthening of $\nabla c$ alignment with $c_a$ under strong actions of flame normal acceleration in the flames with small values of Lewis number, which is consistent with the scaling estimates presented in Table 1 (Gao et al., 2014a). The presence of $(1 - \bar{c})^p$ helps the T3G model to capture the qualitative behavior of across the flame brush. The predictions of the T3G model are compared to extracted from DNS data in Figure 8, which shows that the T3G model reasonably captures both qualitative and quantitative behaviors of $T_3$ when $Le_{H_2}$ and $Le_{H_2O}$ ($D_{OH_2}$ and $D_{OH_2O}$) are used in $\Gamma(Le)$ ($\delta_z$) for $H_2$ and $H_2O$ mass fraction based progress variables, respectively.
The variations of the mean values of \( \frac{1}{2} T_4^4 + f(D) \) conditional on \( \bar{c} \) are shown in Figure 9 for \( \Delta = 0.50 \delta_{th} \) and \( 3.0 \delta_{th} \). The scaling estimates of the resolved (i.e., \( (T_4)_{res} \), \(-D_2)_{res} \), and \( f(D) \) \( \{res \) components of \( T_4 \), \(-D_2) \), and \( f(D) \) are provided in Table 1 according to Gao et al. (2014b), Gao et al. (2015b), and Gao and Chakraborty (2016) utilized \( T_4 + f(D) - D_2 \) together for unity Lewis number flames by extending an existing RANS model (Chakraborty et al., 2008a; 2009; Chakraborty and Swaminathan, 2010, 2013; Mantel and Borghi, 1994), which is referred to as the T4D2FG model in Table 2. The involvement of \( (\bar{c} - c')/[\bar{c}(1 - \bar{c})] \) in the T4D2FG model is required for capturing the qualitative behavior of \( T_4 - D_2 + f(D) \) across the flame brush, whereas \( f_{TD} \) approaches unity for small values of \( \Delta \) as the terms get fully resolved (i.e., \( \lim_{\Delta \to 0} [T_4 - D_2 + f(D)] = \lim_{\Delta \to 0} [(T_4)_{res} - (D_2)_{res} + f(D)]_{res} \)). The change in sign of \( T_4 + f(D) - D_2 \) with increasing \( \bar{c} \) has been accounted for by \( c' \). Table 1 suggests that the magnitude of \( T_4 - D_2 + f(D) \) is expected to increase with a decrease in Lewis number \( Le \). The increased magnitude of \( T_4 + f(D) - D_2 \) for small values of \( Le \) is addressed by \( Le \) dependence of the model parameter \( \beta_3 \) (i.e., \( \beta_3 = 5.7Le^{-0.2} \)). The prediction of the T4D2FG model is shown in Figure 9, which demonstrates that the T4D2FG model

**Figure 8.** Variations of \( T_3 \) conditionally averaged in bins of \( \bar{c} \) along with the prediction of the T3G model for \( \Delta = 0.50 \delta_{th} \) (1st row) and \( 3.0 \delta_{th} \) (2nd row) for \( c_{H_2} \) (1st column) and \( c_{H_2O} \) (2nd column). All of the terms are normalized with respect to the corresponding value of \( \rho_0 S_L^2 / \delta_{th}^2 \).
reasonably captures both qualitative and quantitative behaviors of \( T_4 + f(D) - D_2 \) when \( Le_{H_2} \) and \( Le_{H_2O} \) (\( D_{0H_2} \) and \( D_{0H_2O} \)) are used in \( \beta_3 = 5.7Le^{-0.2} (\delta_z) \) for \( H_2 \) and \( H_2O \) mass fraction based progress variables, respectively.

**Conclusions**

The algebraic and transport equation based closures of Favre-filtered SDR \( \tilde{N}_c \) in the context of LES, which were previously proposed based on simple chemistry DNS data, have been assessed in the current analysis based on a detailed chemistry DNS dataset of a turbulent stoichiometric \( H_2 \)-air V flame. The SDR statistics and closure in the context of detailed chemistry DNS data have been assessed for different choices of reaction progress variable. It has been found that Lewis number \( Le \) of reaction progress variable \( c \) and the choices of \( c \) itself have noticeable influences on the statistical behavior of the unclosed terms of \( \tilde{N}_c \) transport. A recently proposed algebraic closure for \( \tilde{N}_c \), which was previously validated for simple chemistry DNS data for different values of \( Le \), has been found to yield satisfactory prediction also for detailed chemistry DNS data for different choices of reaction progress variable \( c \). The models for the unclosed terms of the SDR transport equation, which were previously proposed based on simple chemistry DNS data, have also been found to satisfactorily predict the unclosed terms obtained from explicitly filtered
DNS data for a range of $\Delta$ for different choices of reaction progress variable in the context of detailed chemistry DNS data. Although the proposed algebraic and transport equation-based closures have been demonstrated to provide satisfactory performance based on the assessment with respect to explicitly filtered DNS data, it is still essential to implement these models in actual LES simulations because the input parameters (e.g., sub-grid turbulent velocity fluctuation $u'_0$) to the combustion models often themselves need closures. Thus, the sensitivity of the combustion model predictions on the modeling inaccuracy of input parameters cannot be assessed based solely on model validation with respect to DNS data. This needs implementation of the models, which have been identified based on the validation using DNS data, in actual LES simulations for the purpose of a-posteriori assessment. However, a-posteriori assessment of the models discussed in this article is beyond the scope of this analysis but it is worth mentioning that numerical inaccuracies interact with modeling errors in a complex manner in actual LES simulations so a-posteriori analyses do not assess the models in isolation and are specific to the numerical schemes used in the computer code employed for LES simulations. Ma et al. (2014a), Butz et al. (2015), and Langella et al. (2015) implemented the algebraic SDR closure discussed in this article for LES simulations of premixed turbulent combustion in rectangular dumped-combustor and bluff body stabilized flames (i.e., ORACLE and VOLVO rigs), turbulent swirl flame (i.e., TECFLAM), and Bunsen-burner configurations and reported satisfactory agreement with experimental data based on a-posteriori assessment. However, this algebraic SDR closure and the closures of the unclosed terms of the SDR transport equation need to be validated further based on actual LES simulations. Further validation of these models will form the basis of future investigations.

**Acknowledgments**

N.C. is grateful to Mr. Jiawei Lai of Newcastle University for his help while preparing this manuscript.

**Funding**

The financial assistance of the Engineering and Physical Science (EPSRC) research council of the UK (EP/I028013/1 and EP/K025163/1) and computational support of ARCHER and N8 are gratefully acknowledged. Sandia is a multi-program laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under Contract DE-AC04-94AL85000.

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