

Simulation of flame-turbulence interactions in premixed combustion

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1. Motivation and objectives

Turbulent combustion is a challenging practical problem where fluid-mechanics and chemistry are strongly coupled. The general motivation of this work is to increase our basic understanding of flame-flow interactions under turbulent conditions. The approach herein consists of applying Direct Numerical Simulation (DNS) methods to turbulent combustion. It is a continuation of previous work by Dr. Poinso (1989, 1990, 1991) and the author (Trouvé 1990).

The objectives in 1991 were twofold:

- investigate the flamelet models used in engineering calculations of turbulent combustion. More specifically, the objective is to study the combined effects of flame curvature and hydrodynamic straining on the structure of premixed turbulent flames with non-unity Lewis number.
- develop a new three-dimensional data base of premixed flames embedded in a variety of basic turbulent flow fields.

1.1 The structure of premixed turbulent flames

Premixed turbulent combustion is the propagation of a chemical reaction zone through a turbulent, molecularly mixed region of fuel and oxidizer. The turbulent flame is characterized by the topology of the region in which reaction occurs: front, pockets, or large volumes. Depending on the relative values of various chemical and turbulence scales, dimensional analysis reveals a range of premixed combustion modes progressing from flamelets to distributed reaction zones to well-stirred reactors (see for example Poinso *et al.* 1990). These modes correspond to different topologies of the reaction zone and require different approaches for both understanding and modeling.

Experimental as well as theoretical evidence suggests that many technologically important flows occur in the flamelet burning mode. Flamelet combustion corresponds to chemical reaction occurring at fast time scales and short length scales relative to the turbulence. In this situation, the flame is confined to relatively thin layers within the turbulent flow field.

In the flamelet regime, much of the interaction between combustion and turbulence is decoupled, and the framework for modeling is, therefore, greatly simplified. It is then convenient to describe the flame-flow interactions in terms of two quantities: the total flame front surface area and the local flame structure. The principle effect of turbulence is for the fluctuating velocity field to wrinkle the flame and greatly increase its surface area. This phenomenon accounts for most of the increase in the overall burning rate due to turbulence. Additionally, turbulent motions can

alter the local flame structure. This secondary effect accounts for local variations of the reaction rate along the flame surface. Under certain conditions, these variations can become critical and lead to partial or total quenching of the flame.

Laminar flame theory indicates that the local flame structure is modified by flow divergence and flame front curvature. Flow divergence is usually characterized by the hydrodynamic strain rate acting in the flame tangent plane. The response of a laminar flame to strain rate and curvature depends strongly on the relative molecular transport of thermal energy and chemical species. This is represented by an effective Lewis number, Le , defined as the ratio of thermal diffusivity to the mass diffusivity of the deficient reactant. When heat and the deficient reactant diffuse identically, i.e. when the Lewis number is unity, the flame structure exhibits a large insensitivity to strain rate and curvature. For non-unity Lewis number, however, differential diffusion of heat and species results in a strong sensitivity of the local flame structure to strain rate and curvature.

Recent studies using DNS have shown that curvature rather than strain rate determines the instantaneous local structure of premixed turbulent flames (Haworth and Poinso 1991, Rutland and Trouvé 1991). The prevailing role of flame curvature is an original and somewhat surprising result. Surprising, since, in current flamelet models, strain rate is the relevant parameter to describe the flame-flow coupling, and curvature effects are simply neglected. This apparent discrepancy lies in the differences between the two levels of analysis. Flamelet models may be viewed as empirical 'subgrid scale' models where the detailed flame front structure remains unresolved. Therefore, although they may appear contradictory, findings pertaining to the instantaneous local structure of the flame front do not necessarily invalidate the assumptions used in the description of the flamelet structure, a description that occurs at a higher level of analysis (at larger scales).

Hence, DNS, revealing strong curvature effects, and flamelet models, based on a dominant role for strain rate, are not contradictory. In fact, they are found to be consistent: DNS results show that curvature effects, however strong at the local level, tend to cancel in the mean, leaving a net statistical effect on space-averaged quantities that is related to strain rather than curvature.

To further document the respective roles of strain rate and curvature on the turbulent flame structure, two different problems were studied in this past year:

- a model flame-vortex interaction problem. Simulations of a premixed laminar flame interacting with a single vortex structure were used to determine whether the prevailing role of flame curvature observed in previous simulations under turbulent conditions could be reproduced in a laminar flow environment. Would that be the case, this would demonstrate that the prevailing role of curvature over strain rate in turbulent flames is essentially a laminar combustion phenomenon (Section 2.1).
- a two-dimensional turbulent problem: simulations of a thick premixed flame zone perturbed by small scale vortices. Previous simulations of premixed flames in isotropic turbulence were representative of fast chemistry conditions (high Damkohler numbers) (Haworth and Poinso 1991, Rutland and Trouvé 1991). In the fast chemistry limit, the reaction occurs in thin layers, and the local flame structure remains

laminar-like. When the chemistry is slow (low Damkohler numbers), however, the flame is dramatically disrupted by small scale, energetic turbulent eddies, and its inner structure differs significantly from the laminar case. The objective of this study was to investigate the persistence of Lewis number effects in low Damkohler number flames, *i.e.* in a situation where turbulent convection competes with molecular transport in the reaction zone (Section 2.2).

1.2 A three-dimensional data base for premixed turbulent combustion

DNS refers to numerical methods with high resolution both in space and time that fully resolve all of the relevant scales of the hydrodynamic flow field. The acoustic field may or may not be resolved. When applied to turbulent combustion, DNS is limited by computational expense to simple reaction schemes. Instead of using a detailed analysis of the complete combustion process, a reduced, finite-rate chemistry model is required. In addition, combustion is an exothermic process, and effects of thermal expansion due to the heat released by chemical reaction should be resolved. However, under the 'constant density' assumption (a numerical artifact that allows using a divergence-free velocity field, see Rutland and Trouvé 1991), these effects are not retained.

Thus, the available choices for DNS of turbulent combustion are:

- low Mach number or fully compressible simulations;
- constant density or variable density simulations;
- simple or complex chemistry.

The present work rests largely on the choices made by Dr. Poinso (1989): heat release and compressibility effects are fully accounted for; the chemistry model is a single step, irreversible chemical reaction with an exponential dependence of the reaction rate on temperature (Arrhenius kinetics).

The finite difference code developed by Dr. Poinso, referred to as the Poinso and Lele code, is limited to two space dimensions. Since the dynamics of two-dimensional and three-dimensional turbulence are known to be so dramatically different, this can be in some cases a severe limitation. One objective in this past year was, therefore, to develop a new code to treat three-dimensional geometries (Section 2.3).

2. Accomplishments

2.1 Flame-vortex interaction

It is our belief that significant improvements in the description of turbulent combustion may be achieved by studying simple problems of laminar flames propagating in non-uniform, steady, or unsteady flow fields. In the present study, DNS methods were used to investigate the modifications of the inner structure of a premixed flame due to the combined effects of hydrodynamic straining and flame curvature, under unsteady flow conditions.

The computational configuration corresponds to a plane laminar flame stabilized obliquely between co-flowing streams of unburnt and burnt gas and perturbed by a vortex core that convects with the flow of fresh reactants (Figure 1). The dynamics of the interaction are simulated in two-dimensions using the Poinso and

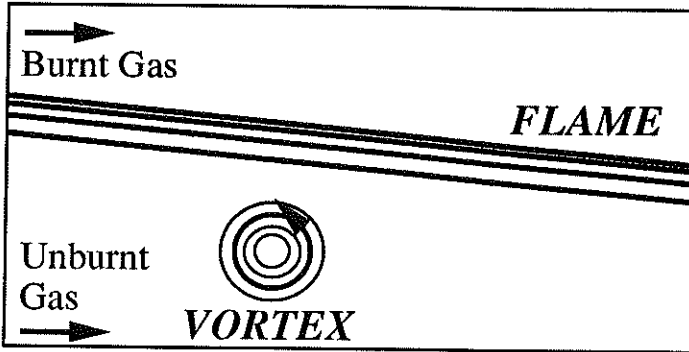


FIGURE 1. Flame-vortex interaction. Schematic of the computational configuration.

Lele code. As discussed below, an important feature of the code is that it accounts for variable transport properties, which means that diffusion coefficients are temperature-dependent.

Diagnostics require defining a flame front, a local flame normal direction, and a local flame speed. The flame surface can be defined using the progress variable, $c = 1 - Y$, where Y is the mass fraction of the deficient reactant. Constant progress variable surfaces are conveniently used to define the flame front location. We use the surface $c = 0.2$. The flame normal direction is then defined using the local gradient of c :

$$\mathbf{n} = \frac{\nabla c}{|\nabla c|} \quad (1)$$

In the range of parameters investigated, contours of c are essentially parallel within the reaction zone and the flame surface and flame normal are defined unambiguously.

Flame curvature, k , is given by the divergence of the flame normal direction:

$$k = \nabla \cdot \mathbf{n} \quad (2)$$

Positive curvature is chosen convex towards the reactants.

The rate of strain, a_T , is computed in the flame tangent plane:

$$a_T = -\mathbf{nn} : \nabla \mathbf{u} + \nabla \cdot \mathbf{u} \quad (3)$$

where \mathbf{u} is the flow velocity.

The reactant consumption speed, S_C , is a local and instantaneous property of the flame front that characterizes the inner structure of the reaction zone. This speed is defined by integrating the reaction rate along the flame front normal direction \mathbf{n} :

$$S_C \equiv \frac{1}{\rho_0 Y_0} \int \dot{w} d\eta \quad (4)$$

where ρ_0 and Y_0 are the density and the reactant mass fraction in the unburnt gas, and the limits of integration are from the local position of pure reactants to that of pure products.

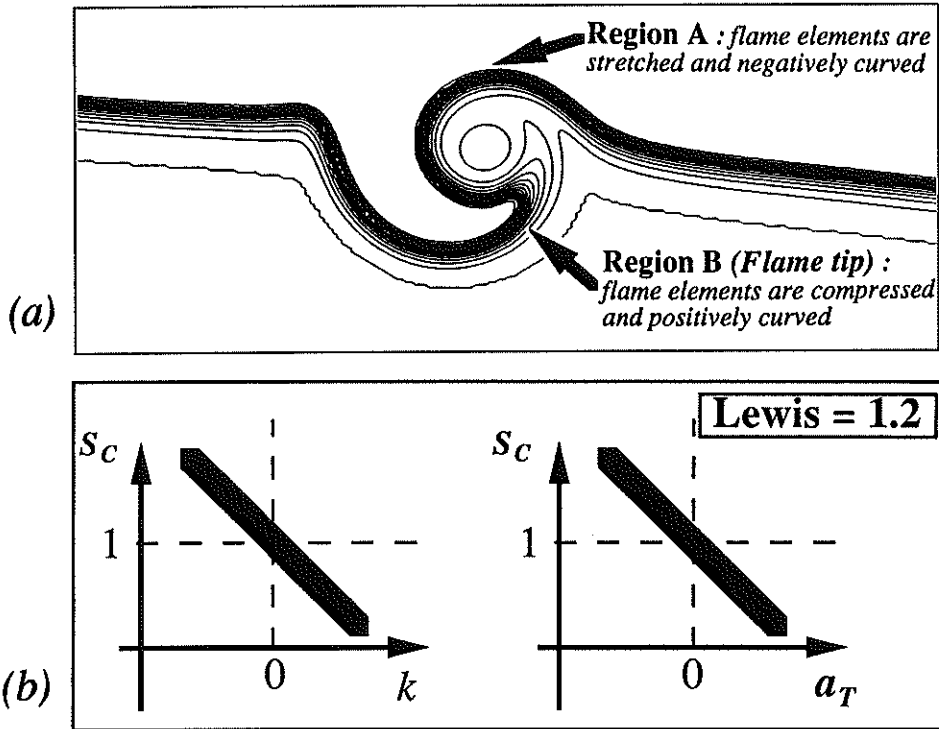


FIGURE 2. Flame-vortex interaction: (a) spatial distribution of curvature, k , and strain rate, a_T , along the flame front; (b) typical flame response to perturbations due to curvature, k , and strain rate, a_T , for $Le > 1$.

Two important aspects of the flame-vortex problem are as follows:

- the tangential strain rate, a_T , and the flame curvature, k , are not independent quantities. As shown in Figure 2a, flame elements in region A are positively strained and negatively curved, while elements in region B are negatively strained and positively curved. Hence, a_T and k are correlated quantities along the flame front, and the correlation is negative.
- the negative correlation between a_T and k results in opposite effects on the flame inner structure. For instance, let us consider a $Le > 1$ flame. In this case, laminar flame theory predicts a decrease (increase) of the local burning rate with positive (negative) strain rate and an increase (decrease) with negative (positive) curvature (Figure 2b). Hence, each flame element in regions A or B experience conflicting influences due to strain rate and curvature. Similar arguments hold for $Le < 1$ flames. Therefore, for non-unity Lewis number, the resulting flame structure is non-trivial.

Our purpose is to unravel the roles of strain rate and curvature at the flame, and the conflict between their respective effects is a rather favorable feature as this provides a mean to delineate between them. Note that, would the vortex core be located in the burnt gas, the correlation between a_T and k would be positive and

the effects on the flame structure would be cumulative, rather than opposite. This choice, however, does not serve our purpose. It also corresponds to much weaker and, therefore, less interesting interactions because: (1) the vortex trajectory is in that case deflected away from the reaction zone by thermally expanding gases; (2) viscosity, which is an increasing function of temperature, is at least an order of magnitude higher in the burnt gas compared to the unburnt value. Thus, the choice of a vortex located in the flow of fresh reactants is deemed more appropriate. In addition, this choice reproduces some of the features observed in past turbulent computations. For instance, the simulations of turbulent flames by Haworth and Poinso (1991) exhibit a negative curvature-strain rate correlation, similar to the present case. This negative correlation may be explained as follows: the simulations account for variable density and variable transport properties; both heat release effects and the increased viscosity in the burnt gas result in asymmetric characteristics of the turbulence close to the flame (high in the pre-flame gases, low in the post-flame gases); this asymmetry is in turn responsible for the negative curvature-strain rate correlation at the flame. Work is currently in progress to further characterize the relationship between the asymmetry of the turbulence at the flame and the curvature-strain rate correlation (Section 2.3). Note that the simulations by Rutland and Trouvé (1991), which assume a 'constant density' flow and do not include variable transport properties and, therefore, do not capture the turbulence asymmetry close to the flame, fail to show any correlation between a_T and k .

The present simulations describe the classical roll-up process observed during a flame-vortex interaction. The inner structure of the reaction zone adapts to vortex driven hydrodynamic perturbations due to flow inhomogeneities, as well as to geometrical perturbations due to the flame wrinkling. The simulations show that the balance between both types of effects is strongly time-dependent. Initial conditions correspond to a plane flame, where curvature effects are absent. Consequently, early times in the computations feature a flame structure where strain rate effects are dominant. a_T is the relevant parameter, and k plays no direct role. As the interaction proceeds, the flame rolls up around the vortex core, and curvature effects become more intense. Also the vortex is affected by viscous diffusion, and the strain rate field becomes weaker in time. A transition, therefore, occurs in the simulations, and late times feature a flame structure where curvature effects prevail. k is then the relevant parameter, and a_T plays no direct role.

This transition is illustrated in Figure 3. The flame response is characterized in terms of the spatial distribution of the local burning rate, S_C , along the flame front. Figure 3 shows the time evolutions of r_1 , the linear correlation coefficient between S_C and a_T , and r_2 , the linear correlation coefficient between S_C and k , for $Le = 1.2$ and $Le = 0.8$. As discussed above, early moments of the interaction correspond to a local flame structure controlled by a_T . Consistent with laminar flame theory, the correlation between S_C and a_T is Lewis number dependent: the correlation is positive when $Le < 1$ (r_1 approaching +1 in Figure 3a), and negative when $Le > 1$ (r_1 close to -1 in Figure 3b). Late times, however, correspond to prevailing effects of

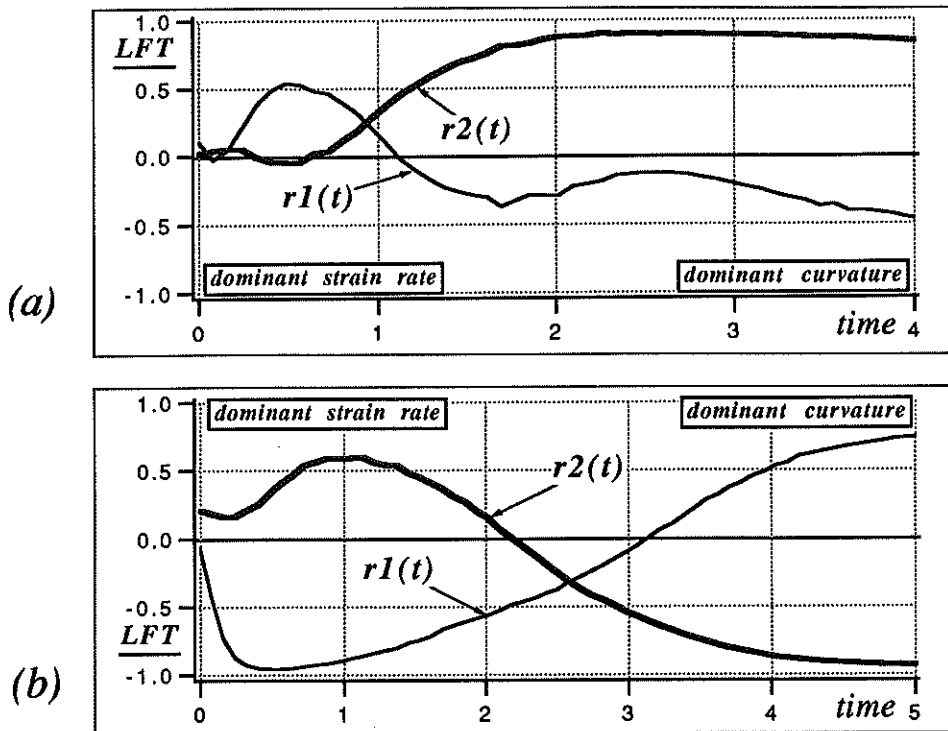


FIGURE 3. Flame-vortex interaction. Time evolution of r_1 and r_2 , defined as the linear correlation coefficients between respectively S_C and a_T , and S_C and k : (a) for a $Le = 0.8$ flame; (b) for a $Le = 1.2$ flame. Time is made non dimensional by the flame time scale. The descriptor LFT on the y axis indicates the range of values for r_1 and r_2 that are consistent with laminar flame theory. Strain rate (curvature) is said to be dominant when r_1 (r_2) is in that range.

the flame curvature, k . Again, consistent with laminar flame theory, the correlation between S_C and k is Lewis number dependent: the correlation is positive when $Le < 1$ (r_2 close to +1 in Figure 3a), and negative when $Le > 1$ (r_2 close to -1 in Figure 3b). Note that since a_T and k are correlated quantities, the flame response, if correlated to a_T , is also correlated to k , and vice versa. This is clearly seen in Figure 3 where the curves $r_1(t)$ and $r_2(t)$ exhibit roughly symmetric behavior. Consistency checks with laminar flame theory are required to decide which of these two parameters, a_T or k , plays a dominant role.

The observation of a transition from a flame structure initially controlled by strain rate to a structure ultimately controlled by curvature is original but not unexpected. This transition is clearly related to our particular choice of initial conditions. It is also related to our choice of a two-dimensional configuration where, in absence of three-dimensional stretching, the vortex strength must decay in time. A more meaningful result is obtained by studying the amount of time required for the transition to occur. This characteristic time, τ , is the key quantity to decide

which of a_T or k is the relevant parameter that controls the local flame structure. Simulations have been performed for a variety of vortex sizes (up to three times the thermal thickness of the unperturbed laminar flame) and a variety of vortex speeds (from two to twenty times the unperturbed laminar flame speed); the characteristic time, τ , always came out to be short compared to the total flame-vortex interaction time. The main observations are that: (1) τ is found to be closely related to the wrinkling of the flame; (2) the flame is only weakly curved when the transition occurs (a typical value for the flame radius of curvature at time τ is five times the laminar flame thickness); (3) τ does not depend significantly on the vortex speed. In other words, as soon as the flame gets wrinkled and irrespective of the vortex strength, a transition in the flame structure is observed. Since the characteristic time, τ , is highly sensitive to curvature but not to strain rate, we are led to the conclusion that the structure of premixed flames (laminar or turbulent) is primarily determined by the flame geometry.

In summary, simulations of a premixed flame interacting with a single vortex structure reveal a structural transition from a strained-type flame to a curved-type flame. The rapidity of that transition is a remarkable result that demonstrates that, locally, curvature is more important than strain rate. These conclusions agree with previous simulations of turbulent flames, and the prevailing role of curvature on the local structure of turbulent flames may, therefore, be viewed as a laminar combustion phenomenon.

2.2 Small scale turbulence acting on a thick flame zone

Previous simulations of flame-turbulence interactions were limited to fast chemistry conditions (Haworth and Poinot 1991, Rutland and Trouvé 1991). Since, in this situation, the local flame structure remains laminar-like, this regime is usually referred to as the laminar flamelet regime. Under slow chemistry conditions, however, the flame-turbulence interactions are more intricate. Slow chemistry conditions correspond to thick flames, *i.e.* thicker than the Kolmogorov-sized eddies. In this situation, small scale turbulent eddies penetrate into the reaction zone, and the structure of flame elements is disrupted in a way that precludes any analogy with laminar flame theory. It is traditionally believed that such conditions correspond to a dramatic change in the flame topology and that the flame will experience a transition from flamelets to a distributed mode of combustion.

The computational configuration is sketched in Figure 4. The left- and right-hand sides of the domain are inflow and outflow boundaries, while periodic boundary conditions are applied at the top and bottom. The calculations are initialized with fresh reactants on one side of the domain and burnt products on the other side; the two are separated by a plane laminar flame. Isotropic turbulence is initially located in the flow of fresh reactants, its velocity field being specified according to a model spectrum. The turbulence is characterized by an integral length scale smaller than the thermal thickness of the laminar flame and a turbulence intensity that is much higher than the laminar flame speed. The initial turbulent Reynolds number is 140, and the initial Damkohler number, defined as the ratio of the integral time scale of the turbulence to the flame characteristic time, is 0.005. The turbulence is decaying

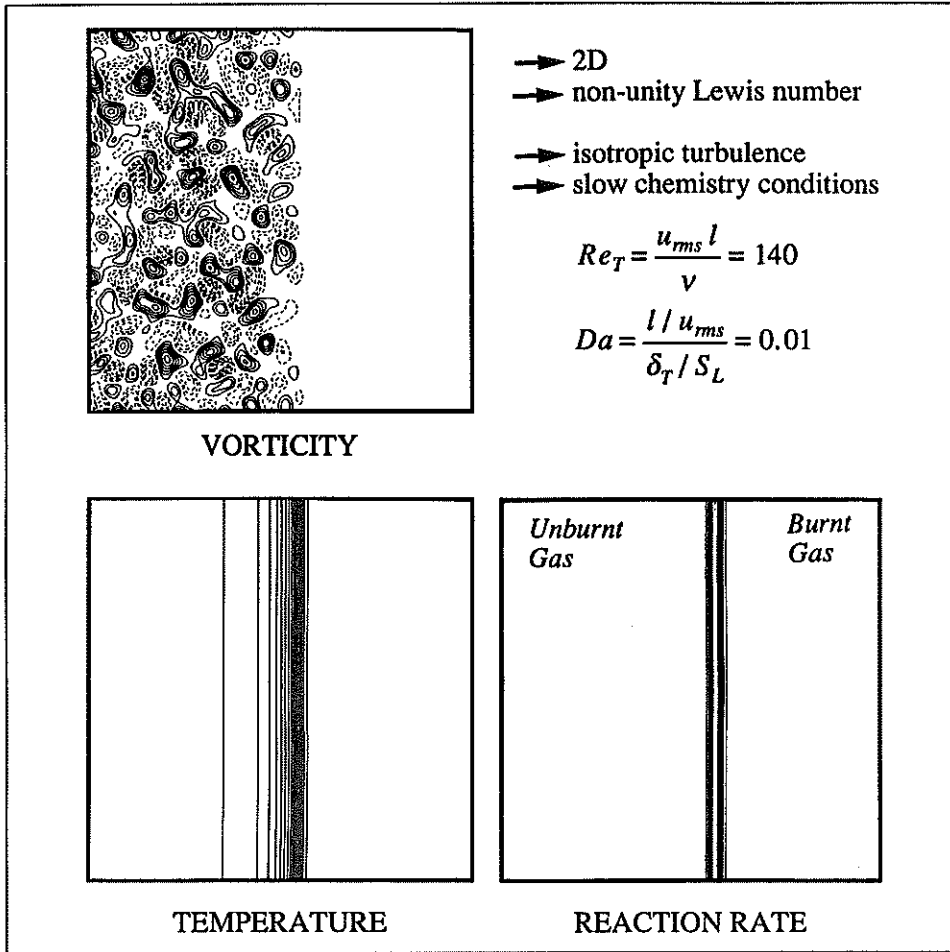


FIGURE 4. Small scale turbulence acting on a thick flame zone. Schematic of the computational configuration. Initial conditions for temperature and reaction rate correspond to a plane laminar flame.

in time, and conditions are non-stationary. The dynamics of the flame-turbulence interaction are simulated in two-dimensions, using the Poinot and Lele code. The grid resolution is 325^2 .

Typical results are shown in Figure 5 for a $Le = 1.2$ flame. Some striking differences with high Damkohler number flames are observed; for instance: (1) the preheat zone is dramatically altered by the small turbulent eddies, and its structure differs significantly from the laminar case; (2) the reaction zone is highly wrinkled by the turbulence, leading to the formation of cusps pointing towards the fresh gases. However, one important similarity with high Damkohler number flames is the strong correlation between the local reaction rate and the flame curvature. In Figure 5, the reaction rate respectively increases or decreases with negative or positive curvature. Opposite trends are observed for $Le = 0.8$ flames. These trends are

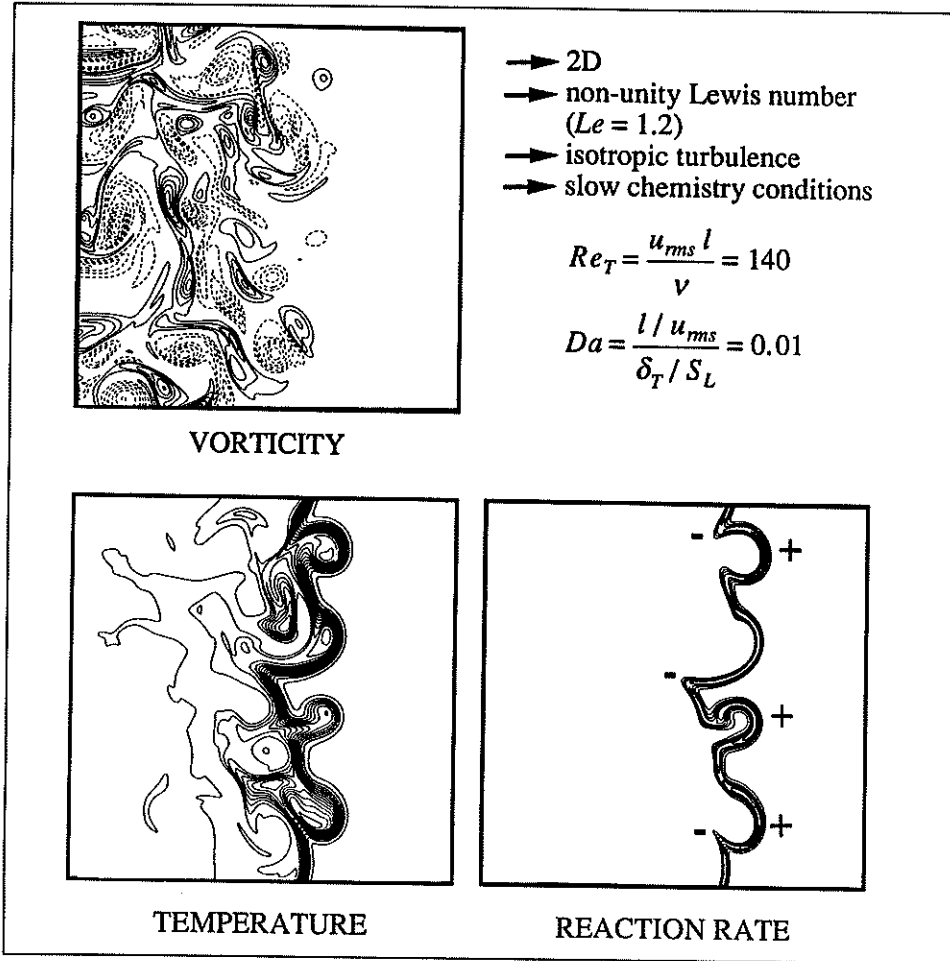


FIGURE 5. Small scale turbulence acting on a thick flame zone. Typical results for a $Le = 1.2$ flame. The plus (minus) signs in the plot of the reaction rate indicate increased (decreased) intensities of the local burning rate and emphasize the strong correlation between the flame structure and curvature.

consistent with curvature-induced Lewis number effects in laminar flame theory.

At this point, conclusions are that:

- Lewis number effects are persistent in low Damkohler number flames. Note that this result is far from being intuitive since, in this situation, turbulent convection competes with molecular transport in the flame zone, and the influence of the Lewis number, a number based exclusively on molecular diffusivities, might have been expected to be diminished;
- the local flame structure is controlled by curvature, not by strain rate. Again, this result is striking when considering the high rates of strain imposed by the turbulent flow field;
- modifications of the flame inner structure occur on a time scale that is related to

the wrinkling process, *i.e.* a turbulence time scale as opposed to a chemical time scale.

These conclusions bear some analogy with the results of Section 2.1 and bring further support to the concept of a local flame structure determined by the flame geometry.

Another question of fundamental interest is the question of the flame topology. This question is related to the definition of the domain of validity of flamelet models. In the following, we propose a mechanism for the transition from flamelet combustion (defined as a surface mode of burning) to a distributed reaction zone (defined as a volume mode of burning), and we show that this mechanism is rather unlikely.

Figure 6 shows contours of the reaction rate at four successive instants from a simulation of a $Le = 0.8$ flame. At times t_1 and t_2 , the intense turbulent motions result in the formation of two pockets of burnt fluid within unburnt, labelled A and B. These pockets correspond to hot material trapped within fresh reactants, and one may wonder whether these conditions are sufficient for ignition of the surrounding reactive fluid. This question is crucial. We believe that the answer to that question determines whether a transition from flamelets to a distributed mode of reaction is likely to occur. Indeed, if pockets like A and B are capable of growth and are found to develop as new flame kernels, the process could repeat and multiply, its rate of occurrence would increase, and a transition to a volume mode of burning might be expected. In any case, the flamelet picture would no longer be valid. As shown in Figures 6 (times t_3 and t_4), however, both pockets A and B are rapidly quenched.

In the above mechanism, the issue of an eventual change in the flame topology is related to the problem of flame ignition in turbulent flows (see Poinso 1991 for a numerical study of this problem). Asymptotic studies of the problem of flame ignition in laminar flows (see Poinso 1991 for references) have shown the existence of a critical radius of curvature below which a flame kernel, cylindrical or spherical, cannot propagate and is led to extinction. A similar mechanism is at play in the present turbulent simulations: the pockets A and B in Figure 6 exhibit characteristic sizes that are too small for combustion to be sustained. Larger length scales are required for flame propagation. This does not mean, however, that large turbulent structures are better suited for promoting a transition to non-flamelet combustion: short flow time scales are also required when producing pockets A and B (the turbulence must prevail over counter-acting effects of laminar flame propagation); large turbulent structures feature longer time scales and are, therefore, unlikely to support the above mechanism.

In conclusion, small turbulent structures are not capable of modifying significantly the flame topology. It is argued that larger structures are unlikely to be more successful. Although we recognize that some other mechanisms are possible for a transition to non-flamelet combustion, for instance mechanisms related to thermal quenching or chemical-kinetic quenching, our results certainly indicate that the domain of validity of the flamelet approach for premixed turbulent combustion is probably larger than previously thought.

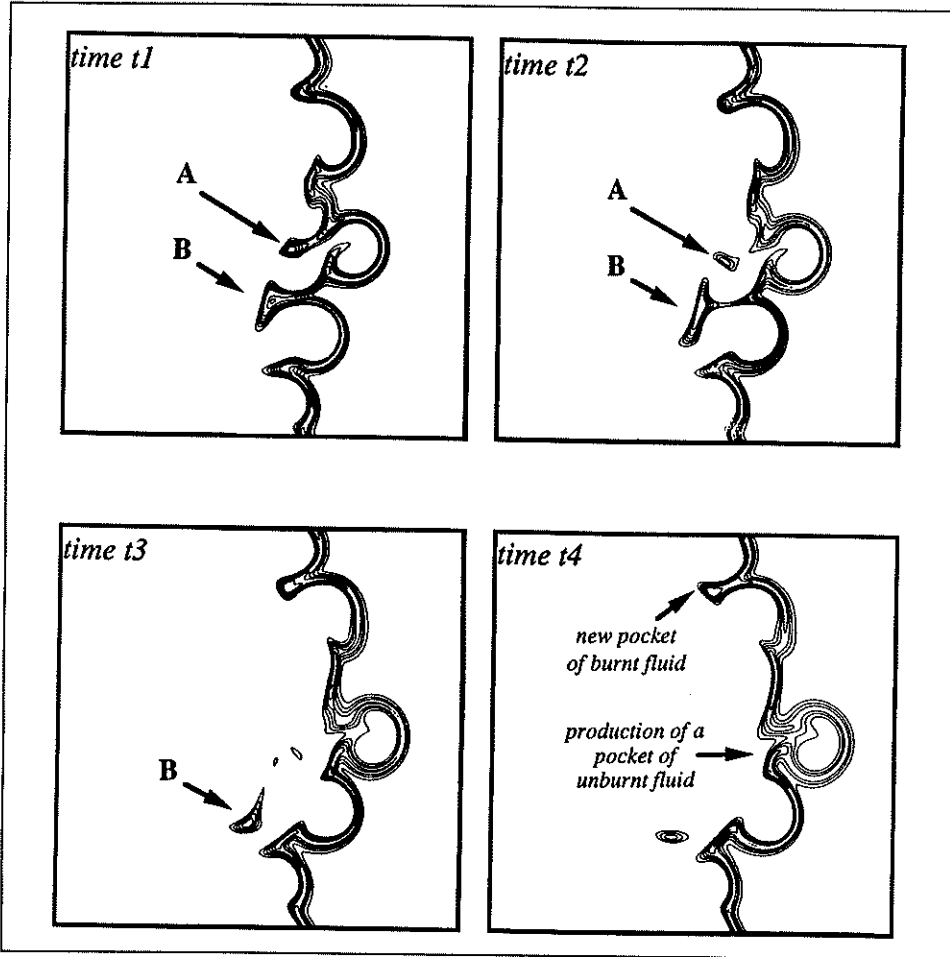


FIGURE 6. Small scale turbulence acting on a thick flame zone. Four successive plots of the reaction rate, for a $Le = 0.8$ flame. These plots describe a dramatic dynamical event: small amounts of burnt material are separated by turbulent motions from the post-flame gases, leading to the formation of pockets A and B (times $t1$ and $t2$); these pockets are not capable of growth and ultimately experience quenching (times $t3$ and $t4$).

2.3 A new three-dimensional data base for premixed turbulent combustion

The Poinot and Lele code is a finite difference code that solves for the unsteady Navier-Stokes equations in non-periodic domains. Time advancement is with a third-order Runge-Kutta scheme. A sixth-order Padé scheme is used for spatial discretization. As discussed in Section 1.2, the simulations include finite chemical reaction, heat release, and compressibility effects.

The code has been used previously to generate a data base for premixed flames in decaying, isotropic turbulence (Haworth and Poinot 1991). Due to the code

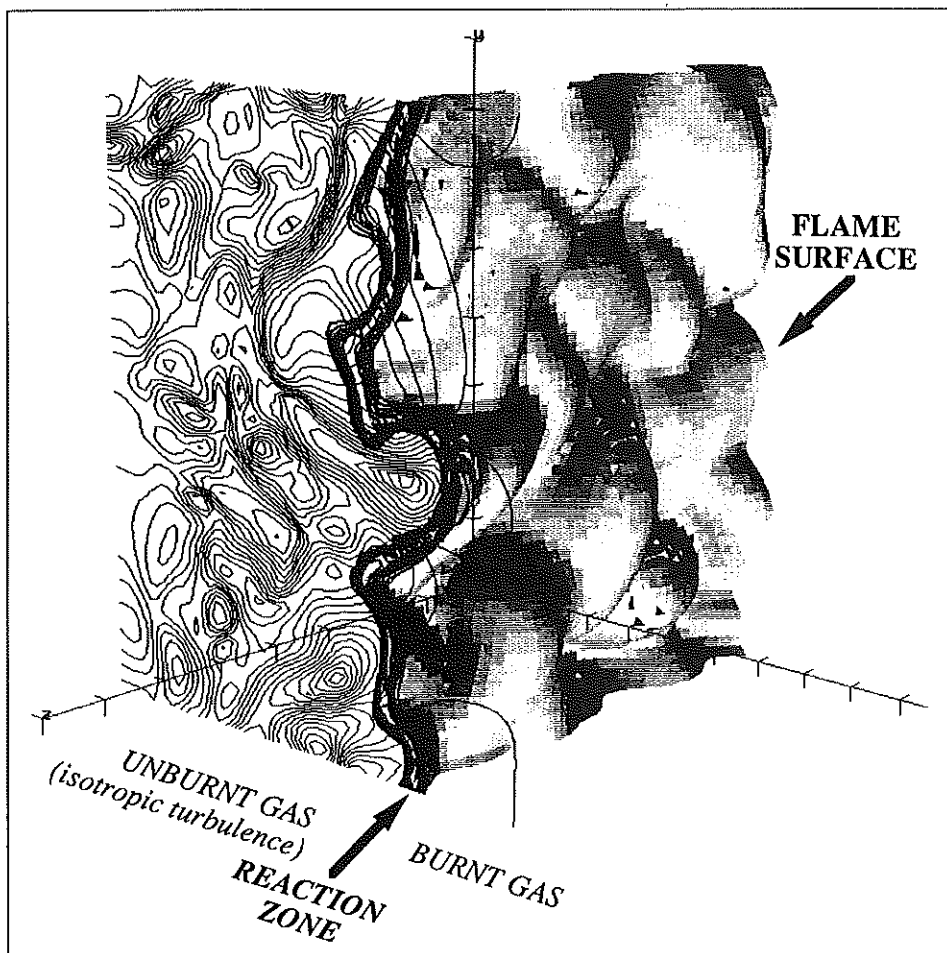


FIGURE 7. Three-dimensional simulation of a premixed flame in isotropic turbulent flow.

features, this data base is quite unique. However, the two major shortcomings of this data base are that: (1) the simulations are limited to two space dimensions; (2) the chemistry model is over-simplified (single step chemistry). In this past year, a new code has been developed to treat three-dimensional geometries. The code can carry a variable number of scalars and can be easily adapted to more complex chemical schemes. This code is referred to as the Trouvé and Lee code.

The Trouvé and Lee code is currently used to study the evolution of premixed flames with single-step chemistry in three-dimensional, decaying, isotropic turbulent flow. The computations are performed for three different Lewis numbers, $Le = 0.8$, 1.0 , and 1.2 . The grid is 129^3 . Figure 7 shows a typical plot from the new data base. Work is in progress to analyze this data base and study some important issues that were left unresolved in previous work, for instance the question of the correlation between strain rate and flame curvature (see Section 2.1).

3. Ongoing and future plans

- a three-dimensional data base for premixed turbulent combustion. As mentioned in Section 2.3, the Trouvé and Lee code is currently used to study the evolution of premixed flames in three-dimensional, isotropic turbulent flow. The first objective in the coming year is to complete this study and extend it to the case of homogeneous shear flow. Both flows are considered as building blocks in the development of turbulent combustion models.

- simple or complex chemistry? Single-step chemistry does not allow for chemical-kinetic extinction, and this is recognized as a severe limitation in problems where quenching is expected to play a central role. Therefore, a second objective in the coming year is to assess the influence of the choice of the chemical model on DNS results. The Trouvé and Lee code will be used with a new two-step chemical scheme. Due to the increased computational cost, this study will be limited to two space dimensions. The flame response to hydrodynamic straining and curvature will be studied both under adiabatic and non-adiabatic conditions, and extensive comparisons will be made between the original single-step and the new chemistry models.

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