Simulation of flame-turbulence interactions in premixed combustion

By A. Trouvé

1. Motivation and objectives

Turbulent combustion is a challenging problem of fundamental interest with numerous practical applications. Direct Numerical Simulation is an attractive tool that provides detailed information on flame-flow interactions and, thereby, provides an ideal basis for testing and developing turbulent combustion models. This report describes the work being undertaken to investigate the laminar flamelet concepts as applied to premixed combustion. More specifically, the present work examines the influence of non-unity Lewis number with emphasis on the effects of hydrodynamic straining and flame front curvature.

The following subsections give a short introduction to the flamelet modeling approach.

1.1 Validity of the flamelet approach

Premixed turbulent combustion is a rather vague terminology that is used to designate very different situations. Dimensional analysis shows that, depending on the flame and turbulent flow characteristic scales, different modes of combustion are expected: flamelets, distributed reaction zones, and well-stirred reactors (Borghi 1984, Peters 1986, Williams 1985). These different modes of combustion correspond to different topologies of the reaction zone (front, pockets, or large volumes) and, consequently, different modeling approaches are required.

Following Poinsot, Veynante and Candel (1990), the flamelet regime corresponds to a situation where the flame front is chemically active everywhere and no quenching occurs. In other words, fresh reactants and burnt products cannot diffuse and mix without triggering reaction. Recent results from direct numerical simulations (Poinsot *et al.* 1990) show that classical arguments based on dimensional analysis underestimate the resistance of flame fronts to flow perturbations. Furthermore, these results suggest that most practical situations feature a flamelet mode of burning.

The definition of a flamelet regime based on the occurrence of quenching is valuable and rigorous, but it is also quite academic. From a practical viewpoint, current flamelet models make use of several assumptions that turn out to be less restrictive or more restrictive than those implied by this definition:

• The domain of application of flamelet models is usually extended to regimes of partially quenched flames. For example, the Coherent Flame Model (Candel *et al.* 1988, Darabiha *et al.* 1989) accounts explicitly for extinction phenomena due to excessive strain. This can only be legitimate if flame quenching is somewhat limited to local effects and does not alter significantly the global picture implied by the flamelet approach (Meneveau and Poinsot 1990).

• Flamelet models use laminar submodels to describe the local properties of the reactive elements. This approach relies on two additional assumptions: each flame element retains an identifiable structure; this structure may be modeled like a laminar reaction zone. When the flame thickness is smaller than all turbulent length scales, flow perturbations acting on the flame zone may be viewed as external perturbations, and the structure of flame elements remains essentially laminar. However, when turbulent eddies are small enough to penetrate into the reaction zone, intuitive ideas suggest that the structure of flame elements may be disrupted in a way that precludes any analogy with laminar theory.

If this holds true, the domain of application of flamelet models is limited by requiring the flame thickness to be smaller than the Kolmogorov length scale. This would be a practical rather than a theoretical limitation. Note that in principle, improved submodels may be developed within the flamelet framework to account for the non laminar behavior of the flamelet elements. Also, it is worth emphasizing that at this stage, little is known on the dynamics of the turbulent small scales and their interactions with the flame zone. Finally, from a practical viewpoint, it remains to be shown how sensitive the results are to the accuracy of the chemical submodel. Therefore, this problem is essentially open.

1.2 Modeling of the mean reaction rate

In the flamelet approach, the reaction occurs in relatively thin layers, and the flame may be considered as a propagating surface separating fresh reactants from burnt products. In the following, we show that the mean reaction rate may then be modeled as a flux term. Let us first introduce the quantities that characterize the flame behavior:

• The turbulent flame speed is a global quantity that measures the mean reaction rate over an arbitrary domain V. For the sake of clarity, we assume that the mean position of the flame is stationary in V (the volume V travels with the flame). In that case, the turbulent flame speed is defined as the total fuel consumption rate in V divided by the total mass inflow of fuel into V:

$$S_T \equiv \frac{\int_V \dot{\omega}_R \, dV}{\rho_u Y_{R,u} \Sigma_0}, \tag{1}$$

where $\dot{\omega}_R$ is the mass of fuel consumed per unit time and per unit volume; ρ_u and $Y_{R,u}$ are respectively the density and the fuel mass fraction in the unburnt gas; Σ_0 is the area of the inlet boundary of V.

• The consumption speed S_C is a local property of the flame front that characterizes the local inner structure of the reaction zone. Assuming that a normal to the flame front can be defined everywhere without ambiguity, the local flame speed is defined by integrating the reaction rate along this normal direction:

$$S_C \equiv \frac{\int_{-\infty}^{+\infty} \dot{\omega}_R \, dn}{\rho_u Y_{R,u}}, \tag{2}$$

where n designates the flame normal direction.

Clearly, the mean reaction rate is determined by the distribution of the local flame speed S_C along the flame surface:

$$S_T = \frac{\int_{\Sigma_T} S_C \, d\Sigma_T}{\Sigma_0}, \tag{3}$$

where $d\Sigma_T$ designates the area of a flame surface element and Σ_T is the total flame surface area within V.

Furthermore, let us define the area-weighted mean of S_C along the flame surface:

$$\langle S_C \rangle = \frac{\int_{\Sigma_T} S_C \, d\Sigma_T}{\Sigma_T}, \tag{4}$$

Combining the last two expressions, it is seen that the turbulent flame speed is essentially a flux term and as such can be expressed as the surface mean of the local fuel consumption speed times the total flame surface area:

$$S_T = \frac{\langle S_C \rangle \, \Sigma_T}{\Sigma_0}, \tag{5}$$

Eq. (5) may be conveniently re-written in terms of the mean reaction rate:

$$\overline{\dot{w}} = \frac{\int_V \dot{\omega}_R \, dV}{V} = \langle \int_{-\infty}^{+\infty} \dot{\omega}_R \, dn \rangle \, \frac{\Sigma_T}{V}, \tag{6}$$

In Eq. (6), the mean reaction rate is the product of the mean fuel consumption rate per unit flame area times the flame surface density (defined as the flame surface per unit volume). Therefore, the closure problem for $\overline{\dot{w}}$ requires modeling of two basic quantities: a speed and a surface. To provide these quantities, two basic ingredients of flamelet models are introduced: (1) a chemical submodel that describes the local properties of reactive elements embedded in the turbulent flow and gives the mean consumption rate per unit flame area; (2) a balance equation for the flame surface density that represents turbulence effects (hydrodynamic straining, convection, turbulent diffusion) and propagation effects (collisions of flame elements, wrinkling, dewrinkling).

1.3 Turbulence acting on the flame: the role of strain

The flamelet ingredients are coupled to a description of the turbulent flow field based on standard transport equations for the flow variables and the main species. A central problem is then to relate the flame properties $\langle S_C \rangle$ and Σ_T to the turbulent flow properties.

An idea shared by all flamelet models is that turbulent straining acting on the flame zone plays an essential role (see Poinsot 1990 for a more detailed discussion of this matter). Strain modifies both the flamelet's structure and the flame surface density. These effects are represented in the models by a single scalar, a mean strain rate ϵ, that influences both quantities $\langle S_C \rangle$ and Σ_T in the following way: (1) $\langle S_C \rangle$ in the flamelet submodel is determined from an analysis of a laminar stagnation point flame where the speed of the counter-flowing reactants and products is adjusted according to the strain rate ϵ; (2) the balance equation for the flame surface density accounts for the stirring process due to turbulent motions through a source term that depends linearly on ϵ.

1.4 Objectives

As discussed in the previous section, flamelet models recognize the importance of strain. However, one shortcoming in these models is the absence of curvature effects. Since curvature is a geometrical parameter that directly affects molecular diffusion processes, a simple way to highlight the nature and importance of this parameter is to study premixed flames featuring different molecular transport properties for different scalars (chemical species, temperature).

The objective of the study of Rutland and Trouvé (1990) is precisely to examine the effects of differential diffusion of heat and chemical species as represented by a single, non-unity Lewis number, Le. This study was performed in collaboration with Prof. Rutland while he was participating in the CTR 1990 Summer Program.

2. Accomplishments

The influence of Lewis number was examined using Direct Numerical Simulation of three dimensional, constant density, decaying isotropic turbulence with a single step, irreversible, finite rate (Arrhenius law) chemical reaction. A modified version of the Rogallo code (1981) was used. More detailed information on the simulations may be found in Rutland (1989) and Rutland and Trouvé (1990). A similar investigation was conducted by Haworth and Poinsot (1990) with a finite difference, two-dimensional, variable density code. Interestingly enough, similar results were obtained. We summarize them in the following sections.

2.1 Curvature effects

Curvature is defined in planes tangent to the flame surface, positive curvature being convex towards the reactants. The main result from simulations is the strong correlation between the local fuel consumption speed S_C and the local flame curvature. This result is presented in the form of joint pdf's in Figure 1. For $Le = 1$, the flame exhibits a large insensitivity to curvature (Poinsot, Echekki and Mungal 1990), and no correlation is observed. For $Le < 1$, the local flame speed is increased (decreased) in regions of positive (negative) curvature. The opposite effect occurs for $Le > 1$.

Also, the pdf's of flame curvature are nearly symmetric with near-zero mean value. Since the correlation of S_C with curvature is roughly linear (Figure 1), curvature effects tend to cancel out in the mean. In other words, the mean flamelet speed $\langle S_C \rangle$ does not exhibit any significant dependence on curvature.

Furthermore, because the distribution of the flame speed S_C along the flame surface tells us about the way the flame propagates in the unburnt gas, these results also indicate that when $Le < 1$ ($Le > 1$), more (less) flame surface Σ_T is produced by turbulent motions.

2.2 Strain effects

Strain effects may already be seen in Figure 1 by slicing the joint pdf's along a line corresponding to zero curvature. When the curvature is zero, only strain effects remain. It is then seen that, depending on the value of the Lewis number, the local flame speeds are shifted from unity: decreased for $Le > 1$ and increased for $Le < 1$.

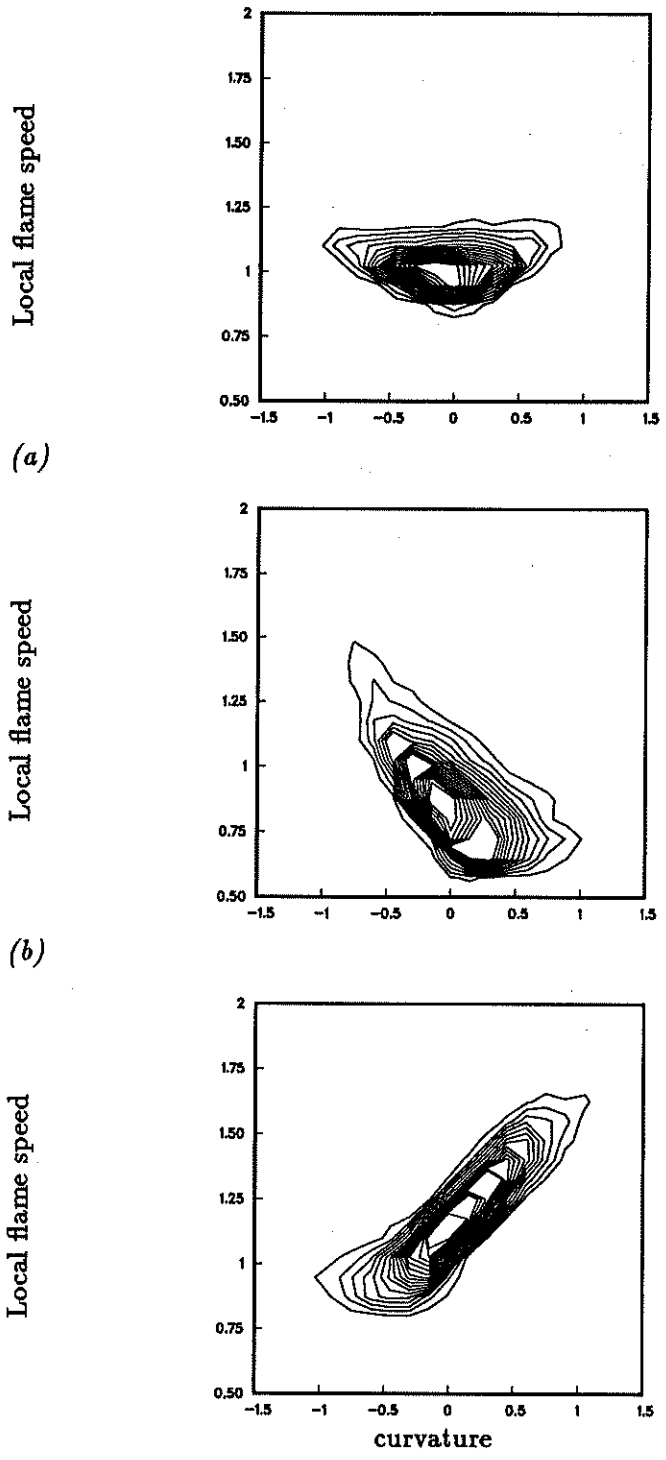

FIGURE 1. Joint pdf of the local flame speed S_C and local flame curvature. Flame speeds are normalized by the unperturbed laminar value. Curvature is normalized by the flame thickness; (a) $Le = 1.0$, (b) $Le = 1.2$, (c) $Le = 0.8$.

These trends are consistent with laminar flame theory (Libby *et al.* 1983), a result that is of primary importance for flamelet models, and with previous simulations (Ashurst *et al.* 1987). It is worth emphasizing that contrary to curvature effects, these trends do not cancel out when averaged along the flame surface, and the mean flamelet speed $\langle S_C \rangle$ is affected by strain.

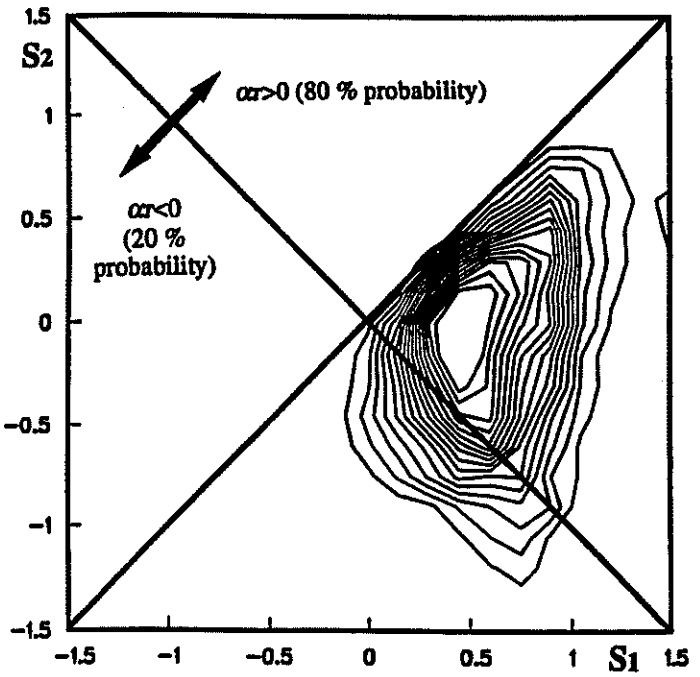

FIGURE 2. Joint Pdf of the principal strain rates in the flame tangent plane, $S_1 \geq S_2$. Strain rates are normalized by the laminar flame timescale. $Le = 0.8$.

An important quantity for the evolution of the flame surface density is the strain rate acting in the flame tangent plane (Candel and Poinsot 1990). Simulations show that independently of the Lewis number, there is an 80 % probability for positive values of this strain rate (Figure 2). This high value brings supports to the flamelet models picture where flame surface is produced by hydrodynamic straining.

A slightly different perspective is obtained when examining the alignment of the principal directions of the strain rate tensor with the flame normal. The strain rate tensor being symmetric, it may be characterized by its three principal directions and three eigenvalues:

$$\alpha \geq \beta \geq \gamma, \tag{7}$$

For incompressible flow, these eigenvalues sum to zero. α is positive and corresponds to the most extensive strain direction. γ is negative and corresponds to the most compressive strain direction. β is the intermediate strain rate and can take positive or negative values. Figure 3 shows that the flame normal tends to align with the most compressive principal direction. This again bears evidence of the effect of hydrodynamic straining on the flame dynamics.

However, contrary to the previous analysis of curvature, it was not possible to show any correlation between the local flame speed S_C and strain. This absence of correlation is believed to be associated with an excessive zooming effect resulting from Direct Numerical Simulation: the strain rate tensor as computed from simulation data is both localized in space (an arbitrary location is selected within the flame zone) and in time (quantities are instantaneous values). This would only be a minor problem if the straining field and the flame zone were always in dynamical equilibrium. However, referring to the idea of persistent straining, it is believed that to significantly modify the flame front structure, strain must act on a time scale that is commensurate with the flame characteristic time. Therefore, the local flame structure is likely to depend on the time history of strain, represented eventually by a time-averaged strain rate, rather than on instantaneous values. Also, among all the turbulent structures present in the vicinity of the flame and which contribute to the strain rate, only a certain class are dynamically active (an active structure would be a structure that satisfies some coherence conditions in space and time). In some sense, the signal to noise ratio is low in fully turbulent simulations.

This study of the effect of strain is now pursued in the context of a flame-vortex interaction problem (see Section 3.1), where some of the above difficulties are removed by considering only one well-characterized flow structure.

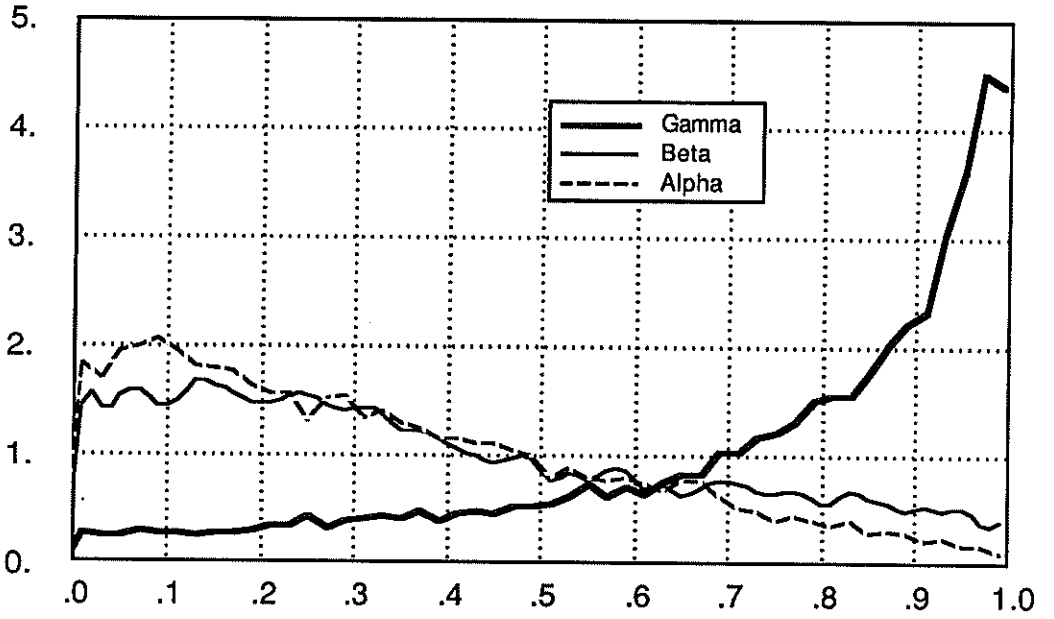

FIGURE 3. Pdf of the cosinus of the angle between the directions of principal strain at the flame and the flame normal. $Le = 0.8$.

2.3 Conclusions

Most notable in the results is the strong correlation between the local flame structure and the flame front curvature. Consistent with laminar flame theory, this

correlation is Lewis number dependent. It may appear at first sight that these findings invalidate some important assumptions used in current flamelet models. In these models, the prototype configuration for flamelet libraries is a strained stagnation point flame, and curvature effects are simply neglected. However, one should keep in mind that turbulent combustion models are developed for engineering applications, where computations are performed on coarse grids. In this context, the model predictions are only required to hold in an average sense (the laminar submodel used in the flamelet approach may be considered as a subgrid scale model). Therefore, fair comparisons between the models predictions and Direct Numerical Simulations should be performed at a global level. At this level, our results indicate that the mean flamelet speed $\langle S_C \rangle$ is affected by strain, not by curvature. In conclusion, while curvature determines the local characteristics of the reaction zone, global features are in good agreement with predictions based on the stagnation point flame picture.

Future work will require studying the effects of differential diffusion at higher Reynolds numbers (in our study the Reynolds number based on Taylor microscale was limited to values around 10). It is worth emphasizing that curvature effects are expected to be strong as long as molecular transport phenomena are important. It may be argued that turbulence wipes out at some point differences in the transport of heat and species (the turbulent Lewis number would then be unity). However, this argument is rather speculative, especially for chemical systems where diffusion processes play a dominant role for sustaining reaction. Therefore, this issue remains open.

3. Ongoing and future plans

3.1 Direct simulation of a single vortex interacting with a flame

It is the essence of flamelet models to reduce turbulent combustion mechanisms to elementary flame problems. It has been recognized for a long time in the combustion community that new insights into turbulent mechanisms could be gained by studying model laminar problems. For example, computations of laminar stagnation point flames provide insight into the effect of a plane strain acting on a flame element (Libby and Williams 1982, 1983). Similarly, situations where isolated vortices interact with laminar flames are considered as generic problems for turbulent combustion.

While at CTR, Dr. Poinsot performed direct simulations of a vortex-pair interacting at right angles with a laminar flame front and reached original conclusions with respect to quenching mechanisms (Poinsot *et al.* 1990, Meneveau and Poinsot 1990). The present study is a continuation of this work as applied to a different geometry: a single vortex structure interacts with a flame stabilized between coflowing fresh reactants and burnt products (Figure 4). This geometry simulates some of the features of practical dump combustors where premixed flames are anchored in shear flows and vortices develop and convect parallel to the reaction zone.

This problem is examined using a high-order, finite difference code for reacting compressible flows developed by Poinsot and Lele. The code features a single step,

irreversible, finite rate (Arrhenius law) chemical reaction with heat release. It is two-dimensional.

Only a few results are available at this time. For $Le = 1$, results indicate that the mean flame speed $\langle S_C \rangle$ is not altered by the vortex-induced perturbations. The total reaction rate is affected because of the production of flame surface resulting from vortex stretching. The increase in the flame surface density scales directly with the vortex lifetime (in the simulations, the vortex strength is continuously decaying because of viscous diffusion).

More results are presently obtained and will be expected in the near future, these include:

- the spatial variations of the fuel consumption speed S_C along the flame surface for various Lewis numbers,
- an analysis of the flame tip created by the vortex motion to characterize curvature effects,
- an analysis of strain effects by monitoring the time history of the strain field along the flame surface,
- the effects of vortices smaller than the flame thickness.

Another possible problem relevant to the control applications consists of simulating a train of vortices rather than a single vortex.

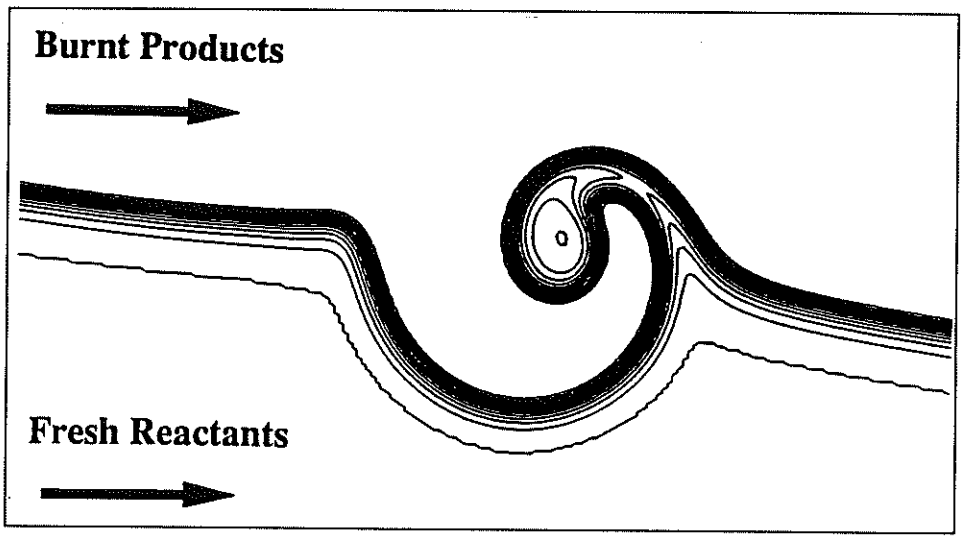

FIGURE 4. Flame-vortex interaction. Temperature contours.

3.2 Development of a three-dimensional code for turbulent combustion

Turbulent combustion problems where three-dimensional effects are important may be classified into two categories: (1) problems where vortex stretching plays a central role (for example: effects of stretched vortices on a flame sheet, effect of streamwise vorticity in reacting shear layers, mixing transition in reacting flows, etc); (2) problems where the flame develops in all space directions (for example:

ignition mechanisms in IC engines). To tackle these problems, it is planned to develop in the coming year a three-dimensional version of the Poinsot and Lele code.

REFERENCES

ASHURST, W. T. 1987 Vortex simulation of unsteady wrinkled laminar flames. *Combus. Sci. and Tech.* **52**, 325

ASHURST, W. T., PETERS, N. & SMOOKE, M. D. 1987 Numerical simulation of turbulent flame structure with non-unity Lewis number. *Combus. Sci. and Tech.* **53**, 339-375

BORGHI, R. 1984 *Recent Advances in Aeronautical Science.* C. Bruno, C. Caseci eds., Pergamon.

BRAY, K. N. C. 1980 *Topics in Applied Physics.* P. A. Libby & F. A. Williams eds., Springer Verlag.

CANDEL, S., MAISTRET, E., DARABIHA, N., POINSOT, T., VEYNANTE, D. & LACAS, F. 1988 *Marble Symposium.* Caltech, Pasadena.

CANDEL, S. M. & POINSOT, T. 1990 Flame stretch and the balance equation for the flame area. *Combus. Sci. and Tech.* **70**, 1-15.

CANT, R. & BRAY, K. 1988 Strained laminar flamelet calculations of premixed turbulent combustion in a closed vessel. *Twenty Second Symposium (International) on Combustion.* The Combustion Institute, p. 791.

CLAVIN, P. & WILLIAMS, F. 1982 Effects of molecular diffusion and of thermal expansion on the structure and dynamics of premixed flames in turbulent flows of large scale and low intensity. *J. Fluid Mech.* **116**, 251.

DARABIHA, N., GIOVANGIGLI, V., TROUVE, A., CANDEL, S. & ESPOSITO, E. 1989 Coherent flame description of turbulent premixed flames. *French-USA Workshop on Turbulent Combustion.* R. Borghi & S. Murthy eds., Springer Verlag.

HAWORTH, D. C. & POINSOT, T. 1990 The influence of Lewis number and non-homogeneous mixture on premixed turbulent flame structure. *CTR Summer Program 1990,* Center for Turbulence Research, Stanford University and NASA Ames Research Center.

LIBBY, P. & WILLIAMS, F. 1982 Structure of laminar flamelets in premixed turbulent flames. *Combus. and Flame.* **44**, 287-303.

LIBBY, P. & WILLIAMS, F. 1983 Strained premixed laminar flames under nonadiabatic conditions. *Combus. Sci. and Tech.* **31**, 1-42.

LIBBY, P., LINAN, A. & WILLIAMS, F. 1983 Strained premixed laminar flames with non-unity Lewis number. *Combus. Sci. and Tech.* **34**, 257-293.

LIBBY, P. & WILLIAMS, F. 1987 Premixed flames with general rates of strain. *Combus. Sci. and Tech.* **54**, 237.

MARBLE, F. E. & BROADWELL, J. 1977 The coherent flame model for turbulent chemical reactions. *Project SQUID.* Report TRW-9-PU.

MENEVEAU, C. & POINSOT, T. 1990 Stretching and quenching of flamelets in premixed turbulent combustion. *Combus. and Flame.* To appear.

PETERS, N. 1986 Laminar flamelet concepts in turbulent combustion. *Twenty First Symposium (International) on Combustion.* The Combustion Institute, p. 1231.

POINSOT, T. 1990 Direct simulation of turbulent combustion. *CTR Annual Research Briefs.* Center for Turbulence Research, Stanford University and NASA Ames Research Center.

POINSOT, T., VEYNANTE, D. & CANDEL, S. 1990 Quenching processes and premixed turbulent combustion diagrams. Submitted to *J. Fluid Mech.*

POINSOT, T., VEYNANTE, D. & CANDEL, S. 1990 *Twenty Third Symposium (International) on Combustion.* The Combustion Institute.

POINSOT, T. , ECHEKKI, T. & MUNGAL, G. 1990 Studies of the laminar flame tip and implications for premixed turbulent combustion. *Combus. Sci. and Tech.* To appear.

POINSOT, T. & LELE, S. 1989 Boundary conditions for direct simulations of compressible viscous reacting flows. *CTR Manuscript 102.* Center for Turbulence Research, Stanford University and NASA Ames Research Center.

POINSOT, T. & LELE, S. 1990 Submitted to *J. of Comput. Phys.*

ROGALLO, R. S. 1981 Numerical experiments in homogeneous turbulence. NASA Technical Memorandum 81315.

RUTLAND, C. J. & FERZIGER, J. H. 1989 27th AIAA Aerospace Sciences Meeting. *AIAA Paper 89-0127.*

RUTLAND, C. J. 1989 Effects of strain, vorticity, and turbulence on premixed flames. Ph.D. Thesis, Stanford.

RUTLAND, C. J. & TROUVE, A. 1990 Premixed flame simulations for non-unity Lewis number. *CTR Summer Program 1990.* Center for Turbulence Research, Stanford University and NASA Ames Research Center.

WILLIAMS, F. A. 1985 *Combustion theory.* 2nd ed. Benjamin Cummings, Menlo Park.

YEUNG, P., GIRIMAJI, S. & POPE, S. 1990 Straining and scalar dissipation on material surfaces in turbulence: implications for flamelets. *Combus. and Flame.* **79**, 340-365.