Algebraic closure of Scalar Dissipation Rate for Large Eddy Simulations of turbulent premixed combustion

Y. Gao[1], N. Chakraborty[1], N. Swaminathan[2]
[1]School of Mechanical and Systems Engineering, Newcastle University
Newcastle-Upon-Tyne, Tyne and Wear, NE1 7RU, United Kingdom

[2]Cambirdge University Engineering Department, University of Cambridge
Trumpington Street, Cambridge, Cambridgeshire, CB2 1PZ, United Kingdom

1 Introduction

The Scalar Dissipation Rate (SDR) based reaction rate closure in turbulent premixed flames has rarely been addressed in the context of Large Eddy Simulations (LES) [1]. In the context of RANS the mean reaction rate $\{\dot{w}\}$ of the reaction progress variable c can be expressed in terms of Favre-averaged SDR (i.e. $\hat{N}_c = \{\rho D \nabla c . \nabla c\}/\{\rho\}$) as: $\{\dot{w}\} = 2\{\rho\}\hat{N}_c/(2c_m - 1)$ [2,3] where ρ, D, $N_c = D\nabla c . \nabla c$ and $\dot{w}$ are the gas density, progress variable diffusivity, instantaneous SDR and reaction rate of c respectively, with $\{Q\}$ and $\hat{Q} = \{\rho Q\}/\{\rho\}$ indicating the Reynolds-averaged and Favre-averaged values of a general quantity Q respectively. The quantity c_m is given by: $c_m = \int_0^1 [\dot{w} c f(c)]_L dc / \int_0^1 [\dot{w} f(c)]_L dc$ where $f(c)$ is the burning rate probability density function (pdf) and the subscript 'L' refers to the values in unstrained planar laminar premixed flames. The analysis by Dunstan *et al.* [1] demonstrated that $\{\dot{w}\} = 2\{\rho\}\hat{N}_c/(2c_m - 1)$ remains valid for large values of the filter size Δ in the context of LES when $\{\dot{w}\}$, $\{\rho\}$ and $\hat{N}_c$ are replaced by $\overline{\dot{w}}$, $\overline{\rho}$ and $\widetilde{N}_c = \overline{\rho D \nabla c . \nabla c}/\overline{\rho}$ respectively, where the overbar suggests an LES filtering operation and the Favre-filtered value of a general quantity Q is denoted by $\widetilde{Q} = \overline{\rho Q}/\overline{\rho}$. The analysis by Dunstan *et al.* [1] has been carried out only for a V-flame DNS with single-step Arrhenius type chemistry and unity Lewis number. Current analysis extends the *a-priori* DNS analysis of Dunstan *et al.* [1] by addressing the SDR based reaction rate closure and the algebraic modelling of $\widetilde{N}_c$ for turbulent premixed flames with different values of heat release parameter τ, global Lewis number Le and turbulent Reynolds number Re_t. In this respect, the objectives of this current analysis are: (i) to extend the SDR based $\overline{\dot{w}}$ closure for a range of different values of τ, Le and Re_t and (ii) to identify an algebraic closure of $\widetilde{N}_c$ which remains valid for a range of different values of τ, Le and Re_t.These objectives have been addressed here by *a-priori* analysis based on a simple chemistry DNS database of statistically planar turbulent premixed flames with a range different values of τ, Le and Re_t..

2 Mathematical Background and Numerical Implementation

A wrinkling factor based on SDR can be defined as [1]: $\Xi_D = \bar{\rho}\widetilde{N}_c \big/ \bar{\rho}\widetilde{D}\nabla\widetilde{c}.\nabla\widetilde{c}$. Dunstan *et al.* [1] explored the possibility of modelling Ξ_D using a power-law in the following manner: $\Xi_D = (\eta_O / \eta_{iD})^{\alpha}$ where η_{iD} is the inner cut-off scale for Ξ_D, whereas the outer cut-off scale η_O for LES can be taken to be the LES filter width Δ. If $\overline{\dot{w}}$ can be considered to be directly proportional to $\bar{\rho}\widetilde{N}_c$, the volume-averaged value of $\overline{\rho N_c}$ should remain independent of Δ, which leads to $\langle \overline{\rho N_c} \rangle = \langle \bar{\rho}\widetilde{N}_c \rangle$ where $\langle \ldots \rangle$ indicates a volume averaging operation. Thus, it is possible to write:

$$\log \Xi_D^V = \log(\langle \bar{\rho}\widetilde{N}_c \rangle / \langle \bar{\rho}\widetilde{D}\nabla\widetilde{c}.\nabla\widetilde{c} \rangle) = \alpha \log \Delta - \alpha \log \eta_{iD} \tag{1}$$

where the superscript V indicates the wrinkling factor based on the volume-averaged quantities: (i.e. $\Xi_D^V = \langle \bar{\rho}\widetilde{N}_c \rangle \big/ \langle \bar{\rho}\widetilde{D}\nabla\widetilde{c}.\nabla\widetilde{c} \rangle$). Dunstan *et al.* [1] also explored the possibility of extending an algebraic model for SDR proposed by Kolla *et al.* [4] in the context of RANS. However, the model by Kolla *et al.* [4] was proposed for unity Lewis number flames, which was extended for $Le \neq 1.0$ combustion by Chakraborty and Swaminathan [5]. The algebraic RANS model proposed by Chakraborty and Swaminathan [5] for the unresolved part of SDR has been extended here for the purpose of LES in the following manner:

$$\widetilde{N}_c = \widetilde{D}\nabla\widetilde{c}.\nabla\widetilde{c} + (1-f)\left[2K_c^* S_L \big/ (Le^{1.88}\, \delta_{th}) + (C_3^* - \tau.Da_\Delta C_4^*)(2u'_\Delta/3\Delta)\right]\widetilde{c}.(1-\widetilde{c})/\beta_c \tag{2}$$

where S_L is the unstrained laminar burning velocity, $\delta_{th} = (T_{ad} - T_0)/Max|\nabla T|_L$ is the thermal flame thickness, $f = \exp[-\theta(\Delta/\delta_{th})^p]$ is a bridging function, C_3^*, C_4^* and β_c are the model parameters, $u'_\Delta = \sqrt{(\overline{\rho u_i u_i}/\bar{\rho} - \widetilde{u}_i\widetilde{u}_i)/3}$ is the sub-grid turbulent velocity fluctuation and $\tau = (T_{ad} - T_0)/T_0$ is the heat release parameter with T, T_0 and T_{ad} being the instantaneous gas, unburned gas and adiabatic flame temperatures respectively. In Eq. 2 K_c^* is given by: $K_c^* = (\delta_{th}/S_L)\int_0^1 [N_c \nabla.\vec{u} f(c)]_L\, dc \big/ \int_0^1 [N_c f(c)]_L\, dc$ [4] and C_3^* and C_4^* are expressed as: $C_3^* = 2.0\sqrt{Ka_\Delta}\big/(1.0 + \sqrt{Ka_\Delta})$; $C_4^* = 1.2(1.0 - \widetilde{c})^{\Phi}\big/\left[Le^{2.57}(1 + Ka_\Delta)^{0.4}\right]$ where $\Phi = 0.2 + 1.5|1.0 - Le|$ with $Da_\Delta = \Delta S_L / u'_\Delta \delta_{th}$ and $Ka_\Delta = (u'_\Delta / S_L)^{3/2}(\Delta/\delta_{th})^{-1/2}$ being the sub-grid Damköhler and Karlovitz numbers respectively. It is worth noting the first term on the right hand side of Eq. 2 was absent in the RANS model by Chakraborty and Swaminathan [5] and the second term featured in Ref. [5] without $(1-f)$. The bridging function $(1-f)$ ensures that $\widetilde{N}_c$ approaches to $N_c = D\nabla c.\nabla c$ for small values of filter size (i.e. $\lim_{\Delta\to 0}\widetilde{N}_c = N_c = D\nabla c.\nabla c$ where $f \approx 1.0$), whereas Eq. 2 approaches to the RANS model expression proposed by Chakraborty and Swaminathan [5] for $\Delta >> \delta_{th}$ where $f \approx 0.0$. The terms $2K_c^*(S_L/\delta_{th})$ and $(C_3^* - \tau.Da_\Delta C_4^*)(2u'_\Delta/3\Delta)$ in Eq. 2 arise due to dilatation and strain rate contributions to the SDR transport, whereas $\widetilde{c}(1-\widetilde{c})/\beta_c$ originates due to the combined reaction and molecular dissipation contributions [5]. The performances of the models given by Eqs.1 and 2 have been assessed here based on *a-priori* analysis of DNS data of statistically planar turbulent premixed flames. The initial values for the root-mean-square (rms) turbulent velocity fluctuation normalised by unstrained laminar burning velocity u'/S_L and the integral length scale to flame thickness ratio l/δ_{th} are presented in Table 1 along with the initial values of Damköhler number $Da = l.S_L / u'\delta_{th}$, Karlovitz number $Ka = (u'/S_L)^{3/2}(l/\delta_{th})^{-1/2}$, turbulent Reynolds number $\mathrm{Re}_t = \rho_0 u'l/\mu_0$, heat release parameter $\tau = (T_{ad} - T_0)/T_0$ and Le, where ρ_0 and μ_0 are the unburned gas density and viscosity respectively. Standard values are taken for Prandtl number Pr, ratio of specific heats $\gamma = C_P / C_V$ and the Zel'dovich number β (i.e. $\mathrm{Pr} = 0.7$, $\gamma = 1.4$, $\beta = 6.0$).

Table 1. Simulation parameters corresponding to the DNS database.

Case	Domain size / δ_{th}^3	Grid size	u'/S_L	l/δ_{th}	τ	Re_t	Da	Ka
A	24.1×24.1 ×24.1	230×230×230	7.5	2.45	3.0	47.0	0.33	13.2
B-F	24.1×24.1 ×24.1	230×230×230	7.5	2.45	4.5	47.0	0.33	13.2
G	36.6×24.1 ×24.1	345×230×230	5.0	1.44	4.5	22.0	0.33	8.67
H	36.6×24.1 ×24.1	345×230×230	6.25	1.67	4.5	23.5	0.23	13.0
I	36.6×24.1 ×24.1	345×230×230	7.5	2.50	4.5	48.0	0.33	13.0
J	36.6×24.1×24.1	345×230×230	9.0	4.31	4.5	100	0.48	13.0
K	36.6×24.1×24.1	345×230×230	11.25	3.75	4.5	110	0.33	19.5

It can be seen from Table 1 Re_t values are comparable for cases A-F and I. The values of heat release parameters are different for cases A and B-K , whereas Le = 0.34, 0.6, 0.8 and 1.2 for cases B, C, D and F respectively and in other cases Le is taken to be unity. In cases G-K the variation of Re_t is brought about by changing either Da or Ka independently of the other. More details on this database can be obtained from Refs. [5,6] The DNS data is explicitly filtered using a Gaussian filter using the following convolution operation: $\overline{Q(\vec{x})} = \int Q(\vec{x} - \vec{r})G(\vec{r})d\vec{r}$ for the purpose of *a-priori* analysis.

3 Results and Discussion

The variations of the mean values of $\overline{\dot{w}} \times \delta_{th} / \rho_0 S_L$ and $2\overline{\rho}\widetilde{N}_c /(2c_m - 1) \times \delta_{th} / \rho_0 S_L$ conditional on $\widetilde{c}$ values for $\Delta \approx 0.8\delta_{th}$ and $\Delta \approx 2.8\delta_{th}$ for cases A-G, I and K are shown in Fig. 1, which shows that $2\overline{\rho}\widetilde{N}_c /(2c_m - 1) \times \delta_{th} / \rho_0 S_L$ does not capture $\overline{\dot{w}} \times \delta_{th} / \rho_0 S_L$ for $\Delta < \delta_{th}$ but $2\overline{\rho}\widetilde{N}_c /(2c_m - 1) \times \delta_{th} / \rho_0 S_L$ captures $\overline{\dot{w}} \times \delta_{th} / \rho_0 S_L$ for $\Delta > \delta_{th}$. Figure 1 shows that the agreement between $\overline{\dot{w}} \times \delta_{th} / \rho_0 S_L$ and $2\overline{\rho}\widetilde{N}_c /(2c_m - 1) \times \delta_{th} / \rho_0 S_L$ improves with increasing Δ. The cases H and J are qualitatively similar to cases I and K respectively and thus are not shown in Fig. 1 and in subsequent figures. The expression $\{\dot{w}\} = 2\{\rho\}\hat{N}_c /(2c_m - 1)$ was originally proposed for $Da >> 1$ where the pdf of c can be approximated as a bi-modal distribution [2]. The variation of Da_Δ conditional on $\widetilde{c}$ values for $\Delta \approx 0.8\delta_{th}$ and $\Delta \approx 2.8\delta_{th}$ are shown in Fig. 2 for cases A-G, I and K. The pdfs of c within the filter volume at $\widetilde{c} = 0.5$ for $\Delta \approx 0.8\delta_{th}$ and $\Delta \approx 2.8\delta_{th}$ are shown in Figs. 2c and d. Figures 1 and 2 demonstrate that the agreement between $\overline{\dot{w}} \times \delta_{th} / \rho_0 S_L$ and

$2\bar{\rho}\tilde{N}_c/(2c_m-1)\times\delta_{th}/\rho_0 S_L$ improves with increasing Da_Δ when there is a significant probability of finding $c \neq \tilde{c}$ within the filter volume.

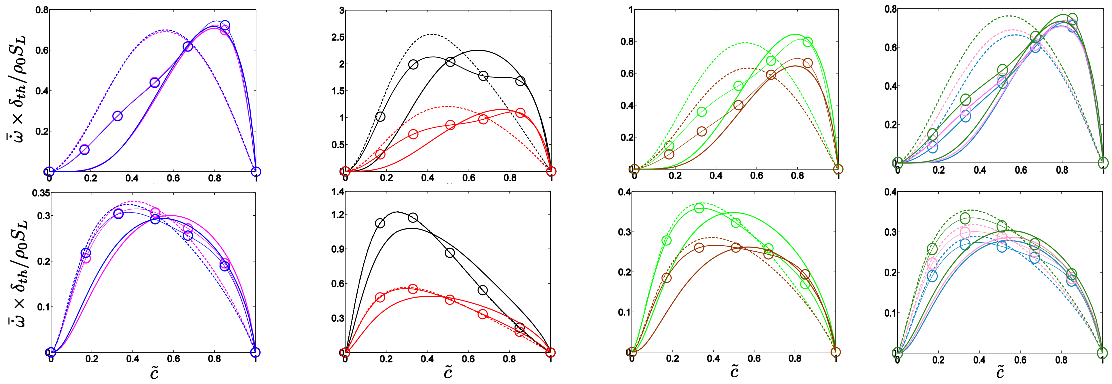

Figure 1: Variation of mean values of $\bar{\dot{w}}\times\delta_{th}/\rho_0 S_L$ (———), $2\bar{\rho}\tilde{N}_c/(2c_m-1)\times\delta_{th}/\rho_0 S_L$ (--------) and the prediction of Eq. 3 (—○—) conditional on $\tilde{c}$ across the flame brush at $\Delta\approx 0.8\delta_{th}$ (1st row) and $\Delta\approx 2.8\delta_{th}$ (2nd row) for case A (——) and E (——) (1st column), case B (——) and C (——) (2nd column), cases D (——) and F (——) (3rd column) and cases G (——), I (——) and K (——) (4th column).

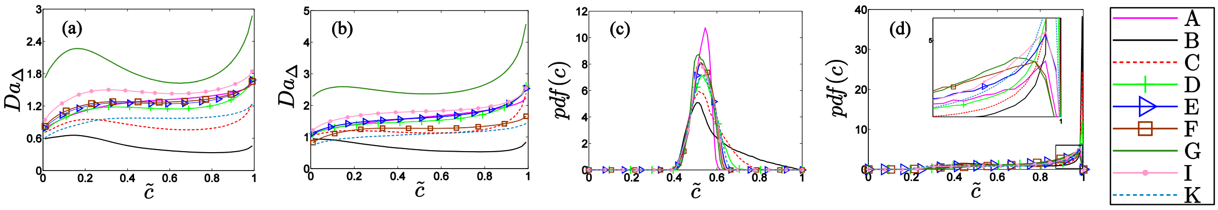

Figure 2: Variation of Da_Δ conditionally averaged in bins of $\tilde{c}$ for cases A-G, I and K for (a) $\Delta\approx 0.8\delta_{th}$ and (b) $\Delta\approx 2.8\delta_{th}$. Pdfs of c within the filter volume for (c) $\Delta\approx 0.8\delta_{th}$ and (d) $\Delta\approx 2.8\delta_{th}$ for cases A-G, I and K.

In order to improve the prediction of $\bar{\dot{w}}$ for $\Delta<\delta_{th}$ and to satisfy the limiting condition given by: $\lim_{\Delta\to 0}\bar{\dot{w}}=\dot{w}$, an alternative expression for $\bar{\dot{w}}$ in the context of LES is proposed here:

$$\bar{\dot{w}} = f_1(\bar{\rho},\tilde{c},\tilde{T})\exp(-\phi\Delta/\delta_{th}) + [1-\exp(-\phi\Delta/\delta_{th})]\{2\bar{\rho}\tilde{N}_c/(2c_m-1)\} \quad (3)$$

where f_1 is such a function, which ensures that $\dot{w}=f_1(\rho,c,T)$ and the model parameter ϕ is given by $\phi=0.56\delta_L S_L/\alpha_{T0}$ where, $\delta_L=1/\max|\nabla c|_L$ and α_{T0} is the thermal diffusivity in unburned gas. Equation 3 ensures that the right hand side becomes $\dot{w}$ when $\Delta\to 0$ (i.e. $\Delta<<\delta_{th}$) and $\bar{\dot{w}}=2\bar{\rho}\tilde{N}_c/(2c_m-1)$ is obtained for $\Delta>>\delta_{th}$. Moreover, Δ/δ_{th} can be taken to scale as: $\Delta/\delta_{th}\sim(u'_\Delta/S_L)Da_\Delta$, which suggests that Eq. 3 tends to $\bar{\dot{w}}=2\bar{\rho}\tilde{N}_c/(2c_m-1)$ for high values of Da_Δ for a given value of u'_Δ/S_L. Figure 1 shows that Eq. 3 satisfactorily predict $\bar{\dot{w}}$ for all cases considered here for both $\Delta<\delta_{th}$ and $\Delta>\delta_{th}$. The satisfactory performance of Eq. 3 indicates that $\bar{\dot{w}}$ can be satisfactorily closed if $\tilde{N}_c$ is adequately modelled. The variations of Ξ_D^V with Δ/δ_{th} for cases A-G, I and K are shown in Fig. 3 on a log-log plot. It is evident from Fig. 3 that a power-law between Ξ_D^V with Δ/δ_{th} (see Eq. 1) can be obtained for $\Delta>\delta_{th}$. The slope of the best fit straight line with the steepest slope provides the value of α and the intersection of this line with the $\Xi_D^V=1.0$ gives the measure of η_{iD}/δ_{th}. Figure 3 demonstrates that α increases with decreasing (increasing) Le (u'/S_L) whereas η_{iD} remains of the order of δ_{th} for all cases considered here. The increase in the extent of flame wrinkling with decreasing (increasing) Le (u'/S_L) is reflected in the increase in α with decreasing (increasing) Le (u'/S_L). The variation of Ξ_D^V with Δ/δ_{th} can be mimicked using the following expression [1]: $\Xi_D^V = \exp(-\theta_1\Delta/\delta_{th}) + [1-\exp(-\theta_2\Delta/\delta_{th})](\Delta/\eta_{iD})^{\alpha}$ where θ_1 and θ_2 are model parameters. This leads to a possible model for $\widetilde{N}_c$:

$$\widetilde{N}_c = \widetilde{D}\nabla\widetilde{c}.\nabla\widetilde{c}\left[\exp(-\theta_1\Delta/\delta_{th}) + [1-\exp(-\theta_2\Delta/\delta_{th})](\Delta/\eta_{iD})^{\alpha}\right] \tag{4}$$

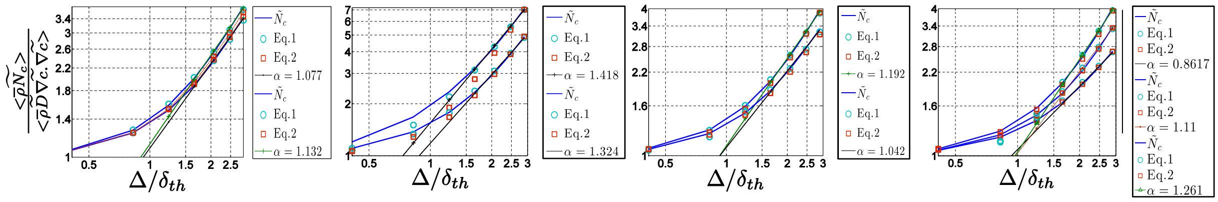

Figure 3: Variations of Ξ_D^V with Δ/δ_{th} on a log-log plot along with the predictions of Eqs. 1 and 2 for case A and E (1st column), case B and C (2nd column), cases D and F (blue) (3rd column) and cases G, I and K (4th column).

According to Eq. 4, $\widetilde{N}_c$ approaches to $D\nabla c.\nabla c$ when the flow is fully resolved (i.e. for $\Delta \to 0$), where $\lim_{\Delta\to 0}\overline{\rho}\widetilde{N}_c = \rho D\nabla c.\nabla c$, and for $\Delta >> \delta_{th}$, Eq. 4 approachs to the power-law $\Xi_D = (\Delta/\eta_{iD})^{\alpha}$ provided suitable values of θ_1 and θ_2 are chosen. The variation of Ξ_D^V with Δ/δ_{th} for optimum values of θ_1 and θ_2 are shown in Fig. 3 for the values of η_{iD} and α extracted from DNS data. The mean values of the predictions of Eq. 4 conditional on $\widetilde{c}$ for optimum values of θ_1 and θ_2, and α and η_{iD} extracted from DNS database are compared with the corresponding $\widetilde{N}_c$ variation extracted from DNS data in Fig. 4 for $\Delta \approx 0.8\delta_{th}$ and $\Delta \approx 2.8\delta_{th}$ for cases A-G, I and K. A comparison between Figs. 3 and 4 suggests that although Eq. 4 satisfactorily captures the variation of Ξ_D^V with Δ/δ_{th}, it does not adequately capture local behaviour of $\widetilde{N}_c$ for large filter widths Δ (i.e. $\Delta > \delta_{th}$). For $\Delta < \delta_{th}$ the first term on the right side of Eq. 4 remains a major contributor and thus Eq. 4 is more successful in capturing the local behaviour of $\widetilde{N}_c$ for $\Delta < \delta_{th}$ than in $\Delta > \delta_{th}$ (see Fig. 4). This suggests that power-law based models with a single global value of α may not be suitable for the LES modelling of $\widetilde{N}_c$, which is consistent with previous findings. [1]. It has been found that Eq. 2 captures the variation of Ξ_D^V with Δ/δ_{th} for $f = \exp[-0.7(\Delta/\delta_{th})^{1.7}]$ provided an optimum value of β_c is used. The optimum value of β_c has been found to increase with increasing τ (i.e. β_c =3.45 to 4.35 from τ =3.0 to 4.5), which is consistent with β_c =2.76 for the model expression given by eq. 2 for the flame with $\tau = 2.52$, analysed in Ref. [1]. By contrast, β_c decreases with increasing Re_t before assuming asymptotic values for $\mathrm{Re}_t \geq 50$, whereas Le does not have any major influence on β_c. The observed τ and Re_t dependences of β_c has been parameterised here as:

$$\beta_c = \left[9.2 - 2.5/\{1+\exp[-10(A-4)]\}\right]\left[\tau/(1+\tau)\right]^{7/3}(\rho_0 D_0/\rho_b D_b)^{0.15}; \text{ where } A = [\mathrm{Re}_{t\Delta}^{0.83} + 0.1]/[(\Delta/\delta_{th})^{1.73} + 0.1] \tag{5}$$

where $\mathrm{Re}_{t\Delta} = 4.0\rho_0 u'_{\Delta}\Delta/\mu_0$ can be taken as the sub-grid turbulent Reynolds number, and ρ_0 and ρ_b (D_0 and D_b) are the unburned and burned gas densities (diffusivities) respectively. The sub-grid turbulent Reynolds number dependence of β_c is consistent with a recent finding in the context of RANS [6]. The predictions of Eq. 2 with the parameterisation given by Eq. 5 are shown in Fig. 4. Figures 3 and 4 show that the model given by Eq. 2 satisfactorily predicts both the global and local behaviours of $\widetilde{N}_c$ for flames with a range of different values of τ, Le and Re_t.

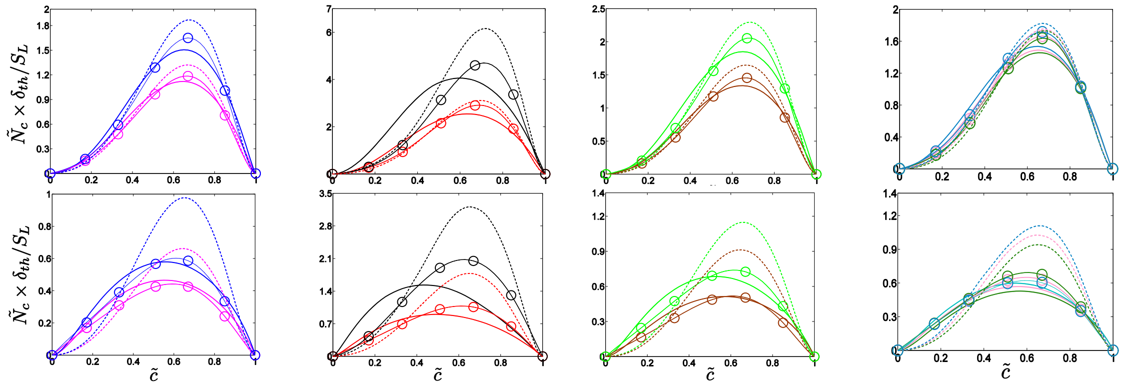

Figure 4: Variation of mean values of $\widetilde{N}_c \times \delta_{th} / S_L$ (———) conditional on $\widetilde{c}$ across the flame brush along with the predictions of Eq. 2 (—○—) and Eq. 4 (--------) at $\Delta \approx 0.8\delta_{th}$ (1st row) and $\Delta \approx 2.8\delta_{th}$ (2nd row) for case A (——) and E (——) (1st column), case B (——) and C (——) (2nd column), cases D (——) and F (——) (3rd column) and cases G (——), I (——) and K (——) (4th column).

4 Conclusions

The SDR based reaction rate closure for turbulent premixed flames has been analysed here by explicitly LES filtering a DNS database of statistically planar turbulent premixed flames with a range of different values of τ, Le and Re_t. Existing algebraic models for $\overline{\dot{w}}$ and $\widetilde{N}_c$ in the context of RANS have been extended here for LES based on *a-priori* analysis of DNS data, so that they can be used for a range of different values of Lewis number, heat release parameter and turbulent Reynolds number. However, the proposed models need to be implemented in actual LES simulations in a configuration for which experimental data is available for the purpose of *a-posteriori* assessment.

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