Dynamics and structure of turbulent premixed flames

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1. Motivation and objectives

In earlier work (Mantel & Bilger, 1994) the structure of the turbulent premixed flame was investigated using statistics based on conditional averaging with the reaction progress variable as the conditioning variable. The DNS data base of Trouvé and Poinsot (1994) was used in this investigation. Attention was focused on the conditional dissipation and conditional axial velocity in the flame with a view to modeling these quantities for use in the conditional moment closure (CMC) approach to analysis of kinetics in premixed flames (Bilger, 1993). Two remarkable findings were made: there was almost no acceleration of the axial velocity in the flame front itself; and the conditional scalar dissipation remained as high, or higher, than that found in laminar premixed flames. The first finding was surprising since in laminar flames all the fluid acceleration occurs through the flame front, and this could be expected also for turbulent premixed flames at the flamelet limit. The finding gave hope of inventing a new approach to the dynamics of turbulent premixed flames through use of rapid distortion theory or an unsteady Bernoulli equation. This could lead to a new second order closure for turbulent premixed flames. The second finding was contrary to our measurements with laser diagnostics in lean hydrocarbon flames where it is found that conditional scalar dissipation drops dramatically below that for laminar flamelets when the turbulence intensity becomes high. Such behavior was not explainable with a one-step kinetic model, even at non-unity Lewis number. It could be due to depletion of H2 from the reaction zone by preferential diffusion. The capacity of the flame to generate radicals is critically dependent on the levels of H2 present (Bilger, *et al.*, 1991). It seemed that a DNS computation with a multistep reduced mechanism would be worthwhile if a way could be found to make this feasible.

Truly innovative approaches to complex problems often come only when there is the opportunity to work close at hand with the (in this case numerical) experimental data. Not only can one spot patterns and relationships in the data which could be important, but one can also get to know the limitations of the technique being used, so that when the next experiment is being designed it will address resolvable questions. A three-year grant from the Australian Research Council has enabled us to develop a small capability at the University of Sydney to work on DNS of turbulent reacting flow, and to analyze data bases generated at CTR. Collaboration between the University of Sydney and CTR is essential to this project and finding

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a workable *modus operandum* for this collaboration, given the constraints involved, has been a major objective of the past year's effort.

The overall objectives of the project are: (1) to obtain a quantitative understanding of the dynamics of turbulent premixed flames at high turbulence levels with a view to developing improved second order closure models; and (2) to carry out new DNS experiments on turbulent premixed flames using a carefully chosen multistep reduced mechanism for the chemical kinetics, with a view to elucidating the laser diagnostic findings that are contrary to the findings for DNS using one-step kinetics. In this first year the objectives have been to make the existing CTR data base more accessible to coworkers at the University of Sydney, to make progress on understanding the dynamics of the flame in this existing CTR data base, and to carefully construct a suitable multistep reduced mechanism for use in a new set of DNS experiments on turbulent premixed flames.

2. Accomplishments

2.1 Accessing the data base

A Fortran 77 program has been written that allows easy access to the DNS data base of Trouvé and Poinsot (1994) from the computers at NAS and also allows efficient computation of derivatives of the data and conditional statistics. It can also be used on the DEC Alpha workstations used at the University of Sydney for this work, but with the limitation that data transfer and storage is limited and further coding has to be written for converting the subroutines that calculate derivatives. So far we have only one field at one time for the unity Lewis number case available in Sydney at 32-bit accuracy. Some processing has been achieved with this at Sydney, but more memory is needed before we can do processing that requires several arrays to be stored at the one time. A further 64 MBytes of RAM will become available soon and this will remove this limitation. It is proposed to write most of the Trouvé and Poinsot data base on tape at 32 bit accuracy and transport it to Sydney in this form.

2.2 Dynamics of the flame

2.2.1 Introduction

During the time that the senior research fellow (Bilger) was at CTR, a good deal of progress was made investigating the velocity and pressure field in the Trouvé and Poinsot flame. It was found that the pressure difference across this flame is small and the acceleration of the mean flow comes from the normal Reynolds stress. This dominance of the normal Reynolds stress makes it seem likely that the use of rapid distortion theory or an unsteady Bernoulli equation will not be successful.

Efforts to progress further were frustrated by apparent anomalies in any balances that contained the reaction rate. This problem took some time to uncover as most balances involve time dependent terms, and these were unavailable without running the original code, the new Fortran 90 version not then being available. The flame is not statistically stationary and the time dependent term in any averaged equation can be quite significant. An equation for the dilatation in the flow was derived which

has no unsteady term, and this showed that there was an error in the parameters being used. This has only been cleared up in the last month or so. The limitations on accessing the data base at Sydney are such that limited processing has only been possible up to now, but it is expected that this problem will be overcome soon.

The results for the dilatation equation are interesting in themselves and are presented here in detail.

2.2.2 Dilatation equation

Instantaneous reaction rate in turbulent flows is related to local value of scalar dissipation rate as demonstrated by Bilger (1976) in the fast chemistry limit and by Peters (1983) for finite rate chemistry for diffusion flames. In the high *Da* (Damkohler number) limit, Bray (1980) showed the same dependency for premixed flames. Hence, scalar dissipation rate is a crucial quantity in reacting flows. Recently, this quantity has attracted a quite a few modeling studies (Chen *et al.* 1989, Girimaji 1992). Mantel and Bilger (1994) analyzed DNS data base of Trouvé and Poinsot (1994) to comprehend the behavior of scalar dissipation rate in turbulent premixed flames. They observed that the behavior of scalar dissipation rate is independent of the position inside the turbulent flame brush. Here, we demonstrate that the conditional scalar dissipation rate can be obtained from the conditional dilatation equation for premixed flames, knowing the probability density function of the progress variable.

To ease the comparisons of the results with DNS, we make all the quantities in the following discussion dimensionless, unless otherwise specified, by using acoustic scales as in Trouvé and Poinsot (1994). One can write the mass conservation equation as

$$\nabla \cdot \mathbf{u} = \rho \frac{\partial (1/\rho)}{\partial t} + \rho \mathbf{u} \cdot \nabla (1/\rho), \tag{1}$$

where ρ and $\mathbf{u}$ respectively denote density and velocity vector. By making use of the equation of state and defining the reaction progress variable c as

$$c = (T - T_u)/(T_b - T_u) = \frac{1-\alpha}{\alpha} \left[(\gamma - 1)T - 1 \right],$$

where α is a heat release parameter (Williams 1985), one can write Eq. (1) as

$$\nabla \cdot \mathbf{u} = \frac{\alpha}{1-\alpha} \left[\rho \frac{\partial c}{\partial t} + \rho \mathbf{u} \cdot \nabla c \right]. \tag{2}$$

Substituting the governing equation for c in Eq. (2), one can obtain

$$\nabla \cdot \mathbf{u} = \frac{\alpha}{1-\alpha} \left[\dot{\omega}_c + \frac{1}{RePr} \nabla \cdot \mu \nabla c \right], \tag{3}$$

where $\dot{\omega}_c$ and μ are respectively the reaction rate of c and the local dynamic viscosity of the fluid (Trouvé & Poinsot 1994). This equation is referred to as the dilatation
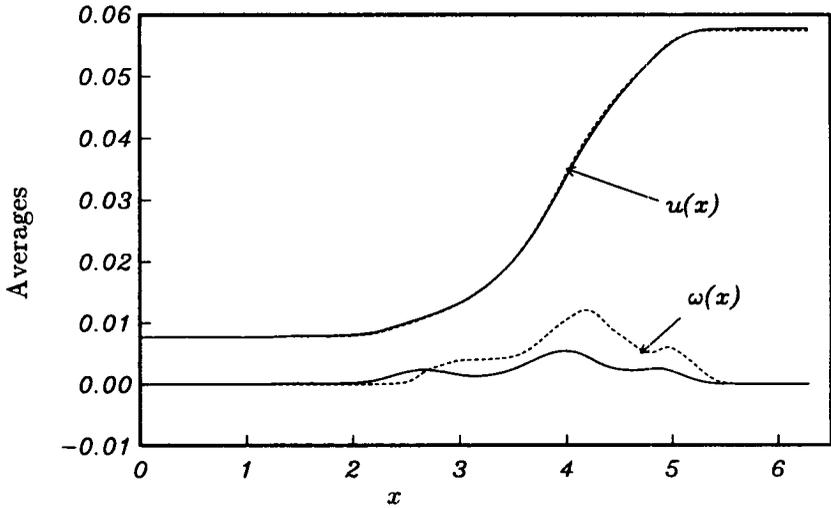
FIGURE 1. Variation of average velocity ($\bar{u}$), reaction rate ($\bar{\dot{\omega}_c}$), and diffusive flux along the inhomogeneous direction x. $\bar{u}$: ——— , DNS; - - - - , Eq.(4), unmarked line diffusive flux. See equation (4).

equation in the following discussions. Averaging this equation, after noting the statistical one-dimensionality of the DNS (Trouvé & Poinsot 1994), yields

$$\bar{u}(x,t) = \bar{u}(-\infty,t) + \frac{\alpha}{1-\alpha}\int_{-\infty}^{x}\bar{\dot{\omega}_c}(x',t)dx' + \frac{\alpha}{1-\alpha}\frac{1}{RePr}\overline{\mu\partial c/\partial x}. \qquad (4)$$

The average velocity $\bar{u}(x,t)$ obtained from the above equation is compared with DNS results in Fig. 1 for $Re = 1000, Pr = 0.75, Le = 1$, and $\alpha = 0.75$ at $t = 4.5$. Time is dimensionless with respect to initial eddy turnover time (Trouvé & Poinsot 1994). The agreement is excellent and encourages us to proceed further.

2.2.3 Conditional dilatation equation

Following Klimenko (1990), the conditioning process can be expressed using a Dirac delta function $\Psi = \delta(c[\mathbf{x},t] - \zeta)$, where c and ζ are respectively progress variable and its sample space variable. Using this notation, the conditional average of any quantity B can be written as $< B\Psi > = < B|\zeta > P_\zeta$, where P_ζ denote the probability density function of progress variable. After applying the rules for the differentiation of the delta function, we can obtain the conditional dilatation equation as

$$\nabla \cdot [< \mathbf{u}|\zeta > P_\zeta] = -\frac{\partial}{\partial \zeta}(< \mathbf{u}\cdot\nabla c|\zeta > P_\zeta) + \frac{\alpha}{1-\alpha} < \dot{\omega}_c|\zeta > P_\zeta$$
$$+ \frac{\alpha}{1-\alpha}\frac{1}{RePr}D_\zeta P_\zeta, \qquad (5)$$

where D_ζ is the conditional diffusion expressed as $D_\zeta = < \nabla \cdot \mu \nabla c | \zeta >$. For statistically 1-D flow (as in the DNS) Eq. (5) can be written as

$$
\begin{aligned}
D_\zeta P_\zeta &= RePr \frac{1-\alpha}{\alpha} \left[\frac{\partial}{\partial x} (< u | \zeta > P_\zeta) + \frac{\partial}{\partial \zeta} (< \mathbf{u} \cdot \nabla c | \zeta > P_\zeta) \right] \\
&\quad - RePr < \dot{\omega}_c | \zeta > P_\zeta \qquad\qquad\qquad\qquad\qquad\qquad (6) \\
&= \frac{\partial}{\partial \zeta} (N_\zeta P_\zeta) + \frac{\partial}{\partial x} \left(< \mu \frac{\partial c}{\partial x} | \zeta > P_\zeta \right) \simeq \frac{\partial}{\partial \zeta} (N_\zeta P_\zeta).
\end{aligned}
$$

The second part of the above equation is obtained by relating the conditional diffusion to conditional dissipation N_ζ. In principle, one can get the conditional dissipation rate from the above equation.

2.3 Multistep reduced mechanism

2.3.1 Formulation

Possibilities of direct numerical predictions of turbulent reacting flows, even in simple geometries, with multistep elementary kinetic mechanisms are remote with the current computational hardware. Hence, researchers often simplify the chemical reactions to a single global step. Direct simulations with single-step chemistry (Trouvé & Poinsot 1994, Swaminathan *et al.*, 1995, Givi 1989), although simplified in certain sense, have given us valuable insight into the different physical processes involved in reacting flows. To further our understanding, direct simulations with a systematically reduced kinetic scheme would be of great interest. Mahalingam *et al.* (1995) have simulated turbulent nonpremixed flames using a two-step chemical scheme which is similar to the Zeldovich-Liñan mechanism. Here, we present a systematically reduced two-step scheme (Peters & Williams 1987, Williams 1991) for hydrocarbon flames from the direct numerical simulation point of view.

Peters (1985) has shown the strategy of reducing full kinetics to a simplified four-step mechanism. Simplification strategy consists of order of magnitude arguments, steady state, and partial equilibrium approximations for appropriate minor species. This reduced mechanism has been used in computational (Bilger *et al.* 1990, Peters & Kee 1987) and asymptotic (Peters & Williams 1987, Seshadri & Peters 1988) studies of laminar flames. These studies improved our understanding of flame structure and extinction mechanisms. For example, a laminar diffusion flame modeled by a single global step extinguishes at high strain rates after allowing fuel to leak through the reaction zone, whereas studies with four-step chemistry indicate that the oxidizer leaks through the reaction zone due to radical depletion on its rich side. These differences indicate that direct simulations with a reduced mechanism would further improve our understanding of turbulent flames and thereby allow us to construct more accurate models for engineering predictions. Due to the computational requirements, we further reduce a four-step mechanism to two steps as discussed below. Reducing a full mechanism to four steps can be found elsewhere (Peters 1991, Bilger *et al.* 1990).

Table 1. Elementary steps involved and their rate constants

Step	Reaction	A	b	E
1	$CH_4 + H \longrightarrow CH_3 + H_2$	6.6E+08	1.6	10840.0
2	$CO + OH \rightleftharpoons CO_2 + H$	1.2E+07	1.4	-730.0
3	$H + O_2 + M \longrightarrow HO_2 + M$	3.6E+17	-0.72	0.0
4	$H + O_2 \rightleftharpoons OH + O$	8.3E+13	0.0	14413.0

$K = AT^b \exp[-E/RT]$, cal-mol-cm-sec-K

Here we start with the four steps given by Bilger *et al.* (1990). These four steps are

$$CH_4 + 2H + H_2O \longrightarrow CO + 4H_2 \qquad\qquad I$$

$$CO + H_2O \rightleftharpoons CO_2 + H_2 \qquad\qquad II$$

$$2H_2 + O_2 \longrightarrow 2H_2O \qquad\qquad III$$

$$3H_2 + O_2 \longrightarrow 2H_2O + 2H. \qquad\qquad IV$$
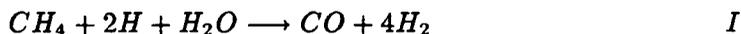
The rates of these four steps are given as linear combinations of some elementary reactions. Excluding all but the most elementary steps, the rate expression given by Bilger *et al.* (1990) can be expressed as

$$\dot{\omega}_I = \dot{\omega}_1, \qquad \dot{\omega}_{II} = \dot{\omega}_2,$$

$$\dot{\omega}_{III} = \dot{\omega}_3, \qquad \dot{\omega}_{IV} = \dot{\omega}_4,$$

where the roman and arabic subscripts respectively denote global and elementary steps. These elementary steps with their rate constants are given in Table 1.

The pressure dependence of elementary step 3 allows us to make a steady state approximation for H atom at pressures typically above one atmosphere. This assumption renders

$$[H]^2 = K_c \frac{[O_2][H_2]^3}{[H_2O]^2} \left[1 - \lambda \frac{[CH_4]}{[O_2]} \right], \qquad (7)$$

where K_c is a combination of equilibrium constants of elementary reactions involved in making partial equilibrium approximation of OH and steady state approximation for O atoms (Bilger *et al.* 1990, Peters & Kee 1987). The ratio of rate constants of elementary steps one to four is denoted by λ and its magnitude is about four for a temperature range of interest. Stoichiometry of the resulting reaction rate expressions of individual species lead us to a three-step mechanism given by (Peters & Williams 1987)

$$CH_4 + O_2 \longrightarrow CO + H_2 + H_2O$$

$$CO + H_2O \rightleftharpoons CO_2 + H_2$$

$$2H_2 + O_2 \longrightarrow 2H_2O.$$
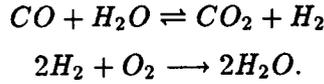
This mechanism can further be reduced to two steps by making partial equilibrium approximations for the water–gas shift reaction. With this assumption, the reaction rates of individual species are given as

$$\dot{\omega}_{CH_4} = -\dot{\omega}_I, \quad \dot{\omega}_{O_2} = -(\dot{\omega}_I + \dot{\omega}_{III})$$

$$\dot{\omega}_{H_2} = -2(\dot{\omega}_I - \dot{\omega}_{III})/(1 + \alpha), \quad \dot{\omega}_{CO} = -2\alpha(\dot{\omega}_I - \dot{\omega}_{III})/(1 + \alpha)$$

$$\dot{\omega}_{CO_2} = -[(1 - \alpha)\dot{\omega}_I + 2\alpha\dot{\omega}_{III}]/(1 + \alpha), \quad \dot{\omega}_{H_2O} = -2[\alpha\dot{\omega}_I + \dot{\omega}_{III}]/(1 + \alpha),$$

where α is ratio of CO to H_2 concentrations at partial equilibrium of water–gas shift reaction and is assumed to be a constant across the reaction zone. Stoichiometry coefficients in the above rate expressions give the two steps as

$$CH_4 + O_2 \longrightarrow \frac{2}{1 + \alpha}[H_2 + \alpha CO] + \frac{1 - \alpha}{1 + \alpha}CO_2 + \frac{2\alpha}{1 + \alpha}H_2O$$

$$O_2 + \frac{2}{1 + \alpha}[H_2 + \alpha CO] \longrightarrow \frac{2\alpha}{1 + \alpha}CO_2 + \frac{2}{1 + \alpha}H_2O.$$
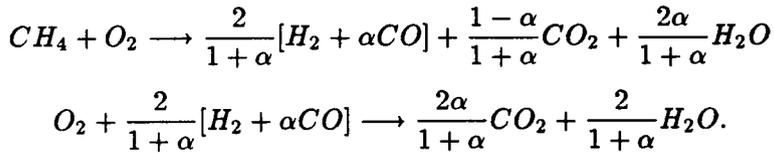
Laminar flame calculations (Bilger *et al.* 1991) with a skeletal mechanism suggest that α is $O(1)$. Hence the above two steps become

$$CH_4 + O_2 \longrightarrow [H_2 + CO] + H_2O$$

$$O_2 + [H_2 + CO] \longrightarrow H_2O + CO_2.$$
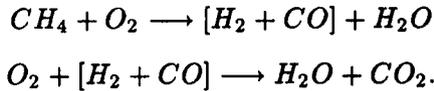
In this mechanism, $[H_2 + CO]$ clearly plays a role of intermediates. Hence, by denoting them as I, CH_4 as F, O_2 as Oxi, H as R, and the remaining species as product P, we get

$$F + Oxi \longrightarrow I + P \qquad\qquad I'$$

$$Oxi + I \longrightarrow 2P. \qquad\qquad II'$$

Reaction rates of these steps, according to the elementary reactions involved, are given as $\dot{\omega}_{I'} = K_1[F][R]$ and $\dot{\omega}_{II'} = K_3'[Oxi][R]$. Radical concentration $[R]$ is given by a modified form of Eq. (7) as suggested by Peters (1995):

$$[R] = K_r[Oxi]^{0.5}[I]^{1.5}\exp(-a\lambda[F]/[Oxi]),$$

where K_r is related to the equilibrium constant K_c, and a is a constant. This form is used to avoid the discontinuity which is implicit in the steady state approximation for H atom (see Eq. (7)) as this will give problems in DNS. By matching the flame speed eigen value for premixed flames (Peters & Williams 1987) or extinction scalar dissipation rate at stoichiometric mixture fraction for diffusion flames (Seshadri & Peters, 1988), one can obtain $a = \sqrt{15/4}$. One can also show that the first and second step of the above two-step mechanism release 40% and 60%, respectively, of the overall heat release. Structure of nonpremixed flames with the above two steps is presented in the following discussions.
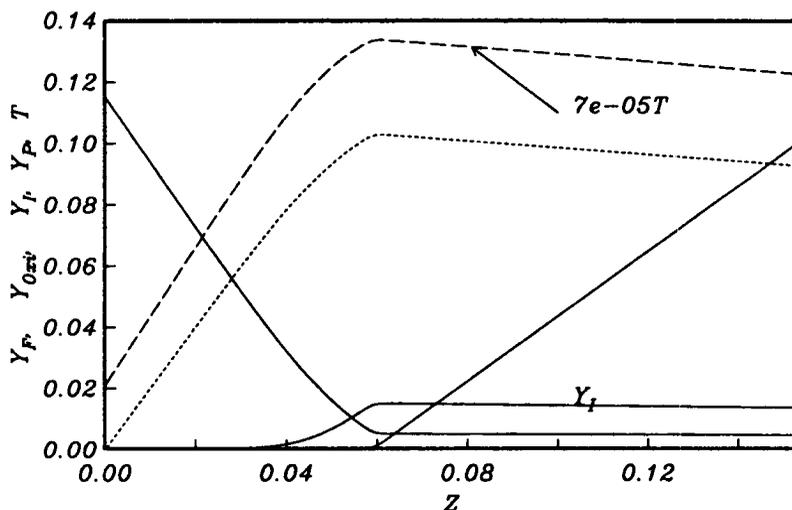
FIGURE 2.   Structure of a laminar (Tsuji) methane-air diffusion flame for a strain rate value of 100 sec^{-1}.
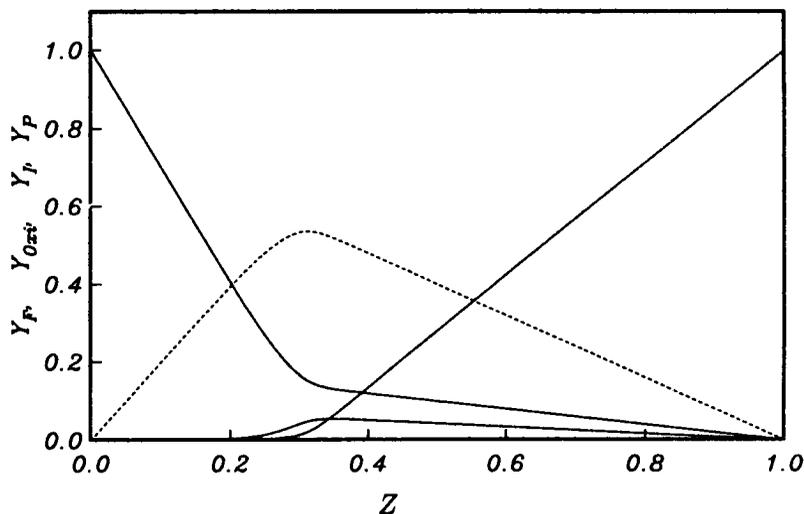
FIGURE 3.   Structure of a laminar diffusion flame used as an initial field for DNS of turbulent nonpremixed flame.

2.3.2 Nonpremixed flame structure

Calculation of Tsuji type laminar diffusion flames are carried out to understand the laminar flame structure and its relation to different rate constants involved. Figure 2 depicts the structure of a methane–air flame at a strain rate of 100 sec^{-1} in mixture fraction space.

The rate constants are derived from those given in Table 1. The specific moles are normalized by the free stream value of fuel species. Radical concentration is about ten times lower than the intermediate concentration. The intermediate is formed
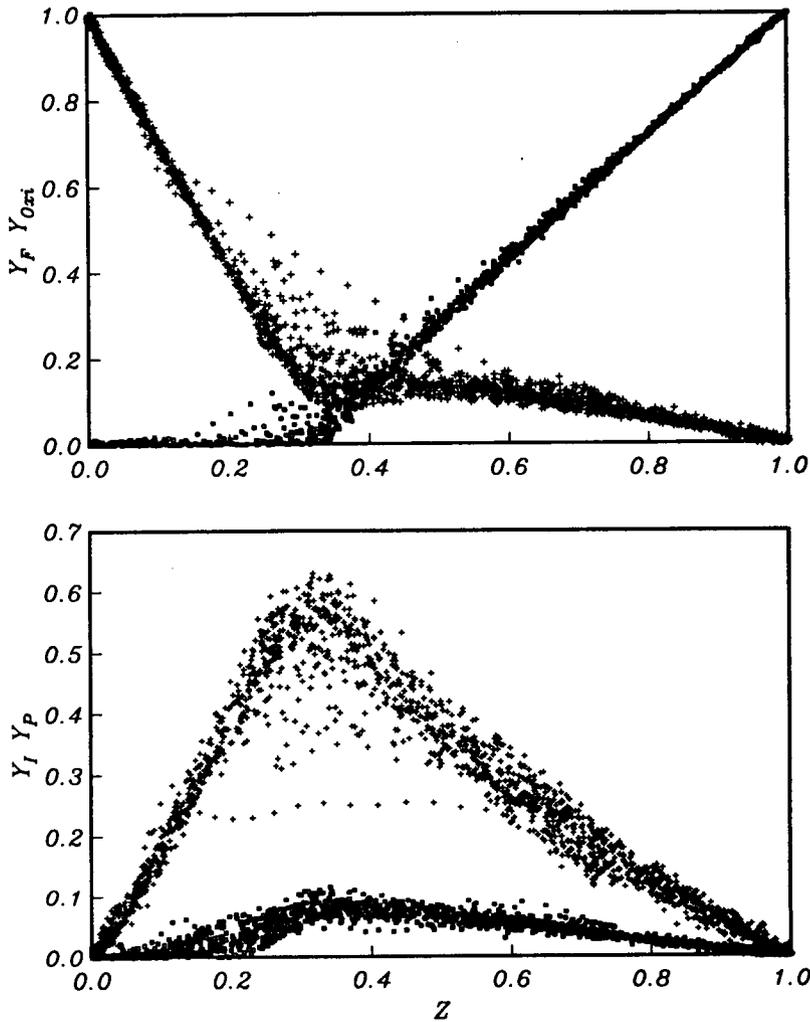
FIGURE 4.   Turbulent nonpremixed flame structure with two-step kinetics at $t = 1.5$. Time t is made dimensionless with eddy turnover time at scalar field initialization.

on the rich side of the reaction zone while it is consumed on the lean side. The maximum temperature is about 1900 K, while the free stream value is 300 K. The size of fuel depletion zone in mixture fraction space is about one fifth of oxidizer consumption zone. This flame structure is consistent with Bilger *et al.*'s (1991) calculation using a skeletal mechanism.

The value of stoichiometric mixture fraction can be increased, to ease resolution requirements in DNS, by diluting the reactant streams. The combination of an oxidizer stream having 50% O_2 and 50% N_2 by weight and a fuel stream of 25% methane and 75% Argon by weight has a mixture fraction stoichiometric value of

1/3. These mixtures have equal molecular weights and densities which are the same as that of air. These attributes are attractive for direct simulations of turbulent nonpremixed flames with low heat release. The structure of a laminar diffusion flame for the above reactants is shown in Fig. 3. The rate constants for this calculation are evaluated at 1800 K. This structure is used to initialize DNS calculations using a psuedospectral algorithm (Swaminathan *et al.* 1995). The structure of the turbulent flame in mixture fraction space is shown in Fig. 4 in the form of scatter plot. The scatter in the values of specific moles is due to unsteady effects. More analysis of this calculation is expected to guide us to design a better experiment.

3. Future work

Our immediate goal is to settle the parameter values to be used in the two-step reduced mechanism for DNS. Laminar and two-dimensional turbulent premixed flames will be tested with the new Fortran 90 compressible code (see Ruetsch and Broadwell 1995, Smith 1995), and then 'production' runs will be made in three dimensions with various values chosen for the Lewis number of the intermediate. The simulation conditions chosen will be similar to those of Trouvé and Poinsot but hopefully with an inflow boundary condition of non-decaying turbulence. Given sufficient computational resources, it is hoped that the 'production' runs can be completed in time for analysis in the 1996 CTR Summer Program.

We will also pursue the goal of making the whole of the existing data base available in Sydney. As soon as the expanded memory for our DEC Alpha is available we will return to analysis of the conditionally averaged momentum, energy, Reynolds stress, and Reynolds flux equations. It is still considered likely that a new approach to second order closure will be found.

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