Statistical analysis and modelling of turbulent fuel mass fraction flux in turbulent stratified flames using Direct Numerical Simulations

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1 Introduction

Stratified mixture combustion [1] has applications ranging from Gasoline Direct Injection (GDI) engines to Lean Premixed Prevaporised (LPP) gas turbines. Often in industrial engineering applications, combustion takes place in a turbulent environment. The modelling of turbulent flows still remains a challenging task, however, the difficulty of analyzing reacting flow systems is augmented by chemical heat release which has significant influences on the turbulent transport of heat, mass and momentum. Computational studies of turbulent reacting flows using the Reynolds Averaged Navier Stokes (RANS) approach requires the modelling of the turbulent scalar flux which originates due to interaction between the turbulent velocity and scalar fluctuations [2,3]. For a passive scalar the turbulent scalar flux is often modeled according to the gradient hypothesis in the following manner [2]:

$$\overline{\rho u_i'' Y''} = -(\mu_t / \sigma)\partial \widetilde{Y} / \partial x_1 \qquad (1)$$

where ρ is the density, u_i is the velocity component in the i^{th} direction, Y is the mass fraction of the scalar in question, σ is the turbulent Schmidt number and $\mu_t = 0.09\overline{\rho}\widetilde{k}^2 / \widetilde{\varepsilon}$ is the eddy viscosity, $\widetilde{k} = u_i'' u_i'' / 2$ is the turbulent kinetic energy and $\widetilde{\varepsilon} = \overline{\mu \partial u_i'' / \partial x_j \cdot \partial u_i'' / \partial x_j} / \overline{\rho}$ is its dissipation rate. In Eq. 1, the notations $\overline{q}$, $\widetilde{q} = \overline{\rho q} / \overline{\rho}$ and $q'' = q - \widetilde{q}$ indicate the Reynolds averaged, Favre averaged and Favre fluctuation of a general quantity q . The gradient hypothesis model given by Eq. 1 often performs satisfactorily in flows involving the transport of a passive scalar. However, in the context of turbulent reacting flows, the turbulent scalar flux of active scalars may exhibit counter-gradient transport under some conditions, which the model given by Eq. 1 cannot account for. Bray *et al*. [4] presented the theoretical explanation of the counter-gradient transport for turbulent premixed flames. Counter-gradient transport in turbulent premixed flames has been observed in both Direct Numerical Simulation (DNS) (e.g. Ref. [5,6]) and experimental (Ref. [7]) studies. In the context of turbulent stratified flame modelling, both active and passive scalar transports need to be accounted for [8-10] and often the fuel mass fraction Y_F is considered to be as the characteristic active scalar [8-10]. The quantity $\overline{\rho u_i'' Y_F''}$ appears explicitly in the transport equation of $\widetilde{Y}_F$:

$$\frac{\partial(\overline{\rho}\widetilde{Y}_F)}{\partial t} + \frac{\partial(\overline{\rho}\widetilde{u}_j\widetilde{Y}_F)}{\partial x_j} = \overline{\frac{\partial}{\partial x_j}\left(\rho D \frac{\partial Y_F}{\partial x_j}\right)} - \frac{\partial(\overline{\rho u_j'' Y_F''})}{\partial x_j} + \dot{\omega}_F \qquad (2)$$

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where D is the diffusivity of fuel and $\dot{\omega}_F$ is the reaction rate of fuel. It is evident from Eq. 2 that one needs to model $\overline{\rho u_i'' Y_F''}$ in order to solve the transport equation of $\tilde{Y}_F$. For statistically planar flames, $\overline{\rho u_1'' Y_F''}$ is the only non-zero component of the turbulent flux of fuel mass fraction. Therefore, the objectives of the current study are:

(i) To study and understand the behaviour of the turbulent flux of fuel mass fraction (i.e. $\overline{\rho u_1'' Y_F''}$) in turbulent stratified flames.

(ii) To identify, a model for $\overline{\rho u_1'' Y_F''}$ through *a-priori* analysis which satisfactorily captures the behaviour of the corresponding quantity obtained from the DNS data.

2 Mathematical background and numerical implementation

In the present study, the reactant inhomogeneity is characterised by a random bi-modal distribution of equivalence ratio ϕ in the unburned reactants as previously done by Eswaran and Pope [11]. The reactant inhomogeneity is introduced ahead of an initially planar laminar premixed flame. Following this, a homogeneous isotropic turbulent velocity field is superimposed on the species distribution and the flame is allowed to interact with background turbulence and upstream reactant inhomogeneity. The turbulent fluctuating velocity field is initialised using a pseudo-spectral method [12] following the Batchelor-Townsend energy spectrum. The chemistry is accounted for by a single-step Arrhenius type reaction in which the activation energy and heat of reaction are taken to be functions of equivalence ratio following Tarrazo *et al.* [13] in order to mimic the unstrained laminar burning velocity $S_{b(\phi)}$ variation with equivalence ratio ϕ in typical hydro-carbon flames. Partially non-reflecting boundary conditions are used in the direction of the mean flame propagation according to the Navier Stokes Characteristic Boundary Conditions (NSCBC) [14] and the transverse boundaries are taken to be periodic. The spatial discretisation and time advancement have been carried out using a higher order central difference scheme and a 3rd order Runge-Kutta method, respectively [15]. The initial values of root-mean-square (rms) turbulent velocity fluctuation normalised by unstrained laminar burning velocity for the stoichiometric mixture $u'/S_{b(\phi=1)}$, integral length scale of turbulence to flame thickness ratio $lS_{b(\phi=1)}/D_0$, the ratio of the integral length scale of species inhomogeneity in unburned gas to the integral length scale of turbulence l_ϕ/l, global mean equivalence ratio $<\phi>$, rms fluctuations of equivalence ratio ϕ', Damköhler number and Karlovitz numbers based on the global equivalence ratio $<\phi>$ (i.e. $Da_{(<\phi>)} = lS_{b(<\phi>)}/u'\delta_{b(<\phi>)}$ and $Ka_{(<\phi>)} = [u'/S_{b(<\phi>)}]^{3/2}[l.S_{b(<\phi>)}/D_0]^{-1/2}$) and the turbulent Reynolds numbers (i.e. $\mathrm{Re}_t = \rho_0 u' l/\mu$) for the cases considered here are listed in Table 1, where D_0 is the unburned gas diffusivity and $S_{b(<\phi>)}$ is the laminar burning velocity at global mean equivalence ratio $<\phi>$. All the cases are run for about 2.5 initial eddy turn-over times ($t = 2.5l/u' = 2.5t_f$) which is greater than or comparable to the chemical time scale $D_0/[S_{b(<\phi>)}^2(1+\rho_0/\rho_{b(<\phi>)})]$. Simulations are carried out using a uniform grid size of $200\times200\times200$ and domain is taken to be cube of size $28D_0/S_{b(\phi=1)} \times 28D_0/S_{b(\phi=1)} \times 28D_0/S_{b(\phi=1)}$. Lewis numbers for all the species are taken to be unity and $(T_{ad}-T_0)/T_0$ is taken to be 3.0 where T_0 and T_{ad} are unburned gas temperature and adiabatic flame temperature of the stoichiometric mixture respectively.

3 Results and Discussion

In the context of stratified flames, the reaction progress variable, c, can be defined as $c = (\xi Y_{F\infty} - Y_F)/[\xi Y_{F\infty} - \max[0,(\xi - \xi_{st})/(1-\xi_{st})]Y_{F\infty}]$ where $Y_{F\infty}$ is the Y_F value in a pure fuel stream, ξ_{st} is the stoichiometric value of the mixture fraction $\xi = (Y_F - Y_O/s + Y_{O\infty}/s)/(Y_{F\infty} + Y_{O\infty}/s)$ with $Y_{O\infty}$ being the oxidiser mass fraction Y_O in pure air and s is the ratio of the oxidiser mass to fuel mass under stoichiometric conditions. The Y_F field at the central $x_1 - x_2$ plane for case C at $t = 2.5t_f$ is shown in Fig. 1a where the contours of reaction progress variable c from 0.1 to 0.9 from left to right in steps of 0.1 are shown by white lines. Figure 1a shows that the value of Y_F does not remain uniform in the unburned reactants and varies across a given c iso-surface. Furthermore, Fig. 1a shows that c contours corresponding to the preheat zone (i.e. $c \le 0.5$) are more distorted than the contours representing the reaction zone (i.e. $0.7 \le c \le 0.9$), which is typical of the thin reaction zones regime combustion [1].

Table 1: List of DNS parameters used in the present study

Case	$u'/S_{b(\phi=1)}$	$lS_{b(\phi=1)}/D_0$	l_ϕ/l	$Da_{(<\phi>)}$	$Ka_{(<\phi>)}$	$<\phi>$	ϕ'	Re_t
A	8.0	4.2	2.2	0.25	10.0	1.0	0.6	57.0
B	4.0	4.2	2.2	0.51	4.0	1.0	0.6	28.5
C	8.0	4.2	2.2	0.05	50.0	0.7	0.6	57.0
D	4.0	4.2	2.2	0.10	18.0	0.7	0.6	28.5

Bray *et al*. [4] showed that in the strict flamelet limit the turbulent scalar flux in premixed flames take the following form: $\overline{\rho u_i'' Y_F''} = \overline{\rho}[(\overline{u_i})_R - (\overline{u_i})_P](Y_{F0} - Y_F)(Y_F - Y_{F\infty})/(Y_{F0} - Y_{F\infty})$ where the subscripts P and R denote the conditional mean values in products and reactants, respectively and the subscripts 0 and ∞ are used to denote the values in unburned and burned gases respectively. This suggests that the statistical behaviour of $\overline{\rho u_1'' Y_F''}$ is dependent upon the behaviour of the slip velocity $[(\overline{u_i})_P - (\overline{u_i})_R]$ such that counter-gradient (gradient) transport will occur when $[(\overline{u_i})_P - (\overline{u_i})_R]$ is positive (negative). The expression for $[(\overline{u_i})_P - (\overline{u_i})_R]$ for premixed flames as proposed by Veynante *et al*. [5] can be written as: $[(\overline{u_i})_P - (\overline{u_i})_R] = -[-\alpha_1\sqrt{2\tilde{k}/3} + (\rho_0/\overline{\rho}_b - 1)\overline{S}_b]M_i$ where $\tilde{k} = \overline{\rho u_i'' u_i''}/2\overline{\rho}$ is the turbulent kinetic energy, α_1 is an appropriate efficiency function [5], $M_i = \partial\tilde{Y}_F/\partial x_i / \left|\nabla\tilde{Y}_F\right|$ is the i^{th} component of the resolved flame normal vector, $\overline{\rho}_b = \int_{\phi_{\min}}^{\phi_{\max}} \rho_{b(\varphi)} p(\phi) d\phi$ is the mean burned gas density and $\overline{S}_b = \int_{\phi_{\min}}^{\phi_{\max}} S_{b(\varphi)} p(\phi) d\phi$ is the mean burning velocity with $\rho_{b(\phi)}$ and $S_{b(\phi)}$ being the burned gas density and the unstrained laminar burning velocity for unstrained laminar flame at equivalence ratio ϕ and $p(\phi)$ is the pdf of equivalence ratio ϕ. This suggests that for $\alpha_1\sqrt{2\tilde{k}/3} < (\rho_0/\overline{\rho}_b - 1)\overline{S}_b$ ($\alpha_1\sqrt{2\tilde{k}/3} > (\rho_0/\overline{\rho}_b - 1)\overline{S}_b$), a counter-gradient (gradient) type transport will be observed. A parameter N_B equivalent to Bray number in the context of stratified flames can be defined as : $N_B = (\rho_0/\overline{\rho}_b - 1)S_b/\sqrt{2\tilde{k}/3}$ and counter-gradient (gradient) transport is obtained for $N_B >> 1$ ($N_B << 1$). As cases A-D in Table 1 are statistically

planar in nature, $\widetilde{c}$ remains a unique function of the co-ordinate in the direction of mean flame propagation (i.e. x_1-direction) and thus the variations of all the relevant terms will henceforth be presented as a function of $\widetilde{c}$. The variations of N_B with $\widetilde{c}$ across the flame brush are shown in Figs. 1b for cases A-D. It is evident from Fig. 1b that N_B varies significantly between cases due the differences in the relative magnitudes of $\sqrt{2\widetilde{k}/3}$ and $(\rho_0/\overline{\rho}_b - 1)\overline{S}_b$. Figure 1b suggests that whilst cases A, C and D are likely to exhibit gradient transport for $\overline{\rho u_1'' Y_F''}$, there is a strong likelihood of counter-gradient behaviour in case B. This can be verified by the variation of $\overline{\rho u_1'' Y_F''} \times \partial\widetilde{Y}_F/\partial x_1 \times D_0/\rho_0 S_{b(\phi=1)}^2$ with $\widetilde{c}$ across the flame brush for cases A-D presented in Fig. 1c where a positive (negative) value of $\overline{\rho u_1'' Y_F''} \times \partial\widetilde{Y}_F/\partial x_1 \times D_0/\rho_0 S_{b(\phi=1)}^2$ suggests counter-gradient (gradient) behaviour. It can be seen from Fig. 1c that $\overline{\rho u_1'' Y_F''} \times \partial\widetilde{Y}_F/\partial x_1 \times D_0/\rho_0 S_{b(\phi=1)}^2$ remains negative throughout the flame brush in all cases, except for a small region (i.e. $\widetilde{c} \approx 0.3-0.45$) in case B as suggested by Fig. 1b.

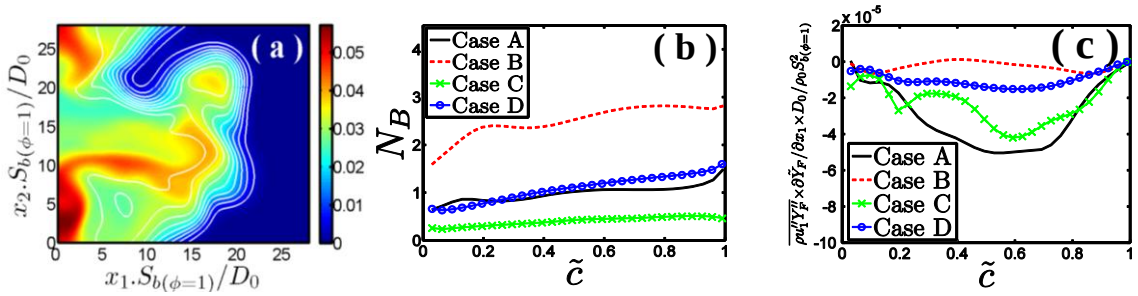

Fig. 1: (a) The fuel mass fraction Y_F field at the central $x_1 - x_2$ plane at $t = 2.5t_f$ for case C. The white lines indicate the contours of c from $0.1-0.9$ from left to right in steps of 0.1. (b) Variations of (b) $N_B = (\rho_0/\overline{\rho}_b - 1)S_b/\sqrt{2\widetilde{k}/3}$ and (c) $\overline{\rho u_1'' Y_F''} \times \partial\widetilde{Y}_F/\partial x_1 \times D_0/\rho_0 S_{b(\phi=1)}^2$ with $\widetilde{c}$ across the flame brush for cases A-D.

The variations of $\overline{\rho u_1'' Y_F''}/\rho_0 S_{b(\phi=1)} Y_{Fst}$ with $\widetilde{c}$ across the flame brush are shown in Figs. 2a-d for cases A-D, respectively. It is evident from Figs. 2a-d that $\overline{\rho u_1'' Y_F''}$ exhibits predominantly positive values throughout the flame brush in all cases except for a small region of the flame brush in case B (i.e. $\widetilde{c} \approx 0.3-0.45$) where counter-gradient transport has been observed (see Fig. 1c) because $\partial Y_F/\partial x_1$ assumes negative values throughout the flame brush. Furthermore, it can be seen from Figs. 2a-d that $\overline{\rho u_1'' Y_F''}$ exhibits non-zero values towards the fresh gas side of the flame brush (i.e. $\widetilde{c} = 0$) due to inhomogeneity in the unburned reactants. The predictions of the gradient hypothesis model for $\overline{\rho u_1'' Y_F''}$ (i.e. $\overline{\rho u_1'' Y_F''} = (\mu_t/\sigma).\partial\widetilde{Y}_F/\partial x_1$) is shown in Figs. 2a-d for $\sigma = 0.2$. It is evident that from Figs. 2a-d that Eq. 1 can account for the qualitative behaviour of $\overline{\rho u_1'' Y_F''}$ obtained from DNS in the cases where gradient transport has been observed throughout the flame brush (i.e. cases A, C and D). However, the value of σ needs to be varied significantly between cases in order to capture the quantitative behaviour of $\overline{\rho u_1'' Y_F''}$ obtained from the DNS data. Moreover, it can be seen that the gradient hypothesis approach cannot capture the correct qualitative behaviour of $\overline{\rho u_1'' Y_F''}$ in certain regions of the flame brush in case B where a counter-gradient transport is observed (see Fig. 1c). Therefore, a new model needs to be proposed for $\overline{\rho u_1'' Y_F''}$ which can adequately account for both

gradient and counter-gradient type transport for both globally fuel-lean and globally stoichiometric conditions.

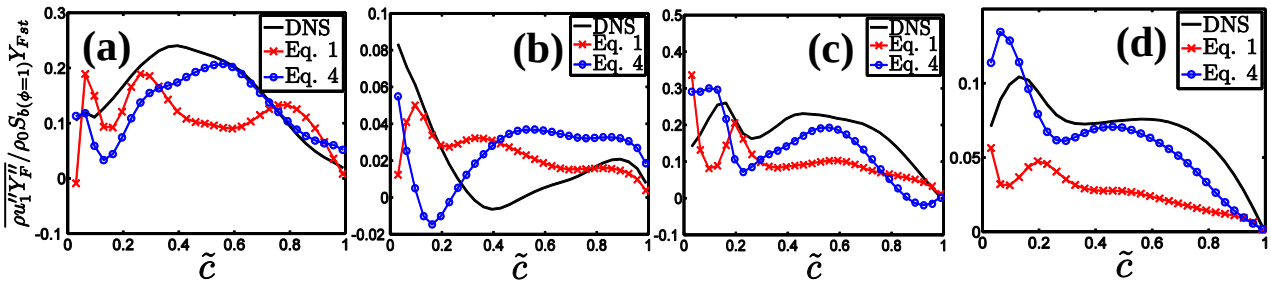

Fig. 2: Variations of $\overline{\rho u_1'' Y_F''} / \rho_0 S_{b(\phi=1)} Y_{Fst}$ with $\widetilde{c}$ across the flame-brush along with the predictions according to Eq. 1 and Eq. 4 for cases: (a) A, (b) B, (c) C and (d) D.

A Favre joint pdf between Y_F and ξ is proposed by Mura *et al*. [10] in the following manner:

$$\tilde{P}(Y_F,\xi) = \rho P(Y_F,\xi)/\overline{\rho} = \lambda_W \tilde{P}(\xi \mid Y_{\max})\delta(Y_F - Y_{\max}(\xi)) + (1-\lambda_W)\tilde{P}(\xi \mid Y_{\min})\delta(Y_F - Y_{\min}(\xi)) + O(1/Da) \quad (3i)$$

where $\lambda_W = (\widetilde{Y}_F - \widetilde{Y}_{\min})/(\widetilde{Y}_{\max} - \widetilde{Y}_{\min})$ is a weighting coefficient [10] and the quantities $Y_{\max}(\xi) = \xi$ and $Y_{\min}(\xi) = A(\xi)(\xi - \xi_{st})$ are maximum and minimum values of Y_F according to the Burke-Schumann diagram, where $A(\xi)$ is given by $A(\xi) = H(\xi - \xi_{st})/(1-\xi_{st})$. The identities $\widetilde{u}_1 = \int u_1 \tilde{P}(Y_F,\xi,u_1)du_1 dY_F d\xi$ and $\overline{\rho u_1'' Y_F''}/\overline{\rho} = \int (u_1 - \widetilde{u}_1)(Y_F - \widetilde{Y}_F)\tilde{P}(Y_F,\xi,u_1)du_1 dY_F d\xi$ yield:

$$\widetilde{u}_1 = [\overline{(u_1)}_R - \overline{(u_1)}_P]\lambda_W(1-\lambda_W) + \overline{(u_1)}_P \quad (3ii)$$

$$\overline{\rho u_1'' Y_F''} = \overline{\rho}[\overline{(u_1)}_R - \overline{(u_1)}_P](\widetilde{Y}_{\max} - \widetilde{Y}_{\min})\lambda_W(1-\lambda_W) + \lambda_W \overline{\rho}\, \widetilde{u_1'' \xi''} + (1-\lambda_W)\widetilde{A}\overline{\rho}\, \widetilde{u_1'' \xi''} \quad (3iii)$$

Chakraborty and Cant [15] proposed an algebraic model for the turbulent flux of reaction progress variable c (i.e. $\overline{\rho u_1'' c''}$) for turbulent premixed flames. Following the analysis by Chakraborty and Cant [6], an algebraic expression can be obtained for $\overline{\rho}[\overline{(u_1)}_R - \overline{(u_1)}_P](\widetilde{Y}_{\max} - \widetilde{Y}_{\min})\lambda_W(1-\lambda_W)$ which in turn can be substituted in Eq. 3iii to yield:

$$\overline{\rho u_1'' Y_F''} = \overline{\rho}\left[-\alpha_{1F}\sqrt{2\widetilde{k}/3} + \beta_F\left[\frac{\partial \widetilde{u}_i}{\partial x_i} + \alpha_{2F}\sqrt{\frac{2\widetilde{k}}{3}}\left|\nabla \widetilde{Y}_F\right|\right]\frac{\delta_b}{\lambda_W(1-\lambda_W)(\widetilde{Y}_{\max} - \widetilde{Y}_{\min})}\right]\lambda_W(1-\lambda_W)(\widetilde{Y}_{\max} - \widetilde{Y}_{\min}) + \lambda_W \overline{\rho u_1'' \xi''} + (1-\lambda_W)\widetilde{A}\overline{\rho u_1'' \xi''} \quad (4)$$

where α_{1F} , α_{2F} and β_F are model parameters and $\delta_b = 2D_0/\overline{S}_b$ is the characteristic flame thickness. The first term in the right hand side of Eq. 4 accounts for the reaction contribution to $\overline{\rho u_1'' Y_F''}$ where as the second and third terms account for the mixing contribution to $\overline{\rho u_1'' Y_F''}$. It is has been found that the model performs satisfactorily for all cases when the model parameters are taken to be $\alpha_{1F} = 0.1(1+Ka_L)^{-1}$, $\alpha_{2F} = 2.0$ and $\beta_F = 0.025[erf(0.08Ka_L)]$ where $Ka_L = (\overline{S}_b)^{-3/2}(\widetilde{\varepsilon}\delta_b)^{0.5}$ is the local Karlovitz number. It is evident from Figs. 2a-d that the model proposed (i.e. Eq. 4) outperforms the gradient hypothesis model (i.e. Eq. 1) in all cases considered in the current study. The model given by Eq. 4 satisfactorily captures both the qualitative and quantitative behaviours of $\overline{\rho u_1'' Y_F''}$ obtained from the DNS data. Moreover, it can be seen in Fig. 2b that the model proposed in Eq. 4 can capture the counter-gradient characteristics of $\overline{\rho u_1'' Y_F''}$ in case B.

4 Conclusions

The statistical behaviour of turbulent scalar flux of fuel mass fraction $\overline{\rho u_i'' Y_F''}$ for globally fuel-lean and stoichiometric (i.e. $<\phi>=0.7$ and $<\phi>=1.0$) stratified flames at different levels rms turbulent velocity fluctuations have been studied using a 3-D compressible DNS database. It has been found that $\overline{\rho u_1'' Y_F''}$ may exhibit a counter-gradient type transport when $N_B = (\rho_0 / \overline{\rho}_b - 1) S_b / \sqrt{2\tilde{k}/3}$ assumes large values, whereas a predominantly gradient type transport is observed for small values of N_B. A model has been identified for $\overline{\rho u_1'' Y_F''}$ in turbulent stratified flames which can account for both gradient and counter-gradient type transports in both globally fuel-lean and stoichiometric conditions. The effects of detailed chemistry and differential diffusion rate of mass and heat are not considered in the present study and the turbulent Reynolds number remains modest. Although the competition between the flame normal acceleration due to heat release and the turbulent velocity fluctuation determines the nature of turbulent scalar transport irrespective of turbulent Reynolds number Re_t, the sensitivity of the proposed model parameters in relation to Re_t needs to be investigated in detail. Therefore, future research in these directions will be necessary for a more comprehensive assessment of the model proposed in this study. Furthermore, the implementation of the proposed models in actual RANS simulations will be necessary for *a-posteriori* assessment.

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