Conditional statistics in a turbulent premixed flame derived from direct numerical simulation

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1. Motivation and objectives

In premixed turbulent combustion modeling, the most common approach is based on averaged transport equations for statistical moments (mean, variance) of thermochemical variables. Most of the recent developments are for systems in the flamelet regime and consider infinitely fast chemical reactions compared to the turbulent mixing (Bray 1980, Peters 1986). Under this assumption, the turbulent flame can be represented as a collection of laminar flamelets stretched and convected by the turbulent flow field. Thus, several authors have proposed to describe the turbulent flame by a transport equation for the surface flame area per unit of volume Σ (Bideaux *et al.* 1994, Candel & Poinsot 1990, Pope 1985-a, Trouvé & Poinsot 1994) or by a transport equation for an arbitrary scalar field (concentration, temperature) $G(x_k, t) = G_0$ which describes the flame sheet as an infinitely thin interface separating fresh and burnt gases (Kerstein *et al.* 1988, Peters 1992, Williams 1985-b). Another possibility is to derive a transport equation for the dissipation of the fluctuations of the concentration leading, in the limit of high Damköhler number, to a balance equation for Σ (Mantel & Borghi 1994).

Another general approach consists of directly calculating the probability density function (pdf) of the thermochemical variables through its transport equation (Borghi 1988, O'Brien 1985, Pope 1985-b). This method avoids the modeling of the chemical reaction rate and can more easily take into account reduced chemical schemes or complete chemical schemes as well (Vervisch 1991). However, the limitation of these models is the high computational cost of the Monte-Carlo method used and the sub-models for the molecular mixing terms.

Recently, Bilger (1993-a,b) has proposed an alternative method based on conditional moment closure (CMC) applied to turbulent reacting flows for both non-premixed and premixed systems. This technique goes beyond the zone conditioning methods developed and applied to non reacting flows in the case of a two-dimensional mixing layer by Libby (1975) and extended to the turbulent mixing of scalars by Dopazo (1977). Like pdf approaches, the CMC method is valid in the different regimes of combustion and can take into account reduced or complete chemical schemes. Moreover, the chemical reaction term can be decomposed using a Taylor expansion (Bilger 1993-b) and can be estimated without modeling. Although CMC methods in turbulent reacting flows are of recent origin and still under development, applications to real configurations for non-premixed combustion have

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been already performed using detailed chemistry (Smith *et al.* 1992). Comparisons with experimental data obtained for a turbulent jet-flame show encouraging results (Smith *et al.* 1993). As in classical flamelet models (Bray 1980), the dissipation rate of a conserved scalar appears in the CMC approach and is a crucial quantity which must be modeled. To validate models for the conditional dissipation rate, Mell *et al.* (1994) use results from direct numerical simulation of a reacting mixture in homogeneous turbulence whereas Li & Bilger (1993) utilize experimental results in a reactive scalar mixing layer. Conditional statistics concerning the dissipation of temperature fluctuations in a non-reacting system are also available (Jayesh & Warhaft 1992).

Nevertheless, for premixed systems only theoretical developments exist (Bilger 1993-b) and certain problems are still unresolved. This is particularly the case for the conditional mean velocity and the conditional mean scalar dissipation rate. This last term characterizes the molecular mixing (or the rate of dissipation of the scalar fluctuations) and must be treated carefully in turbulent premixed combustion as has been shown in Borghi (1990) and Mantel & Borghi (1994).

But, unlike diffusion flames, scalar dissipation is a quantity difficult to measure in premixed flames because of the weak spatial resolution of experimental devices (Bilger 1993-c). Experimental results for the scalar dissipation have not yet been published. Since for premixed systems no data are available, another possibility consists of analyzing results of DNS of turbulent premixed flames. Among the available databases, we cite the pioneering work of Trouvé & Poinsot (1994) who have simulated the interaction between a premixed flame and a three-dimensional isotropic decaying turbulent flow field with realistic heat release. The analysis of these numerical results will provide new information concerning the conditional statistics in turbulent premixed flames and eventually lead to new models for these unclosed terms.

The objective of this paper is to briefly introduce CMC methods for premixed systems and to derive the transport equation for the conditional species mass fraction conditioned on the progress variable based on the enthalpy. Our statistical analysis will be based on the 3-D DNS database of Trouvé & Poinsot (1994) available at the Center for Turbulence Research. The initial conditions and characteristics (turbulence, thermo-diffusive properties) as well as the numerical method utilized in the DNS of Trouvé & Poinsot (1994) are presented, and some details concerning our statistical analysis are also given. From the analysis of DNS results, the effects of the position in the flame brush, of the Damköhler and Lewis numbers on the conditional mean scalar dissipation, and conditional mean velocity are presented and discussed. Information concerning unconditional turbulent fluxes are also presented. The anomaly found in previous studies (Libby & Bray 1981, Moss 1980) of counter-gradient diffusion for the turbulent flux of the progress variable is investigated.

2. Accomplishments

2.1 Equation for the conditional average of the species mass fraction

The transport equation for the conditional average of the mass fraction of a reactive species has been derived by Bilger (1993-b) from the balance equations for the species mass fraction Y_i for the species i and for the progress variable c based on the enthalpy which will be defined below. Its derivation is similar to that used for non-premixed flames (Bilger 1993-a). Klimenko (1990) has a different approach which has not been implemented in premixed flames.

The balance equation for the mass fraction Y_i is:

$$\rho\frac{\partial Y_i}{\partial t} + \rho U_k\frac{\partial Y_i}{\partial x_k} = \frac{\partial}{\partial x_k}(\rho\mathcal{D}_i\frac{\partial Y_i}{\partial x_k}) + \dot{w}_i \tag{1}$$

where $\mathcal{D}_i$ is the molecular mass diffusivity for the species i, ρ the mass density, U_k the velocity vector, and $\dot{w}_i$ the chemical reaction rate.

For the progress variable c, we use the special definition proposed by Bilger (1993-b):

$$c = \frac{h^s - h^s_u - 2h + 2h_u}{\Delta h^s} \tag{2}$$

Here, h is the total enthalpy, h^s represents the sensible enthalpy, and the subscript u characterizes the unburnt gases. The sensible enthalpy rise Δh^s is given by the adiabatic burnt value less the unburnt value. Thus, the progress variable c varies to 0 in the fresh gases to 1 in the fully burnt gases for adiabatic flames. For non-adiabatic flames c can go beyond unity, this being considered useful for studying NO formation and CO burnt out.

The transport equation for h and h^s are respectively:

$$\rho\frac{\partial h}{\partial t} + \rho U_k\frac{\partial h}{\partial x_k} = \frac{\partial}{\partial x_k}(\rho\alpha\frac{\partial h}{\partial x_k}) + \frac{\partial p}{\partial t} - \Phi_R \tag{3}$$

$$\rho\frac{\partial h^s}{\partial t} + \rho U_k\frac{\partial h^s}{\partial x_k} = \frac{\partial}{\partial x_k}(\rho\alpha\frac{\partial h^s}{\partial x_k}) + \frac{\partial p}{\partial t} - \Phi_R + \sum_{i=1}^{N}\dot{w}_i\Delta h_i^f \tag{4}$$

where α represents the thermal diffusivity of the mixture, p the pressure, Φ_R the radiative heat flux, and Δh_i^f the heat of formation for the species i.

According to its definition given in Eq. (2), the equation for c is directly obtained by combining Eqs. (3) and (4):

$$\rho\frac{\partial c}{\partial t} + \rho U_k\frac{\partial c}{\partial x_k} = \frac{\partial}{\partial x_k}(\rho\alpha\frac{\partial c}{\partial x_k}) + \frac{1}{\Delta h^s}\sum_{i=1}^{N}\dot{w}_i\Delta h_i^f \tag{5}$$

Here, the pressure rise and the radiative heat losses have been neglected.

The conditional average of the species mass fraction Y_i conditioned on the progress variable $c(x_k,t)$ being at a chosen value ζ can be defined:

$$Q_i(\zeta, x_k, t) \equiv \langle Y_i(x_k,t) \mid c(x_k,t) = \zeta\rangle = \langle Y_i \mid \zeta\rangle \tag{6}$$

From this definition and from Eqs. (1) and (5), Bilger (1993-a) has obtained the balance equation for Q_i:

$$\langle\rho \mid \zeta\rangle\frac{\partial Q_i}{\partial t} + \langle\rho \mid \zeta\rangle\langle U_k \mid \zeta\rangle\frac{\partial Q_i}{\partial x_k} = \frac{1}{Le_i}\langle\rho \mid \zeta\rangle\langle\alpha\frac{\partial c}{\partial x_k}\frac{\partial c}{\partial x_k} \mid \zeta\rangle\frac{\partial^2 Q_i}{\partial \zeta^2} + \langle\dot{w}_i \mid \zeta\rangle + e_Q + e_y - \frac{1}{\Delta h^s}\left(\sum_{i=1}^{N}\Delta h_i^f\langle\dot{w}_i \mid \zeta\rangle\right)\frac{\partial Q_i}{\partial \zeta} \quad (7)$$

with

$$Le_i = \frac{\alpha}{\mathcal{D}_i} \quad (8)$$

$$e_Q = \frac{\partial}{\partial x_k}(\rho\mathcal{D}_i\frac{\partial Q_i}{\partial x_k}) + \langle\{\rho\mathcal{D}_i\frac{\partial Q_{,c}}{\partial x_k}\frac{\partial c}{\partial x_k} + \frac{\partial}{\partial x_k}(\rho\mathcal{D}_i(1-Le_i)\frac{\partial c}{\partial x_k})\} \mid \zeta\rangle \quad (9)$$

$$e_y \approx -\frac{1}{P_c(\zeta)}\frac{\partial}{\partial x_k}(\langle\rho u_k y_i \mid \zeta\rangle P_c(\zeta)) \quad (10)$$

Here, Le_i represents the Lewis number for the species i, u_k and y_i are the fluctuating parts of respectively U_k and Y_i about their conditional means, and $Q_{,c}$ is the derivative of Q with regards to c. The probability density function of c defined at $c = \zeta$ is given by $P_c(\zeta)$.

If the Reynolds number of the flow is sufficiently high, the molecular diffusion fluxes present in e_Q are negligible compared to the turbulent flux (Bilger 1993-a). The conditional turbulent flux e_y has been observed negligible in the case of a reacting mixing layer (Bilger 1993-a) and can probably be neglected in premixed flames.

The conditional mean chemical reaction rate can be approximated using a Taylor expansion for $\langle\dot{w}_i \mid \zeta\rangle$ (Bilger 1993-b). This technique has been used by Smith *et al.* (1992) for the prediction of radicals and NO in a turbulent diffusion jet flame and comparisons with experimental data lead to satisfying agreements.

Even after these approximations, some terms of Eq. (7) remain unclosed and need to be modeled. Our attention will be focused principally on the conditional mean velocity $\langle U_k \mid \zeta\rangle$ and on the conditional mean scalar dissipation N_ζ defined by:

$$N_\zeta = \langle\alpha\frac{\partial c}{\partial x_k}\frac{\partial c}{\partial x_k} \mid \zeta\rangle \quad (11)$$

These two terms are also crucial quantities in models using pdf methods. They appear explicitly in the transport equation for the pdf $P(\zeta)$:

$$\langle\rho \mid \zeta\rangle\frac{\partial P}{\partial t} + \langle\rho \mid \zeta\rangle\langle U_k \mid \zeta\rangle\frac{\partial P}{\partial x_k} = \frac{\partial}{\partial \zeta}(\langle\dot{w}_c \mid \zeta\rangle P) + \frac{\partial^2}{\partial \zeta^2}(\langle\rho \mid \zeta\rangle N_\zeta P) \quad (12)$$

where $\dot{w}_c$ is the last term appearing on the right hand side of Eq. (7).

2.2 The numerical experiment of Trouvé £ Poinsot (1994)

Since measurements in premixed flames are limited due to spatial resolution problems (Bilger 1993-c), DNS offers the possibility of having access to specific quantities of statistical interest such as unconditional and conditional moments (mean, variance, etc). The numerical results used in the present analysis come from the DNS of turbulent premixed flames performed by Trouvé and Poinsot (1994). These authors have studied the interaction between an initially planar premixed laminar flame with realistic heat release and a three-dimensional decaying isotropic turbulent flow field. Their code fully resolves the compressible Navier-Stokes equations using a sixth order spatial scheme (Lele 1992) and a third order temporal scheme (Wray 1992). Due to the heat release and the resulting gas expansion, the boundary conditions in the direction of propagation of the flame are inflow/outflow non-reflecting (Poinsot and Lele 1992), whereas periodicity is used in the two other directions.

The chemistry is described by a single-step irreversible reaction using a classical Arrhenius law. Following the notation of Williams (1985-a), the reaction rate for the deficient species (subscript R) can be expressed:

$$\dot{w}_R = \Lambda \rho Y_R \exp\left(-\frac{\beta(1-\Theta)}{1-\varphi(1-\Theta)}\right) \tag{13}$$

where:

Θ	$=(T-T_u)/(T_b-T_u)$	is the reduced temperature
φ	$=(T_b - T_u)/T_b$	represents the heat release parameter
β	$=\varphi E_a/R^0 T_b$	is the Zel'dovich number
Λ	$=B\exp(-\beta/\varphi)$	is the pre-exponential factor

The subscripts u and b represent respectively the unburnt and burnt gases and E_a the activation energy of the reaction, R^0 being the universal gas constant.

Moreover, in the simulations, the temperature dependence of the transport coefficients is taken into account by a power law:

$$\frac{\mu}{\mu_u} = \left(\frac{T}{T_u}\right)^b \tag{14}$$

where μ represents the dynamic viscosity and b is a constant equal to 0.76. The thermal conductivity and molecular diffusivity of the reactants are determined by considering constant Prandtl and Schmidt numbers.

Different simulations have been performed for various Lewis number (0.8, 1.0, 1.2), the other physical parameters being the same for all the configurations. At time $t = 0$, the turbulent Reynolds number based on the Taylor microscale λ is $Re_\lambda = 50$ and the initial Damköhler number (defined by $Da = (\lambda/u')/(\alpha_u/S_{L_0}^2)$) is $Da = 0.4$. Here, α_u represents the thermo-diffusivity in the fresh gases, S_{L_0} the laminar flame, speed and u' the rms turbulent velocity. These initial conditions

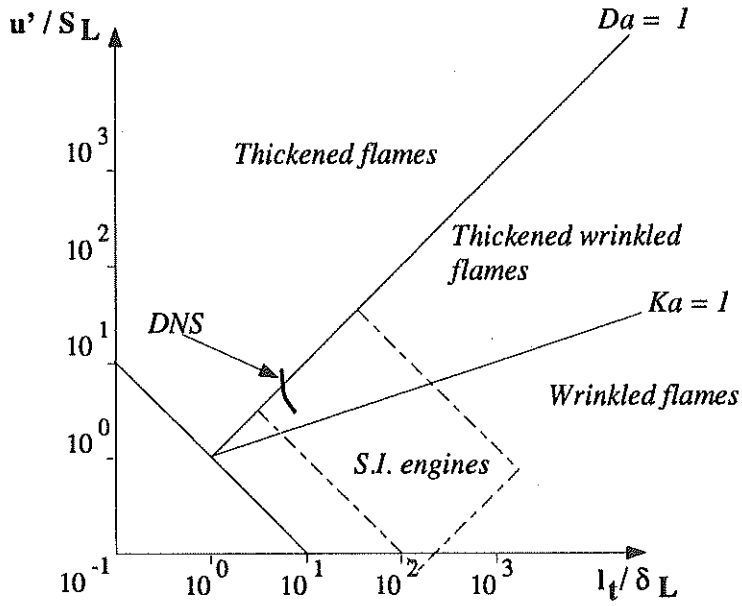

FIGURE 1. Evolution of the DNS in the diagram of premixed turbulent flames - comparisons with the operating domain of classical experimental devices and S. I. engines.

correspond to the ratios $u'/S_{L_0} = 10$ and $l_t/\delta_F = 5.2$ (l_t is the integral length scale of the turbulence and δ_F the laminar flame thickness defined by $\delta_F = \alpha_u/S_{L_0}$).

The flames investigated in the DNS evolve in the thickened wrinkled flames regime of the Borghi diagram for turbulent premixed flames (Borghi 1985) as is shown in Fig. 1. Also schematically shown in this diagram is the operating domain of classical experimental devices and S. I. engines (Abraham 1985).

In the following analysis, all of the cited turbulence quantities are obtained from a simulation of 3-D decaying isotropic turbulence with no combustion. All cases have been performed using a 129^3 computational domain.

2.3 Statistical analysis

In our analysis, since radiative heat losses and pressure rise are neglected and the specific heat is constant, the progress variable c defined in Eq. (2) is equivalent to $c = (T - T_u)/(T_b - T_u)$ and is equal to 0 in the fresh gases and to 1 in the fully burnt gases. In the calculation of the scalar dissipation $N = \alpha(\partial c/\partial x_k)(\partial c/\partial x_k)$, the thermo-diffusivity α is temperature dependent according to the relation (14) and by using the constant Prandtl number ($Pr = 0.75$).

In the determination of the conditional statistics, the progress variable space ζ is divided into 100 sub-domains. In each point of the computational domain, the variables of interest are calculated and stored in arrays corresponding to the sub-domain of ζ at this point. Conditional averages are then obtained by dividing the variable contained in the arrays by the number of samples of each sub-domain.

Since in the DNS the direction of propagation of the flame front is following the x direction, only $\langle U_1 \mid \zeta \rangle$ is of interest and will be investigated in the present analysis.

For the unconditional statistics, since we have access to only one realization, the problem is assumed to be homogeneous in the $y-z$ directions (x being the direction of propagation of the flame front). Then, the computational domain is divided into slices perpendicular to the x direction, and statistics are calculated for each plane through the turbulent flame front. The averaging of a variable Q varying spatially and temporarily is then estimated as it is proposed by Trouvé & Poinsot (1994):

$$\langle Q(x,t) \rangle = \frac{1}{L_y L_z} \int Q(x,y,z,t) dy dz \tag{15}$$

where L_y and L_z are the size of the computational box in the y and z directions.

Through the flame brush $\widetilde{c}$, the density weighted mean of c increases monotically with x. Consequently, the results will be presented using the mean progress variable $\widetilde{c}$ instead of the x coordinate.

2.4 Results

2.4.1 The conditional dissipation rate N_ζ

Because it represents the small scale mixing or molecular dissipation of a scalar (concentration, temperature), the dissipation rate of the progress variable N is a crucial quantity in turbulent combustion (Borghi 1990, Bray 1980, Mantel & Borghi 1994). In the case of turbulent premixed combustion, the mean reaction rate is directly proportional to $\widetilde{N}$ as has been demonstrated by Bray (1980) in the limit of high Damköhler numbers. Often, this term is modeled utilizing the dissipation time scale of the turbulent kinetic energy and a suitable constant, so that $\widetilde{N} \propto \widetilde{c''^2}/\tau_t$ (Bray 1980, Spalding 1971). However, further studies have shown that the proportionality constant depends on at least two parameters describing the structure of the premixed flame such as the Damköhler and turbulence Reynolds numbers (Mantel & Borghi 1994, Said & Borghi 1988). In those studies, it appears that the ratio of the two dissipation time scales $R = \tau_t/\tau_c$ (τ_c represents the dissipation time scale of the scalar) is a function of the ratio $k^{1/2}/S_{L_0}$, which can also be defined by $k^{1/2}/S_{L_0} \propto (Re_t/Da)^{1/2}$ (k represents the turbulent kinetic energy). Said & Borghi (1988) proposed an algebraic formula for R whereas Mantel & Borghi (1994) have derived a transport equation for $\widetilde{N}$.

For the conditional dissipation rate, few theoretical developments exist, and experimental and numerical data are only available for non-premixed combustion or non-reacting flows. Both Mell *et al.* (1994) in their numerical simulations and Li & Bilger (1993) in their experimental study have modeled the conditional dissipation of a conserved scalar N_η using the unconditional one and a frequency related to the large scales of the turbulence:

$$N_\eta \approx \widetilde{N_z} = R\widetilde{Z''^2}\frac{\epsilon}{k} \tag{16}$$

where R is the time scale ratio assumed to be constant, ϵ represents the dissipation of the turbulent kinetic energy, Z is the mixture fraction in the physical space, and η the mixture fraction in the domain of phase. These authors conclude that this classical closure gives good predictions for their experimental and numerical results, although more detailed modeling of N_ζ is better (Mell *et al.* 1994).

However, this kind of closure apparently valid for non-premixed systems cannot be applied for premixed flames because the turbulent mixing is not the only cause of scalar variance annihilation. Chemical reaction is also involved and has to be considered in the modeling of N_ζ. This is illustrated in Fig. 2 which shows the evolution of R across the flame brush. The ratio R varies significantly through the flame brush ranging from 0.3 to 1.5. This is consistent with the values found by Beguier *et al.* (1978) in the case of non-reacting flows. Only a slight effect of the Lewis number is observed on R (see Fig. 2-a). As the time goes on, we note in Fig. 2-b that R is less than unity in the most part of the turbulent flame front ($0.1 \leq \widetilde{c} \leq 0.9$). This indicates that the turbulence dissipates more rapidly than the fluctuations of $\widetilde{c}$. In such a case, it clearly appears that the well-known Eddy Break-Up model will significantly overestimate the mean reaction rate since $\widetilde{\dot{w}}_{ebu} \propto \widetilde{c}(1-\widetilde{c})/\tau_t$.

Fig. 3 shows the form of $\hat{N}_{\zeta_{lam}} = N_{\zeta_{lam}}\tau_{ch}$ (τ_{ch} represents a chemical time scale defined by $\tau_{ch} = \alpha_u/S_{L_0}^2$) in a planar laminar flame front for different Lewis numbers. As expected, $\hat{N}_{\zeta_{lam}}$ is insensitive to the Lewis number since the progress variable is expressed in terms of temperature instead of the concentration of fuel, for instance. Unlike Bilger (1993-b), $\hat{N}_\zeta$ does not have a symmetric shape, but has a maximum value towards the burnt gases. This asymmetry is due to the high activation energy for the kinetics, whereas Bilger (1993-b) is for a full kinetic mechanism. We can note the quadratic behavior of $\hat{N}_{\zeta_{lam}}$ in the preheat zone ($\zeta < 0.6$) as given by the convection diffusion balance:

$$\rho_u S_{L_0}\frac{dc}{dx} = \frac{d}{dx}\left(\rho\alpha\frac{dc}{dx}\right) \tag{17}$$

which leads directly to $\hat{N}_{\zeta_{lam}} = (T/T_u)^{1-b}.\zeta^2$.

Fig. 4 shows the evolution of N_ζ (normalized by the laminar value $N_{\zeta_{lam}}$) for the turbulent flame with $Le = 1.0$ versus ζ for different times (t/τ_0 ranges from 1.4 to 4.5, τ_0 being the eddy turn-over time). At the earliest time results are shown after one eddy turn-over time, and thus the flame has had the time needed to adapt itself to all the spectrum of the turbulence. Since in the DNS positive stretch occurs (on average) more often than negative stretch (Trouvé & Poinsot 1994), the profiles of concentration and temperature are steepened, and we can expect higher values for N_ζ than in the laminar case. At earlier times, this enhanced mixing appears to be very strong in the preheat zone but also may be dependent on the Damköhler number. Since the Damköhler number is low, the instantaneous flame front does not respond immediately to the turbulent flow field, and in the preheat zone, N_ζ is 2 or 3 times greater than the laminar value. The reaction zone, however remains almost unaffected by the turbulent mixing, and we observe an only slight increase

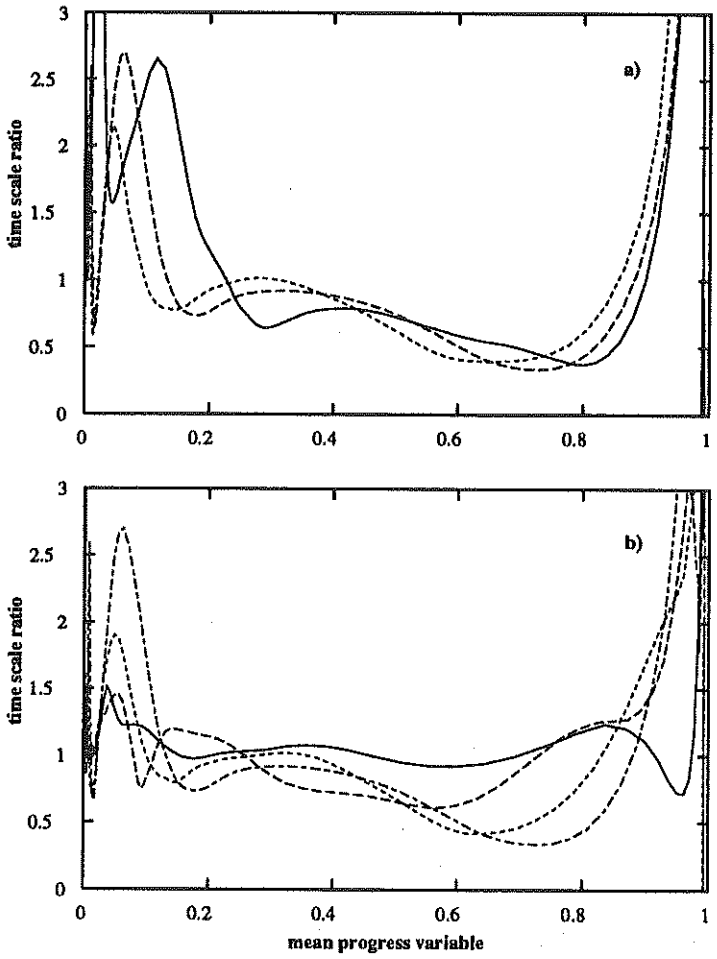

FIGURE 2. Profiles of $R = \tau_t/\tau_c$ versus $\widetilde{c}$. a) for different Lewis number at $t/\tau_0 = 4.5$: $Le = 0.8$: ——— ; $Le = 1.0$: ---- ; $Le = 1.2$: ------ . b) for different times and $Le = 1.0$: $t/\tau_0 = 1.4$ - $Re_t = 50$ - $Da = 0.5$:——— ; $t/\tau_0 = 2.7$ - $Re_t = 33$ - $Da = 0.6$:---- ; $t/\tau_0 = 3.6$ - $Re_t = 29$ - $Da = 0.8$:------ ; $t/\tau_0 = 4.5$ - $Re_t = 25$ - $Da = 1.0$:— — —

of N_ζ of approximately 20%. As the time goes on, the Damköhler number increases due to the decay of the turbulence. Thus, the turbulent flame comes more into the flamelet regime and N_ζ behaves more and more as in the laminar case. At this point, there is no distinction between the preheat zone, and the reaction zone and $N_\zeta/N_{\zeta_{lam}}$ is almost constant and close to unity in all of the domain of ζ.

The variation of $N_\zeta/N_{\zeta_{lam}}$ across the flame brush is represented in Fig. 5 for different values of ζ. It appears that $N_\zeta/N_{\zeta_{lam}}$ is almost constant through the turbulent flame front and is only weakly dependent on $\widetilde{c}$. Thus, conditional statistics for N_ζ can be extracted from all the computational domain rather than in $y - z$ planes.

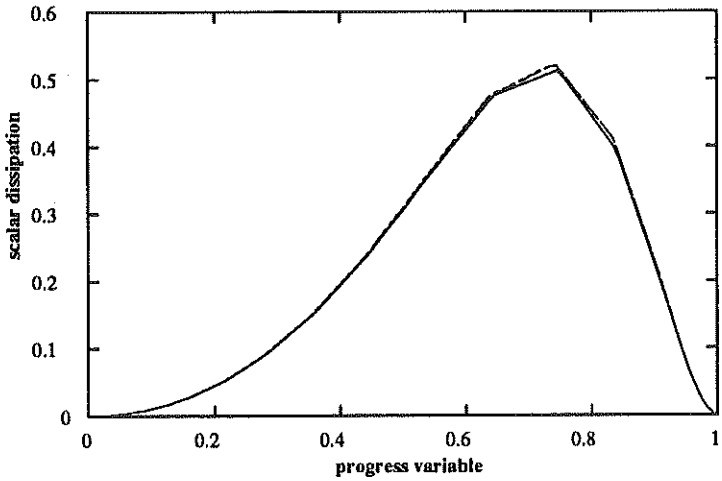

FIGURE 3. Profiles of $\hat{N}_\zeta$ for laminar flame versus ζ given by DNS. $Le = 0.8$: ——— ; $Le = 1.0$: ---- ; $Le = 1.2$: ------

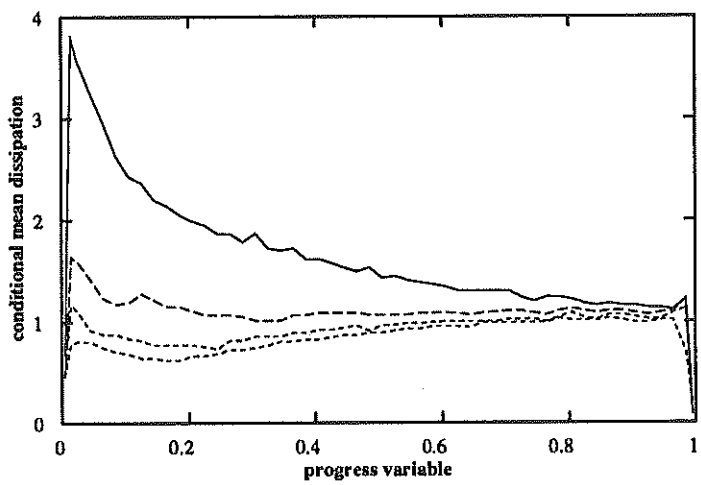

FIGURE 4. Profiles of $N_\zeta/N_{\zeta_{lam}}$ versus ζ for $Le = 1.0$. $t/\tau_0 = 1.4$: ——— ; $t/\tau_0 = 2.7$: ---- ; $t/\tau_0 = 3.6$: ------ ; $t/\tau_0 = 4.5$: —-— . See Fig. 2 for the corresponding Damköhler numbers.

The influence of the Lewis number on N_ζ is also investigated and presented in Fig. 6 for 2 different times of the interaction. At time $t/\tau_0 = 1.4$ (corresponding to $Da = 0.5$), we notice a significant effect of the Lewis number in the reaction zone ($\zeta > 0.7$). In the preheat zone, no effect of the Lewis number is observed. The turbulent mixing predominates and diffusivities (of species and temperature) are too slow compared to the chemistry to allow the profile of c to behave like in the laminar case. In the reaction zone, the end of the temperature profile seems to be affected, illustrating an effect of the Lewis number. The gradients of c are

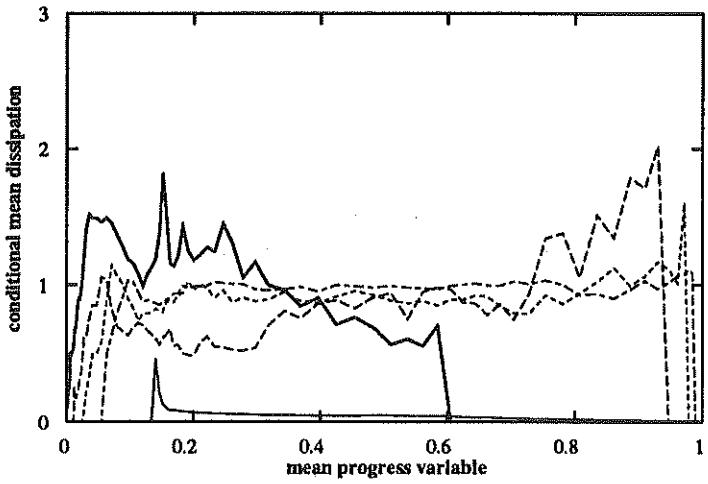

FIGURE 5. Evolution of $N_\zeta/N_{\zeta_{lam}}$ versus $\widetilde{c}$ for different values of ζ at $t/\tau_0 = 4.5$ and $Le = 1.0$. $\zeta = 0.0$: ——— ; $\zeta = 0.25$: ---- ; $\zeta = 0.5$: ····· ; $\zeta = 0.75$: —·— ; $\zeta = 1.0$: ———

steeper for $Le = 0.8$ and flatter for $Le = 1.2$ (for $Le = 1.2$, we can note that N_ζ decreases significantly below the laminar value). There is no clear explanation for such behavior. We can argue that for a positive stretch, the local reaction rate increases (decreases) when the Lewis number is smaller (greater) than unity and affects the end of the temperature profile increasing (decreasing) the gradients of c.

For time $t/\tau_0 = 4.5$ (which corresponds to $Da = 1.0$), N_ζ is affected uniformly by the Lewis number and no distinct behaviors exist between the preheat and reaction zones. The gradients of c are steeper everywhere in the ζ space for $Le = 0.8$ and weakly flatter (especially in the reaction zone) for $Le = 1.2$. This result is quite surprising because we can expect that when the Damköhler number increases, the turbulent flame behaves more and more in the flamelet regime. Thus locally the flame should have the structure of a laminar flame, and consequently the 3 curves of Fig. 6-b should merge together. This comment concerns mainly the case $Le = 0.8$ for which the gradients of c are significantly higher than the two others cases. Since in this case the Lewis number is smaller than unity, we can hypothesize that thermo-diffusive instabilities have become non-negligible and provoke additional stretch that is not present in the cases $Le = 1.0$ and $Le = 1.2$.

In conclusion, from the Fig. 6, it appears that the ratio $N_\zeta/N_{\zeta_{lam}}$ depends strongly on the Damköhler number, particularly in the preheat zone. At this point, we cannot make a conclusion on the dependency on Lewis number since we are not able to separate the effects of the turbulence and the effects of thermo-diffusive instabilities.

In order to get more information on the role of the mixing on the structure of the flame, the product $\widetilde{P}(\zeta;\widetilde{c}).N_\zeta$ is extracted from the DNS for $Le = 1.0$ at $t/\tau_0 = 4.5$. Fig. 7 shows $\widetilde{P}(\zeta;\widetilde{c}).N_\zeta$ (non-dimensionalized by τ_{ch}) as a function of ζ

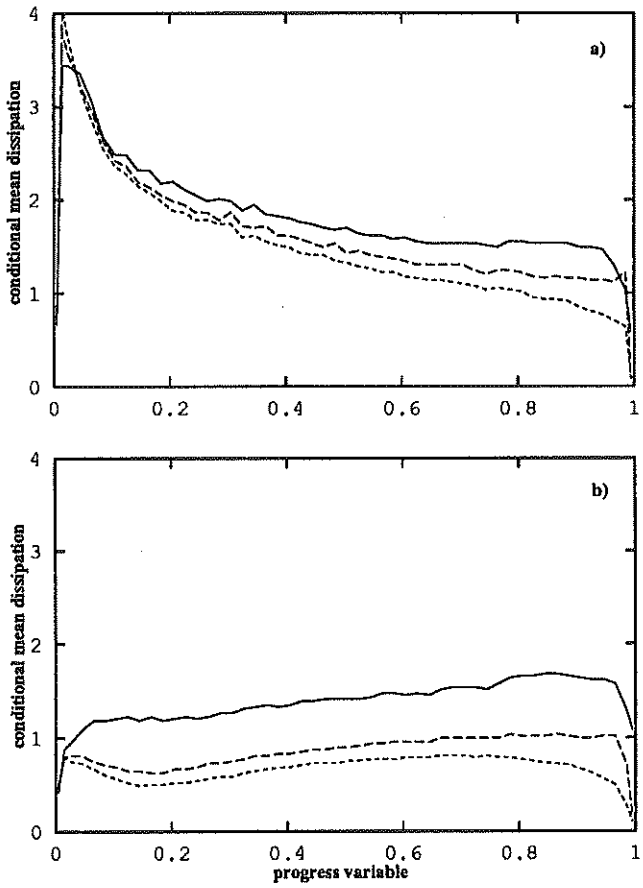

FIGURE 6. Profiles of $N_\zeta/N_{\zeta_{lam}}$ versus ζ. a) $t/\tau_0 = 1.4$ - b) $t/\tau_0 = 4.5$ $Le = 0.8$: ——— ; $Le = 1.0$: ---- ; $Le = 1.2$: ------

at different locations across the flame front. It appears that the dissipation occurs almost everywhere in the progress variable space, but most of it takes place in the reaction zone associated with values of ζ comprised between 0.6 and 0.9. Higher dissipation occurring in the preheat zone is only observed in regions of the turbulent flame located near the fresh gases.

The density-weighted pdf $\widetilde{P}(\zeta)$ is shown in Fig. 8 for different sections of the flame brush at different instants and Lewis number. For all the cases studied here, the pdf $\widetilde{P}(\zeta)$ exhibits a strong bimodal shape corresponding to fresh and fully burnt gases. However, $\widetilde{P}(\zeta)$ is not purely bimodal and a broad peak on the fresh gas side (which characterizes regions of the flame brush where instantaneous flame fronts are thickened) is observed. Between these two peaks (for $0.3 \leq \zeta \leq 0.9$), the shape of $\widetilde{P}(\zeta)$ is rather flat and ranges from 0.2 to 0.8. This represents intermediate events occurring in the instantaneous flame fronts. This behavior can be expected according to the schematical description given in Fig. 1 concerning the regime of

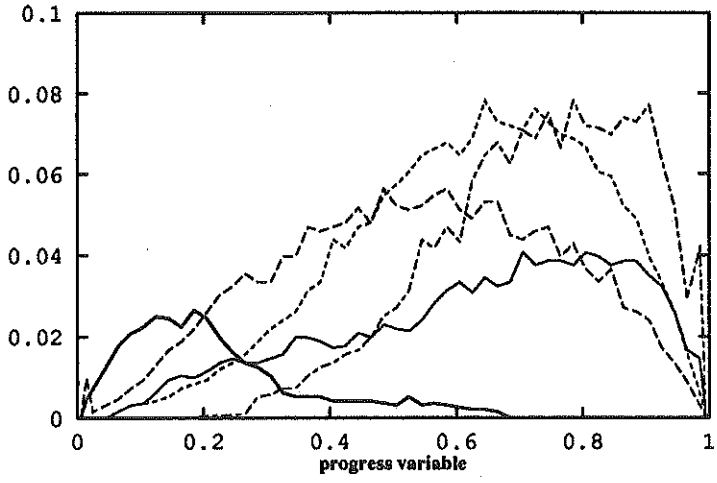

FIGURE 7. Evolution of $\widetilde{P}(\zeta).N_\zeta$ (non-dimensionalized by τ_{ch}) versus ζ across the flame front at $t/\tau_0 = 4.5$ and $Le = 1.0$. $\widetilde{c} = 0.05$: ——— ; $\widetilde{c} = 0.25$: ---- ; $\widetilde{c} = 0.5$: ------ ; $\widetilde{c} = 0.75$: — — — ; $\widetilde{c} = 0.95$: ———

propagations of these flames.

Since most of the available data for turbulent premixed combustion are obtained using unconditional statistics, it is of interest to calculate unconditional variables from their conditional values. The unconditional statistics for a variable Q can be directly obtained from the conditional value $\langle Q \mid \zeta \rangle$ and the probability density function $\widetilde{P}(\zeta)$:

$$\widetilde{Q} = \int_0^1 \langle Q \mid \zeta \rangle \widetilde{P}(\zeta) d\zeta \tag{18}$$

If $\langle Q \mid \zeta \rangle$ is known, it appears that the pdf $\widetilde{P}(\zeta)$ has to be carefully estimated. As we said in the introduction, the pdf $\widetilde{P}(\zeta)$ can be directly obtained by solving its transport equation (an expression for $\widetilde{P}(\zeta)$ can be found in Borghi 1988, Pope 1985-b) or estimated by assuming realistic shapes for $\widetilde{P}(\zeta)$ (Borghi 1988, Bray 1980) and predicting only its first two moments, $\widetilde{c}$ and $\widetilde{c''^2}$.

A way to estimate $\widetilde{P}(\zeta)$ is to choose a β function as proposed by Janicka & Kollmann (1978):

$$\widetilde{P}(\zeta) = \frac{\zeta^{a-1}(1-\zeta)^{b-1}}{\displaystyle\int_0^1 \zeta^{a-1}(1-\zeta)^{b-1} d\zeta} \tag{19}$$

with $a = \widetilde{c}\left(\dfrac{\widetilde{c}(1-\widetilde{c})}{\widetilde{c''^2}} - 1\right)$ and $b = a\dfrac{1-\widetilde{c}}{\widetilde{c}}$. Fig. 9 represents the comparison between the pdf $\widetilde{P}(\zeta)$ given by the DNS and the pdf estimated from Eq. (19) for different positions across the turbulent flame brush. The parameters a and b are calculated using $\widetilde{c}$ and $\widetilde{c''^2}$ extracted from the DNS. The agreement between the

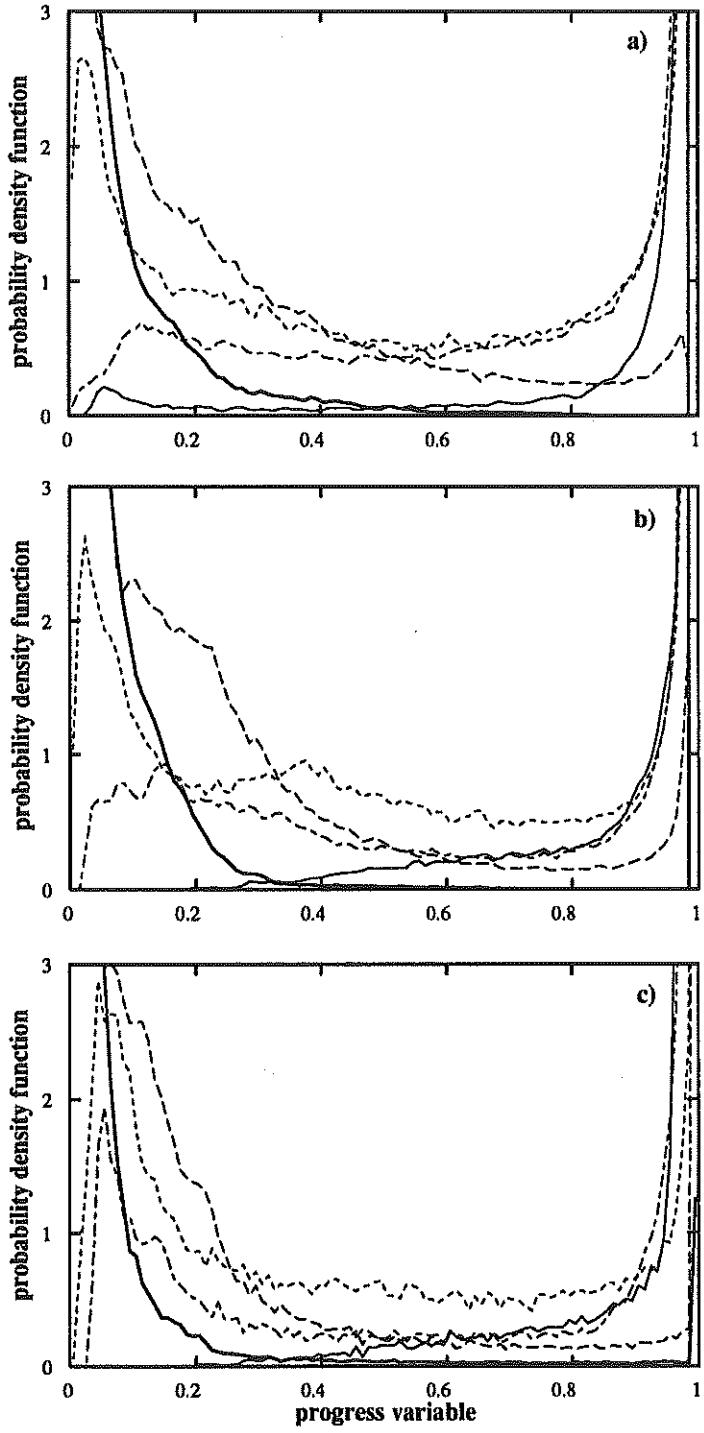

FIGURE 8. The pdf $\widetilde{P}(\zeta)$ versus ζ at: a) Le = 1.0 - t/τ_0 = 1.4, b) Le = 1.0 - t/τ_0 = 4.5, c) Le = 0.8 - t/τ_0 = 4.5. $\widetilde{c} = 0.05$: ——— ; $\widetilde{c} = 0.25$: - - - - ; $\widetilde{c} = 0.5$: ····· ; $\widetilde{c} = 0.75$: — - — ; $\widetilde{c} = 0.95$: ———

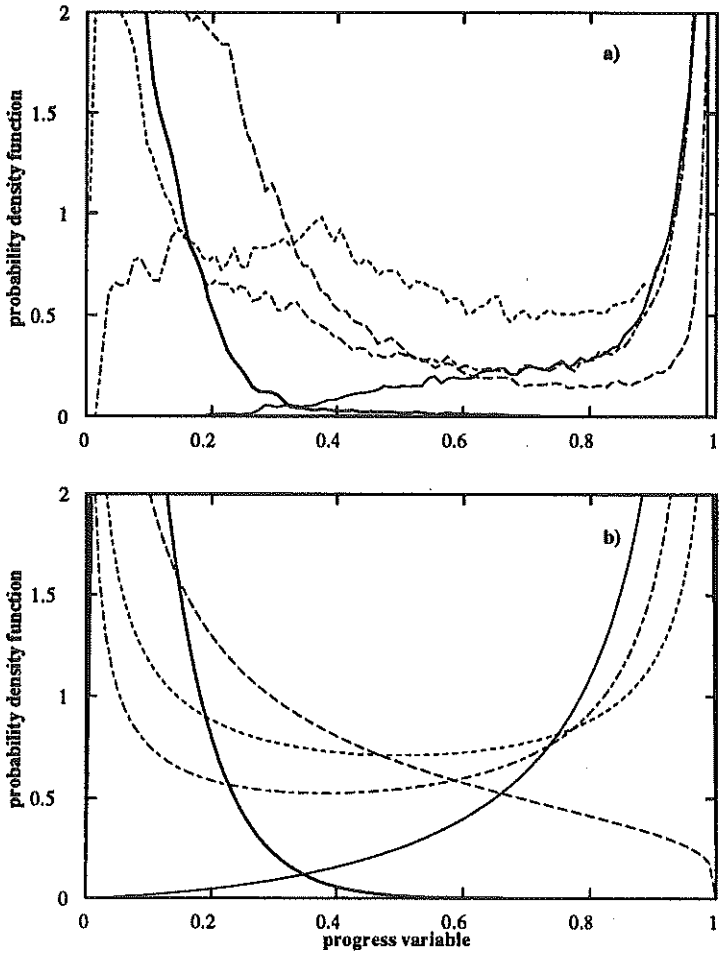

FIGURE 9. Profiles of the pdf $\widetilde{P}(\zeta)$ versus ζ across the turbulent flame front at $Le = 1.0$ and $t/\tau_0 = 4.5$. a): DNS ; b): β function. $\widetilde{c} = 0.05$: ——— ; $\widetilde{c} = 0.25$: - - - - ; $\widetilde{c} = 0.5$: ····· ; $\widetilde{c} = 0.75$: — - — ; $\widetilde{c} = 0.95$: ———

DNS and the model of Eq. (19) is relatively satisfying for each of the five sections studied across the turbulent flame front. The β function constitutes an interesting approach to estimating $\widetilde{P}(\zeta)$ in a presumed pdf approach applied to turbulent premixed combustion.

As we have already mentioned, the pdf $\widetilde{P}(\zeta)$ appears strongly bimodal, but a significant fraction of events occurs between the two spikes located at $\zeta = 0$ and $\zeta = 1$. This is probably a consequence of the low Damköhler number. Thus, the pdf present between $\zeta = 0$ and $\zeta = 1$ can become a crucial quantity in the estimation of some terms which are equal to 0 for $\zeta = 0$ and $\zeta = 1$. This is particularly the case for the conditional dissipation rate for which we have $\langle N_\zeta \mid \zeta = 0 \rangle = \langle N_\zeta \mid \zeta = 1 \rangle = 0$.

The unconditional dissipation rate defined by:

$$\widetilde{N} = \int_0^1 \langle N_\zeta \mid \zeta \rangle \widetilde{P}(\zeta) d\zeta \tag{20}$$

is strongly dependent on the value of $\widetilde{P}(\zeta)$ between the two spikes, especially when Da is low as in this DNS.

In order to estimate how far we are from a purely bimodal combustion regime, we have also studied the fluctuation level parameter g defined by Bray (1980):

$$g = \frac{\widetilde{c''^2}}{\widetilde{c}(1-\widetilde{c})} \tag{21}$$

This parameter varies from 0 for no fluctuation to 1, the maximum possible value corresponding to a purely bimodal pdf. In this last case, only fully burnt or fresh gases are present in the flow.

The results in Fig. 10 show that even if the level of fluctuations is high, g is significantly below the maximum value of 1.0. Thus, in some regions of the flow, intermediate states occurs quite frequently as has already been shown in Fig. 10-a where the pdf shows a plateau of about 0.5 when $\widetilde{c} = 0.5$.

Because different models for turbulent premixed combustion relate directly the mean reaction rate to $\widetilde{c}(1-\widetilde{c})$ and a suitable frequency, this result is important from a modeling point of view. In cases such as this, these models will overestimate the mean reaction rate. This is particularly the case in the Eddy Break-up formulation (Spalding 1971) and for the BML approach (Bray & Libby 1986). An alternative possibility is to directly calculate $\widetilde{c''^2}$ from its transport equation. However, this approach requires a good model for the dissipation rate $\widetilde{N}$, which is not an easy task. We have already discussed the difficulties and the different possibilities of estimating this quantity (Mantel & Borghi 1994, Said & Borghi 1988).

2.4.2 The conditional mean velocity

Like the conditional dissipation rate N_ζ, the conditional mean velocity $\langle U_k \mid \zeta \rangle$ appearing in Eq. (7) has to be modeled. Since very little is known concerning $\langle U_k \mid \zeta \rangle$, information from experimental data or from DNS is of interest in order to propose realistic closure for this term.

The conditional mean velocity $\langle U_k \mid \zeta \rangle$ can be obtained from the conditional pdf $P(V_k \mid \zeta)$ of U_k and c:

$$\langle U_k \mid \zeta \rangle = \int_{-\infty}^{\infty} V_k P(V_k \mid \zeta)\, d\zeta\, dV_k \tag{22}$$

where V_k represents the stochastic vector variable related to the velocity vector $U_k(x_k, t)$. According to Bayes theorem, $P(V_k \mid \zeta)$ is obtained from the joint pdf of V_k and ζ $P(V_k; \zeta)$ and the pdf for ζ $P(\zeta)$:

$$P(V_k \mid \zeta) = P(V_k; \zeta)/P(\zeta) \tag{23}$$

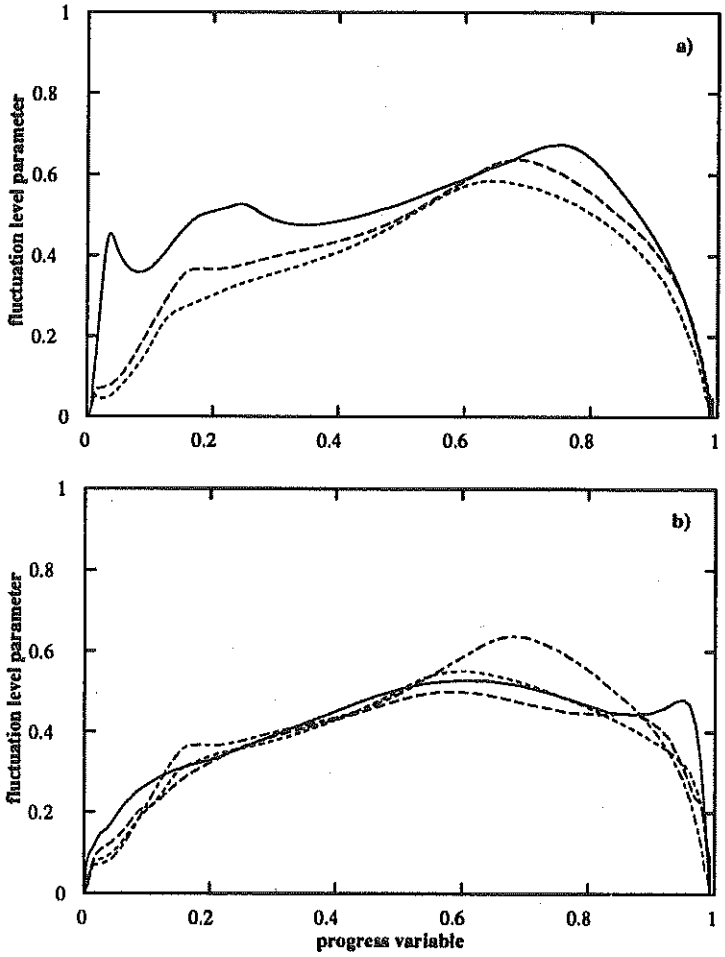

FIGURE 10. Variation of the fluctuation level parameter g versus $\widetilde{c}$. Same legend as in Fig. 2.

The joint pdf of V_k and ζ can be modeled by presuming realistic shapes for P (Borghi & Dutoya 1978) or by calculating its transport equation (see Pope 1981-1985 for the derivation and the modeling of this equation).

The conditional mean velocity can be extracted from the DNS for the different available cases. Since in the y and z directions the conditional mean advection term is zero from homogeneity, only the conditional mean velocity in the direction of propagation of the flame (x direction) is investigated.

Fig. 11 represents the variation of the conditional velocity $\langle U_1 \mid \zeta \rangle$ across the turbulent flame front for different values of ζ. During the simulation, the velocity conditioned on the fresh gases is higher than the one conditioned in the burnt gases. Thus, the slip velocity (which is the difference between the mean velocity conditioned in the burnt gases and the mean velocity conditioned in the fresh gases) is always negative and indicates that the flame displacement is strongly correlated

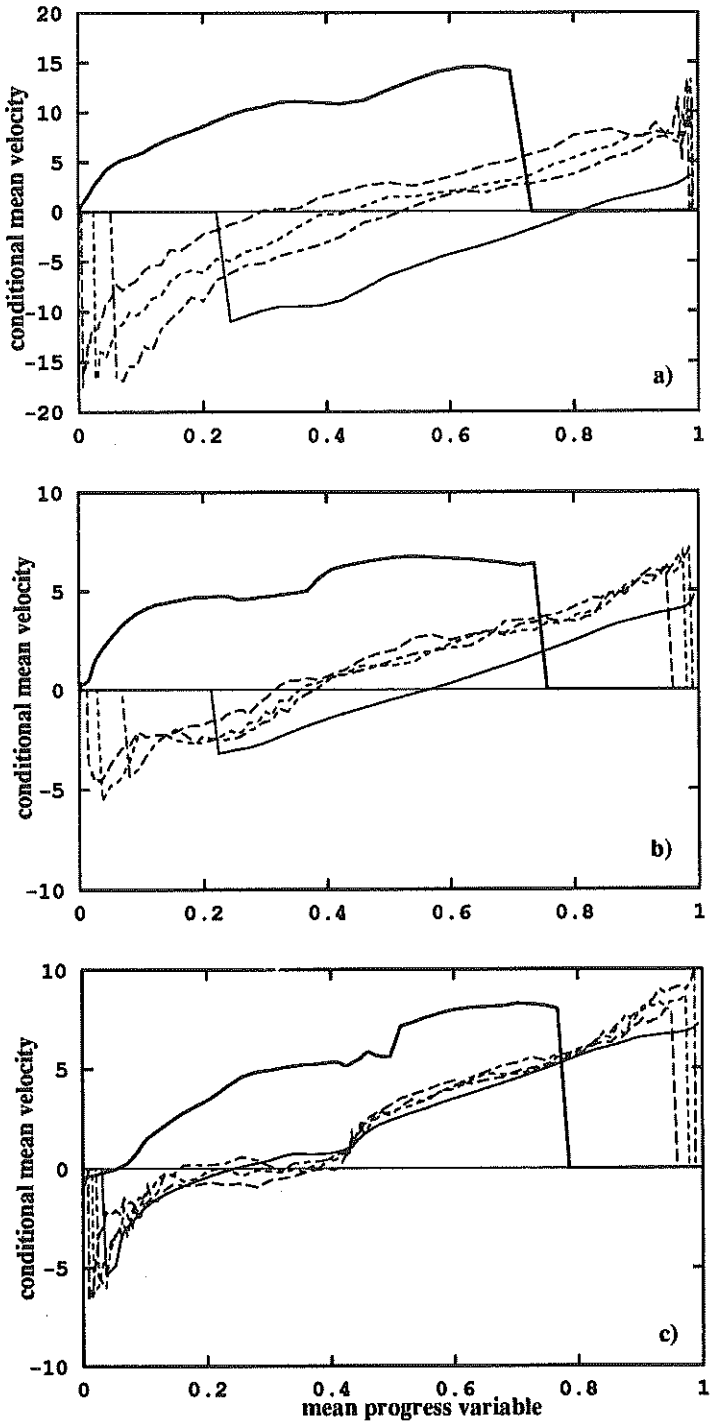

FIGURE 11. Profiles of $\langle U_1 \mid \zeta \rangle$ versus $\widetilde{c}$. a) Le = 1.0 - t/τ_0 = 1.4 b) Le = 1.0 - t/τ_0 = 4.5 c) Le = 0.8 - t/τ_0 = 4.5. ζ = 0.0: ——— ; ζ = 0.25: ---- ; ζ = 0.5: ------ ; ζ = 0.75: — — — ; ζ = 1.0: ———

with the velocity fluctuations in the unburnt gas. Thus, on most part of the flame front, the burnt gases are animated with negative velocities (toward the fresh gases) whereas the fresh gases move with positive velocities (toward the burnt gases). In the turbulent flame front, fingers of fresh gases appear in the burnt gases (and conversely).

We can also notice only a slight acceleration of the gases through the laminar flame front. All the isopleth contours are moved with the same displacement velocity. This is probably due to the fact that the pressure difference across the instantaneous flame front is insufficient to produce significant acceleration of the fluid through the instantaneous flame front in the x direction. Acceleration of the burnt gas occurs in the mean pressure gradient across the turbulent flame brush as a whole rather than in the instantaneous flame fronts. It seems that the instantaneous flame fronts adjust themselves to provide dilatation without acceleration. If this finding is sustained in other studies, it could be an important hypothesis on which to base a new approach to the theory of turbulent premixed flame propagation. It is evident that the variation of $\langle U_1 \mid \zeta \rangle$ through the flame brush will be significant in CMC modeling.

2.4.3 Turbulent diffusion fluxes

In turbulent combustion modeling, the turbulent fluxes of the mean progress variable are classically closed using a gradient transport approximation:

$$-\widetilde{u_k'' c''} = \frac{\nu_t}{Sc_t} \frac{\partial \widetilde{c}}{\partial x_k} \tag{24}$$

where ν_t is the eddy viscosity and Sc_t a Schmidt number. From previous studies, it is known that such modeling is not always sound for turbulent premixed flames (Borghi & Dutoya 1978, Libby & Bray 1981, Mantel & Borghi 1994, Moss 1980). Both Dutoya & Borghi (1978) and Mantel *et al.* (1993) found that the Schmidt number Sc_t is not constant and varies significantly across the turbulent flame front. Moreover, the modeling of the turbulent flux strongly affects the structure of the turbulent flame brush. In their study, Mantel *et al.* (1993) show that the turbulent flame thickness is over-estimated by about 50% by the gradient transport approximation. Libby & Bray (1981) have even formulated a model for counter-gradient diffusion due to the large variation of density occurring in reactive flows in accordance with the experimental results of Moss 1980). With a sufficiently high heat release ($\tau = T_b/T_u - 1 > 3$), the authors show that a pressure gradient present in the flow can preferentially accelerate the low density gases and then create counter-gradient diffusion processes. However, the pressure gradient is not the only candidate able to provoke counter-gradient diffusion. In a recent study, Trouvé *et al.* (1994) show that while counter-gradient diffusion is present at low turbulence, in the presence of strong turbulence the flame brush tends to become more and more wrinkled and thickened, leading to classical gradient diffusion transport. The authors also show that the wrinkling of the turbulent flame brush is a crucial parameter controlling gradient and counter-gradient diffusion.

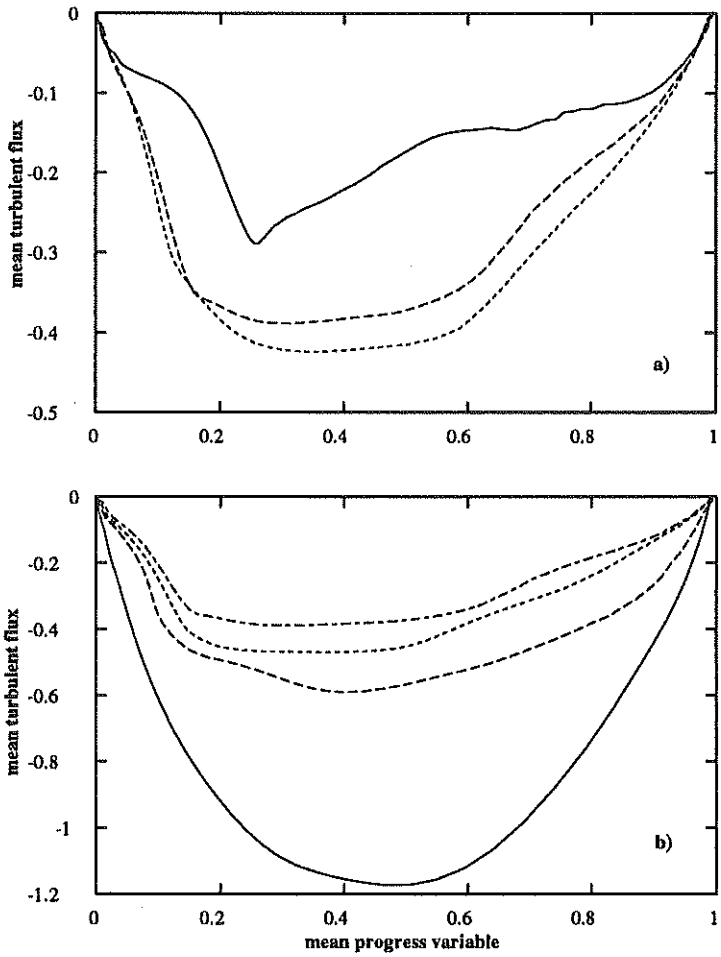

FIGURE 12. Profiles of $\widetilde{u''c''}$ versus $\widetilde{c}$. Same legend as in Fig. 2.

From the DNS, we have computed the turbulent fluxes $\widetilde{u''c''}$ and $\widetilde{u''c''^2}$ across the flame brush at different times of the interaction and Lewis number (see Figs. 12 and 13). For the same heat release as in Libby & Bray (1981), no counter-gradient diffusion is observed for $\widetilde{u''c''}$ from the DNS. Similarly, no counter-gradient diffusion is observed for the turbulent flux $\widetilde{u''c''^2}$.

3. Conclusion

Conditional statistics for the scalar dissipation N_ζ and the mean velocity $\langle U_1 \mid \zeta \rangle$ have been extracted from direct numerical simulation. The simulations used in this study have been performed by Trouvé & Poinsot (1994) and describe the interaction between a premixed flame with realistic heat release and an isotropic decaying turbulent flow field. The turbulence intensity is at the high end of the range of interest and the Damköhler numbers at the low end.

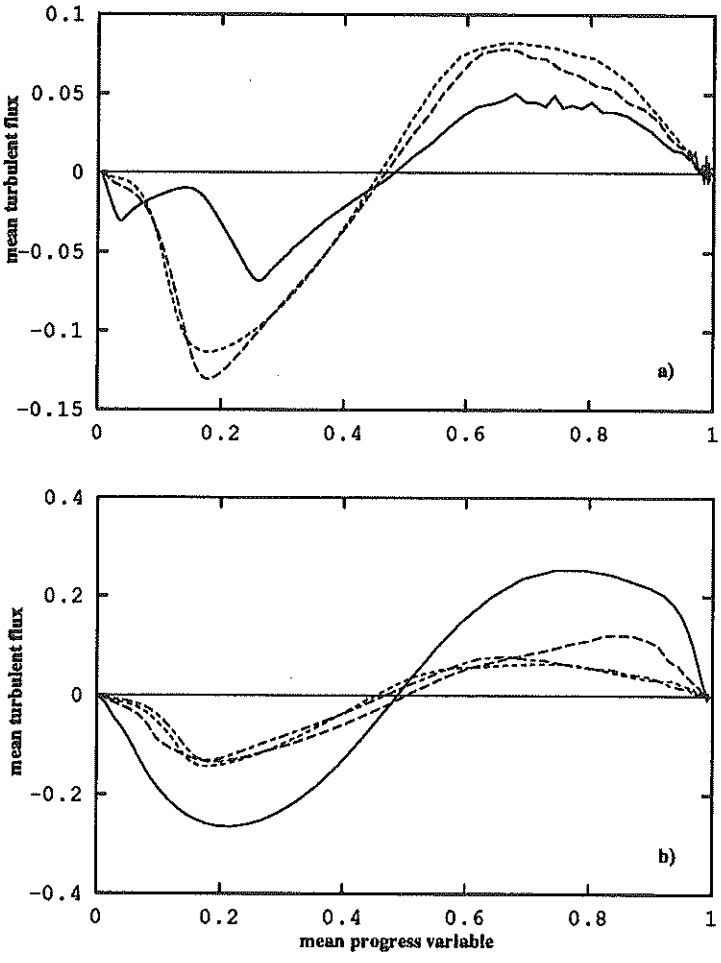

FIGURE 13. Profiles of $\widetilde{u''c''}$ versus $\widetilde{c}$. Same legend as in Fig. 2.

The conditional scalar dissipation N_ζ behaves differently in different parts of the instantaneous flame fronts. In the reaction zone, N_ζ is weakly affected by the turbulent mixing whereas in the preheat zone, the local gradients of the progress variable ζ are steeper due to the stretch effects which tend to increase N_ζ. This is particularly notable when the Damköhler number is low. As the time goes on, Da increases (due to the decay of the turbulence in the simulations), and locally, the instantaneous flame fronts resemble more the laminar flamelet.

As expected from the heat release, the conditional mean velocity (x-component) $\langle U_1 \mid \zeta \rangle$ evolves almost linearly through the turbulent flame brush. We also notice a negative slip velocity, which characterizes the wrinkling of the turbulent flame. We found that in this simulation, burnt gases are moved towards the fresh gases and vice versa, producing a highly wrinkled flame as can be observed in Trouvé & Poinsot (1994). Due to a weak local pressure gradient, only a slight acceleration of the gases across the instantaneous flame fronts is observed.

The weighted pdf $\widetilde{P}(\zeta)$ derived from the DNS shows a strongly bimodal shape (for $\zeta = 0$ and $\zeta = 1$). Between these two peaks, non-negligible values for $\widetilde{P}(\zeta)$ are observed (typically 0.2) which characterize intermediate states. A satisfying agreement is observed between $\widetilde{P}(\zeta)$ estimated from a β function and $\widetilde{P}(\zeta)$ extracted from the DNS.

The turbulent fluxes $\widetilde{u_1''c''}$ and $\widetilde{u_1''c''^2}$ across the flame brush are derived from the DNS. Contrary to previous studies (Libby & Bray 1981, Moss 1980), no counter-gradients have been found in these simulations. According to the recent study of Trouvé *et al.* (1994), the presence of a strong wrinkling of the turbulent flame brush is more favorable to gradient diffusion.

The present study constitutes a first analysis of conditional statistics in premixed turbulent flames. Further experimental and numerical studies have to be done in order to provide new information, notably at higher Reynolds and Damköhler numbers.

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