Progress in Direct Numerical Simulations of Turbulent Reacting Flows

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A description of the emerging field of direct numerical simulations of turbulent, chemically reacting flows is presented. The types of direct numerical simulations, physical issues related to implementing the simulations, as well as the various numerical methods used are described. Examples of recent applications of direct numerical simulations to a variety of problems, displaying both the potential of the method and also some of its limitations, are presented. Finally, our view of the potential role of direct numerical simulations in future research on turbulent, chemically reacting flows is presented.

Introduction

TURBULENT flow dynamics are often a critical element in combustion processes. For example, in non-premixed reactions, the overall rate of product formation is usually controlled by the ability of the turbulence to mix the reacting species down to the microscale. The present ability to model turbulence in combustion processes is very limited, however, due to the lack of understanding of the physical processes involved. This has led Waltrup[1] (see also Northam[2]), in a discussion of the development of liquid-fueled, supersonic combustion ramjets, to list research into turbulent shear layers and turbulent boundary layers as the highest priority items deserving further research.

Most modeling of turbulent reacting flows to date is based on either the Reynolds (or Favre) averaged equations or the probability density function equations (or some combination of the two). Both approaches suffer from the closure problem and, hence, rely heavily on empirical models, which are of questionable validity and generality, especially for combustion processes. An alternative predictive approach to this problem, which avoids some of the problems of these other methods, is direct numerical simulations. This approach, as applied to chemically reacting flows, is in its infancy. A significant amount of work using this methodology has been initiated over the past few years, and the method has tremendous potential in the future, as the speed and memory of computers increase and as numerical methods become more efficient and more accurate. The objective of this paper is to explain the basic methodology of direct numerical simulations when applied to turbulent, chemically reacting flows. The discussion will include the various methods of approach, the different numerical methods presently used, and the problems that can and cannot be addressed with this methodology. Since we are emphasizing the methodology, this paper is not meant to be a complete review of past and current work. We will draw on examples from this work to the extent that it helps to explain the methodology.

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Direct numerical simulations involve the numerical solution of the time development of the detailed, unsteady structures in a turbulent flowfield. Using very efficient numerical methods and, usually, supercomputers, the fully nonlinear governing equations are solved directly so that, at most, only the smaller-scale motions need to be modeled. Statistical data then are obtained by performing averages over the computed flowfields. The procedure is analogous to laboratory experiments but has the following advantages: 1) most of the physical quantities of interest are known and their relevant statistical properties can be computed since the entire flowfield is known at every time step, 2) the parameters can be varied easily, and 3) experimental conditions are more controllable. The advantages over other numerical approaches are that the closure problem can be circumvented partially or totally and the behavior of large-scale structures can be addressed directly. The main disadvantage is the limited spatial and temporal resolution available, which limits the range of space and time scales (and, hence, maximum Reynolds and Damköhler numbers) that can be included in the simulations. Furthermore, if modeling the effects of the subgrid-scale motions is required, reasonable models can be very difficult to develop, especially for reacting flow problems. At the present time, direct numerical simulations are limited to use as a research tool. However, it is possible that within the next decade certain types of direct numerical simulations will be used in applications.

The approach has been used successfully in the study of turbulent, nonreacting flows. For example, it has been applied to testing turbulence theories, from analytic theories[3,4] to second-order closure modeling assumptions.[5-7] Important advances have been made in the study of the atmospheric boundary layer[8] as well as of neutral boundary layers,[9] of homogeneous shear and homogeneous straining flows,[10] and of density-stratified flows.[11,12] The method has been validated by comparing simulation results with laboratory data for the cases of homogeneous, turbulence decay,[13] turbulent wakes,[14] turbulent mixing layers,[15] and turbulent boundary layers.[9]

In this paper, first we discuss in detail the methodology involved in direct numerical simulations of chemically reacting turbulent flows. This involves discussion of the various types of direct simulations, of some physical issues related to the implementation of direct simulations, and of the numerical methods employed in simulations to date. Next, we discuss examples of direct simulations, pointing out, in particular, some of the ways that direct simulations can be used to address important issues. Finally, we discuss how we believe

the methodology should be used in the future, including the critical areas of research in further developing the methodology, and problems that are best addressed by this methodology. For an excellent review of the methodology and applications of direct numerical simulations to nonreacting flows, see Ref. 16.

Methodology

As the field of direct numerical simulations has developed over the past 17 years, a variety of implementations has emerged, and several different numerical methods have been employed. In this section, we discuss these different implementations and the numerical methods used, as well as several physics issues that must be addressed if one is to properly apply the methodology.

Direct Numerical Simulations

By the term "direct numerical simulation," we mean a numerical calculation that solves for the time development of the detailed, unsteady structures in a turbulent flowfield. In particular, we exclude any calculation using the Reynolds (or Favre) averaged equations, even if applied to a statistically unsteady turbulent flow. There are several implementations of direct numerical simulations, which can be classified as follows.

Full turbulence simulations (FTS) are calculations in which all of the dynamically significant length and time scales of motion are included. This implies resolving length scales ranging from the size of the domain of interest down to scales smaller than those at which viscous dissipation and chemical reaction occur. We can obtain an estimate of this range of scales for *nonreacting* flows by examining the ratio of a length scale characterizing the energy-containing range (L_e) to the Kolmogorov length scale (L_k), which characterizes the dissipation range. The Kolmogorov length scale is defined by $L_k = (\nu^3/\epsilon)^{3/4}$, where ϵ is the energy dissipation rate. Estimating ϵ by u'^3/L_e,[17] where u' is an rms turbulent velocity scale, the ratio of the energy-containing scale to the Kolmogorov scale is approximately

$$\frac{L_e}{L_k} \sim \frac{L_e}{(\nu^3\epsilon)^{1/4}} \sim \left(\frac{u'L_e}{\nu}\right)^{3/4} \tag{1}$$

We see that this ratio of length scales is roughly proportional to $R_L^{3/4}$, where $R_L = u'L_e/\nu$ is a Reynolds number based on the energy-containing range of scales. Therefore, the number of grid points N in a particular direction is expected to be proportional to $R_L^{3/4}$, so that, in a three-dimensional simulation, the total number of grid points will be proportional to $(u'L_2/\nu)^{9/4}$. Most technological flows have Reynolds numbers in the tens of thousands or more, which would require more grid points than computers of the present or near future could handle. With present-day supercomputers, the maximum Reynolds numbers achieved in such simulations are in the range of several hundred. This limits this approach to basic research studies.

Full turbulence simulations originated with the work of Orszag and Patterson,[3] who studied homogeneous decaying turbulence and the validity of certain analytical theories of turbulence. The approach has been employed further in many basic research issues, including turbulent diffusion,[18] magnetic turbulence,[19] the behavior of pressure/strain-rate correlations,[6,20] turbulent wakes,[14,21] turbulent mixing layers,[15] and turbulent boundary layers.[9] Examples of FTS of chemically reacting flows are the work of Riley et al.[22] and McMurtry et al.,[23,24] and will be discussed in the following section.

In order to avoid the Reynolds number limitations inherent in FTS, Lilly[25] and Deardorff[26] introduced the methodology that is now known as large-eddy simulations (LES). In this approach, the equations of motion are prefiltered to eliminate the scales of motion smaller than those resolvable on the computational mesh. This produces equations analogous to the Reynolds-averaged equations; only the averaged (filtered) terms now represent the unresolved motions. Models are proposed for the filtered terms, and then the equations are solved for the resolvable scales of motion (large eddies).

The advantage of this approach over FTS is that it has the potential to treat very high Reynolds numbers and very fast reaction flows. The disadvantage is that ad hoc models are necessary to close the equations, which introduce some uncertainty into the validity of the results. The advantage of the method over solving the usual Reynolds-averaged equations is that the large-scale turbulent motions are treated directly, and only the smaller scales are modeled. In the Reynolds-averaged approach, all turbulence scales are modeled. Therefore, it would be expected that the LES would provide a more accurate simulation of the turbulence, that the LES results would be less sensitive to modeling assumptions (since scales comprising only a small percentage of the energy are usually modeled), and that this sensitivity would decrease as the resolution increases. It should be noted, however, as discussed subsequently, that the difficulties inherent in modeling the effects of the subgrid scales may be much more severe for reacting flow problems. Another advantage of LES is that information about the detailed structures of the larger-scale motions is provided. The disadvantage is that lengthy computations of unsteady three-dimensional (or possibly two-dimensional) flows are required, whereas, in the Reynolds-averaged approach, usually steady-state and lower-dimensional equations are considered. Furthermore, a much larger range of length and time scales is necessary in the LES approach, so that a significantly greater computational effort is required.

Large-eddy simulations can be classified into two categories, two-dimensional (or axisymmetric) and three-dimensional. In two-dimensional LES, in addition to filtering out the subgrid-scale motions, the equations are also averaged in one spatial direction. This results in a much simpler numerical problem. More of the scales of motion need to be modeled, however, decreasing the reliability of the model. Furthermore, key three-dimensional aspects of turbulence, e.g., vortex-tube stretching, are eliminated, which considerably limits the dynamics that can be simulated. Two-dimensional LES have been applied mainly to the study of plane turbulent mixing layers, where it is argued that a significant portion of the turbulence dynamics are two-dimensional. Studied have been carried out of both nonreacting[11,15,27–29] and reacting flows.[23,30,31]

Three-dimensional LES have been used in a variety of problems, beginning with the boundary-layer studies of Deardoff,[8,26] and continuing with calculations of homogeneous decay,[13] channel flows,[9,32] and more recent work on the atmospheric boundary layer.[33] At present, no three-dimensional LES of chemically reacting turbulent flows have been performed.

Some Physics Issues

In direct numerical simulations, it is important to estimate the length scales of the physical phenomena of interest so that an appropriate choice of the approaches discussed earlier can be made, and so that the phenomena can be adequately resolved numerically. This is particularly true when FTS are employed. Usually, it is also important to estimate the parameter range for which the simulations can accurately predict the phenomena of interest.

Given the performance of supercomputers available now and in the near future, approximately two decades of length scales can be resolved in a three-dimensional simulation. As mentioned in the previous section, using Eq. (1) to estimate the maximum Reynolds number in terms of the ratio of the largest to the smallest length scales that can be resolved, the maximum Reynolds number is found to be several hundred for an FTS.

When chemical reaction is included, additional physical parameters are involved. We shall use a non-premixed reaction to demonstrate how the physical parameters related to chemical reaction may affect the scaling and, thus, the technique for direct numerical simulations. For convenience in our discussion, we assume that the Prandtl and Lewis numbers are both unity, so that only one dissipative coefficient—namely, the viscosity—is an independent parameter. The chemical reaction is characterized by the Damköhler number Da_I, defined as

$$Da_I = (rC_\infty L_C)/u' \tag{2}$$

where r is the rate coefficient, C_∞ a characteristic value of the chemical concentration field C, and L_C a length scale characterizing C. The Damköhler number gives an estimate of the ratio of the reaction terms to the advection terms in the conservation equation for the chemical concentration. When it is on the order of unity, the diffusion length scale, i.e., the Batchelor length scale $(D\nu/\epsilon)^{1/2}$, and the thickness of the reaction zone are of the same order. (Here D is the molecular diffusivity of C.) A simulation that resolves the diffusion scale then will resolve the reaction zone. At high Damköhler numbers, for binary reactions, the ratio of thickness of the reaction zone to the diffusion length scale decreases as $\mathcal{O}(Da_I^{-1/3})$.[34] Inside the reaction zone, the species concentration is small and of the same order in Da_I as the thickness of the reaction zone. Assuming a mesh capable of resolving phenomena down to about one-third of the Batchelor length scale, the well-designed direct numerical simulations can probably handle up to about $Da_I = 30$ without losing numerical accuracy.

For very high Damköhler numbers, the reaction zone cannot be resolved using currently available computers. It is well known, however, that the rate of chemical reaction is controlled by the rate of diffusion of the reactants into the reaction zone, which, in this case, is extremely thin. If the reaction zone is treated as a sheet with zero thickness, the gradient of the concentration of the reactants is discontinuous there. The numerical solutions of the species concentration equation may thus encounter loss of accuracy. Fortunately, a conserved scalar, which is smooth across the reaction sheet, can be defined for cases in which the species diffusion coefficients are equal and the Lewis number is unity.[35] The species concentrations, including the reaction product, can be inferred from the conserved scalar. For a flow with constant density, accurate results can be obtained by numerical simulations using this approach.[22]

For a high-Damköhler-number flow in which chemical heat release affects the fluid dynamics by producing local variations in density, the situation is somewhat different. Although the species concentrations as well as the temperature field, and thus the density field, still can be inferred from the conserved scalar, the first spatial derivatives of these quantities are discontinuous at the reaction sheet. In the solution of the conservation equations for a variable density flow, spatial derivatives of the density field are required. Numerical inaccuracy due to the Gibb's phenomena may, thus, result near the reaction sheet in any numerical method intended to capture the reaction sheet. This discontinuity in derivatives is due to the discontinuous nature of the relationship between the conserved scalar and temperature (see Fig. 1) and may be circumvented by smoothing this relationship. (In a realistic reversible chemical reaction, this is actually smoothed by the existence of the reverse reaction.) In physical space, this smoothing process broadens the reaction zone into a region of finite thickness with artificial structure. If the smoothing process can be contained within a scale small with respect to the diffusion length, the effects of the artificial broadening of the reaction zone on the fluid dynamics as well as on the species diffusion may not be affected. Since the reaction is diffusion controlled, it is expected to be independent of the structure of temperature and density field within the artificial reaction zone. An alternative method is to develop a nonoscillating upwind scheme that contains the slope discontinuity of the variables in two or three grid points (e.g., the ENO scheme of Harten et al.[36]). The potential of using a conserved scalar for variable density flows has yet to be explored.

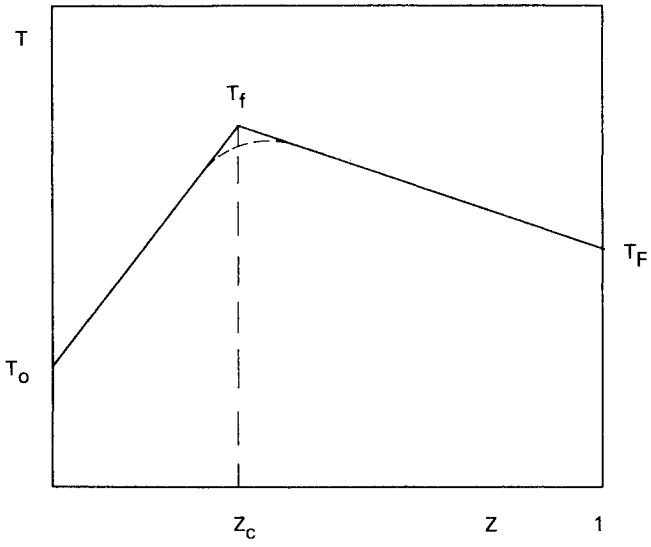

Fig. 1 Relationship between temperature T and conserved scalar Z.

For a reaction with an Arrhenius temperature-dependent rate, an additional parameter, E—the activation energy nondimensionalized by the adiabatic flame temperature—is present. This additional parameter is usually large so that the large activation energy asymptotic analysis[35,37] can provide valuable information. Since the Damköhler number, the nondimensional activation energy, and the Reynolds number are all large, there is a relative ordering among these parameters that determines the structure of the flame. It is known that in a flowfield where the local dissipation rate is high enough, flame extinction occurs.[38,39] Heat is diffused away from the flame rapidly enough so that the chemical heat release fails to sustain the flame temperature at a value above which chemical reaction occurs. Because of the exponential nature of the temperature-dependent reaction rate, the heat release is reduced rapidly once the temperature falls below the flame temperature. To establish the relative ordering of the parameters involved, we start with the known scaling of the flame thickness of $\mathcal{O}(E^{-1})$ when the flame extinction occurs.[38] The species concentration in the flame sheet is also of the same order in E. Therefore, the balance between the diffusion term and the reaction term gives

$$\nu/(L_k^2 E^{-2}) \sim r_f C_\infty E^{-1} \exp(-E) \tag{3}$$

where r_f is the frequency factor of the chemical reaction. This relation can be rewritten in terms of a redefined Damköhler number, $\tilde{D}_a$, as

$$\tilde{D}_a = \frac{Da_I R_L^{-1/2}}{E^3 e^E} = \mathcal{O}(1) \tag{4}$$

where Eq. (1) has been used, and Da_I only includes the frequency factor r_f. This is a relative ordering among the three parameters R_L, Da_I, and E for local flame extinction to occur. In this parameter range, the assumption of chemical equilibrium in the region outside of the flame sheet is no longer valid, as part of the flowfield is chemically frozen. If the Damköhler number is so large that the preceding relation is not satisfied, the chemical reaction is again in equilibrium and the flame thickness is scaled by an additional factor of $\tilde{D}a^{-1/3}$.

In many practical flows, both the Reynolds number and the Damköhler number are very large and are beyond the range

for accurate FTS. However, interesting information on flame extinction occurring in a high-Reynolds-number, high-Damköhler-number flow may be obtained by a simulation with a moderate Reynolds number, Damköhler number, and activation energy if the preceding relation can be satisfied. This conclusion, of course, is based on the assumption that a high enough Reynolds number can be attained in the simulations so that the estimate given by Eq. (1) can be employed. With continued improvement in the computational power of supercomputers, the accurate simulation of the dissipation range of a turbulent flow at moderate Reynolds numbers becomes increasingly possible.

Numerical Methods

With an understanding of the length scales of the physical phenomena involved and of the accuracy requirements of various approaches of direct numerical simulations, an appropriate numerical scheme must be chosen for resolving the physics. Various numerical schemes can be used in direct numerical simulations of turbulent reacting flows. These methods can be classified into three main categories: spectral and pseudospectral methods, finite-difference and finite-volume methods, and vortex methods. These methods vary in accuracy, computing efficiency, and flexibility in treating boundary conditions. Each method has certain advantages and disadvantages, with no one method the obvious choice for all problems. In selecting a numerical method for a specific problem, it is important to understand the properties of these methods, so that one may make the optimum choice for the particular problem of interest.

Much of the work on direct numerical simulations of nonreacting turbulent flows has employed spectral or pseudospectral numerical methods. (In fact, this has led to some confusion: some people have tended to equate direct numerical simulations with spectral numerical methods.) The application of these methods to turbulent reacting flows was initiated by Riley et al.[22] and was continued by McMurtry et al.,[23,24] Givi et al.,[39] and Leonard and Hill.[40]

In the spectral or pseudospectral method (see Refs. 41 and 42 for rather complete discussions of these methods), the dependent variables are expanded in truncated series of orthogonal functions satisfying the required boundary conditions. Spatial derivatives then are evaluated locally in the transformed domain, while nonlinear products are evaluated locally in the physical domain. Up to now, mainly Fourier series and Chebyschev polynomials have been used (although Legendre polynomials, Jacobian polynomials, and other series have sometimes been employed). With these functions, the mapping between the physical space and the configuration space can be performed efficiently using a fast Fourier transform algorithm. The spectral method, which is equivalent to a Galerkin method, involves eliminating entirely the aliasing errors that arise in evaluating the nonlinear terms. The pseudospectral method, which is equivalent to collocation, retains some of these aliasing terms. The pseudospectral methods, which are much easier to implement and run several times faster, have been used most often, although not exclusively.[3,10,43] Various time-stepping schemes have been employed with these methods, including leapfrog, Adams-Bashforth, and higher-order Runge-Kutta schemes.

Spectral and pseudospectral methods have the advantages that phase errors are very small and rates of convergence are very high. If the dependent variable is sufficiently smooth and the orthogonal functions have been chosen properly, then as the number of orthogonal functions N becomes large, the truncation error decreases faster than algebraically.[41] Various authors[44,45] have found that the pseudospectral methods are at least twice as accurate in each spatial dimension compared to finite-difference schemes using the same resolution.

In order to explore the capabilities of pseudospectral numerical methods when applied to chemically reacting flows, Riley et al.[22] applied the method to the color problem with diffusion and reaction. It was found that both diffusive and dispersive errors decay rapidly with N (the number of Fourier modes) when a sufficiently small time step is used. Because of this high convergence rate and the lack of phase errors, high gradient regions could be computed accurately and efficiently with a moderate number of Fourier modes. This property of the method is important for simulations of a reacting flow where the molecular diffusion is of primary concern. When the number of modes was not sufficient to resolve the dependent variables, a buildup of amplitude near the cutoff wave number occurred, leading to significant errors in the solutions.

There are several drawbacks with this method. The class of complete basis functions, which allow matching the boundary conditions and also possess the properties of rapid convergence, are limited. The application of Fourier series is restricted to problems with periodic or free-slip boundary conditions. Although Chebyschev polynomials can be applied to problems with arbitrary boundary conditions, the distribution of collocation points for the method may not be ideal for many problems. These collocation points are densely packed near the boundary with spacing of $\mathcal{O}(N^{-2})$. Additional mapping is required, particularly in the far field, to adjust the spacing to a more reasonable distribution. The method in its original form is limited in its capabilities for computing flows around complex geometrical shapes and for treating inflow and outflow boundary conditions. However, recent work on the spectral element method[46,47] has made considerable progress in removing these limitations. Spectral methods, because of their inherent nonlocal properties, also have difficulty in capturing discontinuities such as shocks while maintaining spectral accuracy. Gibb's phenomenon develops at the discontinuities, degrading the accuracy of the solution.

Finite-difference methods can be constructed to arbitrarily high orders of accuracy but with increasing computational effort. In general, second- or fourth-order schemes are used in computing complex flowfields. Unfortunately, the large dispersive and dissipative errors in second-order central-difference schemes produce results that are not acceptable for moderately high Reynolds-number flows or for flows with shock waves. Spurious oscillations occur near regions with large gradients, possibly causing the numerical computations to become unstable. To circumvent this problem, either explicit artificial dissipation is added to the scheme, or the scheme is constructed in such a way that artificial dissipation is implicitly included. Examples of the former can be found in Refs. 48 and 49, and those of the latter in MacCormack's[50] scheme and the Quadratic Upstream Interpolation for Convective Kinematics (QUICK) scheme.[51] Thus, the methods can be applied to smooth flows at moderate Reynolds number with numerical stability and reduced spurious oscillations. Sharp gradients are smoothed over several grid points. In fact, many schemes can compute flow with extremely high Reynolds number while retaining numerical stability. The Reynolds number in these computations probably loses its meaning, however, as the numerical viscosity dominates the molecular viscosity. Therefore, only large-scale phenomena may be captured accurately using such a method at high Reynolds number. Hence, in applying these schemes to reacting flows, one should be careful in the interpretation of the results. Examples of using MacCormack's scheme for large-eddy simulations can be found in the flow simulations in a propulsion device.[28,29]

To prevent artificial viscosity from smearing discontinuities (e.g., shocks) over a large number of grid points while eliminating spurious oscillations around a discontinuity, a class of numerical schemes has been developed. Boris and Book[52] were the first to construct a finite-difference scheme, the Flux-Corrected Transport scheme, which preserves the monotonicity of flow variables in a high-gradient region. The recently developed schemes, called Total Variation Diminishing (TVD) schemes,[36,53–56] also belong to this category. The

essential feature of these schemes is a "smart" artificial viscosity, in the form of a flux limiter, which is small in the region of smooth flow but reduces the numerical scheme to low order near sharp gradients. The solution can thus "negotiate" the sharp gradient without producing spurious oscillations. Study of the dissipative properties of TVD schemes using the color problem was discussed by Smolarkiewicz.[57] It was found that the solution maintained the monotonicity property. Dissipative errors, however, were substantial. Again, molecular diffusion cannot be treated accurately for a high-Reynolds-number flow, even when the computations are stable. This type of scheme is quite successful in computing very complex patterns of detonation waves.[58] Its applications to other reacting flows can be found in Ref. 59, where the flow is assumed inviscid and the chemical reaction is modeled.

Some attempts have been made to combine monotonicity-preserving schemes (in particular the Flux-Corrected Transport scheme) with spectral methods in order to treat problems with sharp gradients or discontinuities.[44] The results appear promising, but further work is required to determine the efficacy of this approach.

For an FTS of a reacting flow in which no phenomenological model is desirable, the detailed molecular dissipative processes are essential elements of the physics. Thus, the careful construction of a finite-difference scheme with sufficiently small numerical dissipation in high-gradient regions is important. The Reynolds number, the Damköhler number, and the activation energy for these simulations then will be restricted to moderate values. These restrictions are likely to be more stringent for finite-difference methods than for pseudospectral methods. For large-eddy simulations, however, the numerical dissipation can be considered as a crude subgrid-scale model.

Finite-difference methods have advantages over spectral methods in several respects. It is easier to construct a finite-difference code than a pseudospectral code for flow with complex geometry. If properly implemented, shock waves can be captured more accurately with finite-difference schemes. Finally, for the same number of grid points, the computational efficiency of a finite-difference scheme is generally higher than for a pseudospectral scheme.

An interesting numerical method for solving thermofluid problems is the vortex method, or, perhaps more appropriately, the distributed singularity method. Examples of the application of this method to reacting flows can be found in the research of Refs. 30, 31, and 60 for two-dimensional flows. Applications to three-dimensional nonreacting flows are just emerging.[61–63] Only two-dimensional flows will be discussed here. In solving the governing equations subject to the small-Mach-number approximation, the velocity field is decomposed into a solenoidal part and a potential part as follows:

$$\boldsymbol{u} = \nabla \wedge \boldsymbol{\Psi} + \nabla\Phi \tag{5}$$

If the vorticity distribution is discretized and its spatial distribution is known, then the solenodial velocity field can be obtained using a Green's function, which satisfies the required boundary conditions and is singular at a convex corner. The heat of combustion produces a local dilatation, which is idealized as a source term in the Poisson equation governing the potential field Φ. Since, in many cases, the density is considered constant, this source term amounts to a mass source. Again, a Green's function approach can be employed to find the potential flowfield. The combined flow velocity induced by each discrete vortex and dilatation source convects these sources to new locations. If a convex corner is present, then new vortices must be shed at the corner in order that the Kutta condition be satisfied there. Similarly, in order to match a no-slip boundary condition, vortices must be shed from the solid surfaces. Viscous diffusion is simulated by a random walk of the discrete vortices.

In its application to the combustion of a premixed gas, the flame sheet is treated as a discontinuous surface, and its location is tracked using the local laminar flame velocity.[64] It is equivalent, in spirit, to the shock-fitting method in the computation of compressible flows with shock waves. The smoothing of flame location, however, may be required to prevent a sawtooth instability.[65] This is the equivalent of adding some form of artifical dissipation, of which the effects on computational accuracy are not understood.

Since the flowfield away from the sources is expressed analytically in terms of Green's functions, only highly complex source regions require discretized numerical computations. Because the method is essentially grid free, and only the essential aspects of the flow are followed in detail, then presumably the computations can be made much more efficient than the numerical solution of the primitive equations. However, no direct comparison between the computational efficiencies of the distributed singularity method and the discretized field methods is available.

The methodology described earlier applies to constant density flows, but with concentrated mass sources to represent local volume expansion due to heat release. Certain dynamics are lost, however. For a flow with density discontinuity, such as a flame front in a premixed reaction, the velocity induced by the vortices and computed on each side of the discontinuity by the Biot-Savart law will be equal. Therefore, the dynamic boundary condition at the density discontinuity cannot be satisfied unless new vortices are introduced there. This is the manifestation of the effect of the baroclinic torque. Recently, the generation of vorticity at the flame front was taken into consideration by Pindera[65] using the vorticity jump condition across a discontinuity derived by Hayes, and by Ghoniem et al.[66] by indirectly computing the baroclinic torque term. In both cases, the effects of this baroclinic torque on the evolution of the flowfield were shown to be very strong.

The vortex method presents a useful tool to compute in two spatial dimensions the large-scale features of complex phenomena associated with reacting flows. The method can be very easy to code, and the computations are stable for very high Reynolds numbers. Whether the resulting flowfield, however, contains all features of a high-Reynolds-number turbulent flow is still a subject for debate. The results of simulations using this method in two dimensions must be interpreted in the context of a large-eddy simulation. Applications of this method to three-dimensional nonreacting flows have just begun, and the three-dimensional vortex stretching mechanism can thus now be simulated.[61–63] As discussed in the previous section, the spectral bandwidth of a flow increases as the Reynolds number increases. Therefore, although the vortex method may produce stable computations, in order to describe all turbulence scales accurately, the number of singular vortex elements may increase with Reynolds number at a similar rate as the computational elements in a pseudospectral or a finite-difference calculation.

Examples

In this section, we introduce examples of direct numerical simulations in order to demonstrate how such simulations can be used in the study of turbulent, chemically reacting flows. We begin with a sequence of related numerical experiments. This discussion will emphasize non-premixed reactions, although significant advances also have been made for premixed reactions.[31,64,65]

Step-by-Step Sequence

Perhaps the best way to illustrate the use of direct numerical simulations of reacting turbulent flows is to describe some examples from the recent literature. These examples are not meant to be exhaustive but are chosen to illustrate the general approach. We shall begin with a series of studies in which we have been directly involved. This series starts with the very simple case of a constant density flow, and the complexity of

the physical model is increased gradually. In doing so, each of the physical mechanisms can be turned on and off in order to isolate their individual effects on the overall behavior of the flow and chemical reaction. In this manner, a systematic understanding of the physics of turbulent reacting flows can be obtained.

The series started with the work of Riley et al.[22] The flow under consideration is a two-stream mixing layer with one reactant on each side. The fluid is assumed to be of constant density, so that the fluid dynamics are independent of chemical reaction. The species concentrations are influenced by advection, molecular diffusion, and chemical reaction. The chemical reaction is taken as a binary, single-step, irreversible reaction with a constant rate coefficient. (Hence, in particular, the reaction rate is temperature independent.) This simple model addresses effects of the fluid dynamics on the chemical reaction but not vice versa. In order to avoid the significant numerical difficulties associated with inflow and outflow boundary conditions, and to take advantage of Fourier pseudospectral numerical methods, the flow is assumed to be periodic in the streamwise direction. Therefore, the temporally growing mixing layer is studied, whereas in laboratory flows the spatially growing layer is investigated. However, the temporal problem is closely related to the spatial problem when viewed in a reference frame moving at the average velocity, and many of the dynamic characteristics of the spatial problem are contained in the temporal case. Full turbulence simulations in three spatial dimensions were performed using a $64 \times 64 \times 65$-point Fourier decomposition of the flow variables. Typical values of important parameters for the simulations are $Re = \Delta U L_{1/2}/\nu = 92$, $Da_I = rC_\infty L_C/U = 0.25$, and $Sc = \nu/D = 0.6$. (Here ΔU is the velocity difference across the mixing layer, and $L_{1/2}$ is the mean velocity half-width.) Also, cases with infinite Damköhler number were computed using a conserved scalar approach.

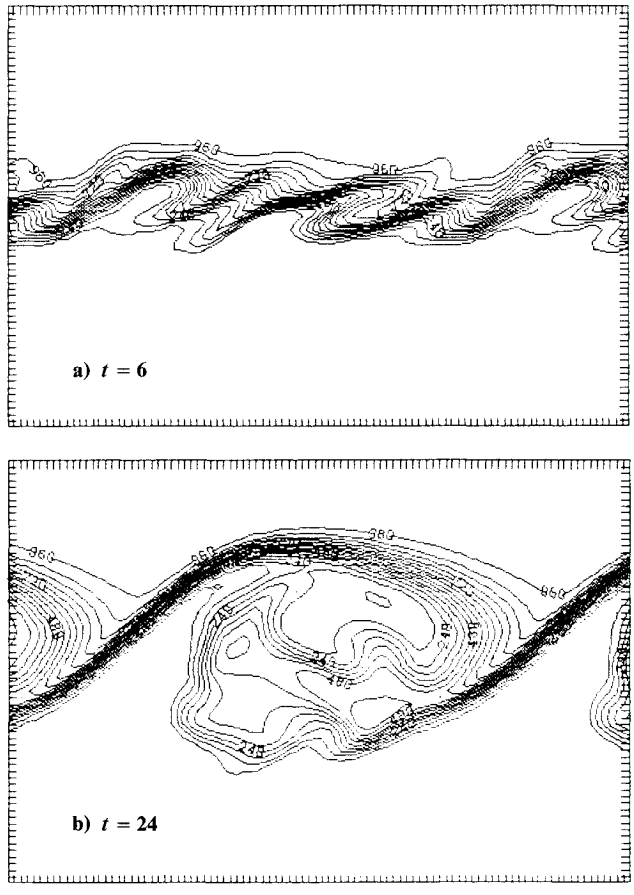

Fig. 2 Concentration contours in streamwise section at early and late times for an isothermal reaction.

Figure 2 shows two concentration contour plots in a streamwise section, displaying the time development of the layer and, in particular, the general behavior of the reaction zone. Even with this limited range of parameters, several important observations and conclusions are obtained concerning the fluid dynamical effects on chemical reactions. Qualitatively, the coherent structures in a turbulent flow increase the interface between the two species, thus increasing the overall reaction rate. Quantitative information is obtained by taking (spatial) averages of flow variables from the results of simulations. Mean product thicknesses are computed at various times and show that the profiles of chemical species concentrations are approximately self-similar. A most interesting result is obtained from the averages of the reaction term at various times. With constant reaction rate, the reaction term can be averaged to give

$$\overline{rC_AC_B} = r\overline{C_A}\,\overline{C_B} + r\overline{C'_AC'_B} \tag{6}$$

The individual components of this relation as a function of the cross-stream coordinate are given in Fig. 3. The two terms on the right-hand side are of the same order of magnitude and of opposite sign. It is very clear that the modeling of the correlation of the fluctuations of species concentration must be performed carefully to ensure that the overall chemical reaction rate is computed accurately. A surprising result from the study is the weak dependence of the product thickness on the Damköhler number. The product thickness for the infinite-reaction-rate case, which is completely diffusion controlled, is only about 10% greater than for cases with moderate Damköhler numbers. Finally, the similarity profiles for the average product, computed from the infinite-reaction-rate case, compared favorably with the experimental results of Mungal,[67] giving some confidence in the results of the simulations.

The parameter range investigated in these experiments was very limited. The effects of Damköhler number can probably be examined in further detail by performing simulations with values of up to about 20–30. The behavior of solutions can be studied as the reaction rate is increased systematically. The grid resolution has restricted the turbulence scales being simulated. With a supercomputer such as the National Aerodynamic Simulator, a $256 \times 256 \times 256$ grid-point simulation is possible and would greatly enhance the understanding of the physical processes at higher Reynolds and Damköhler numbers.

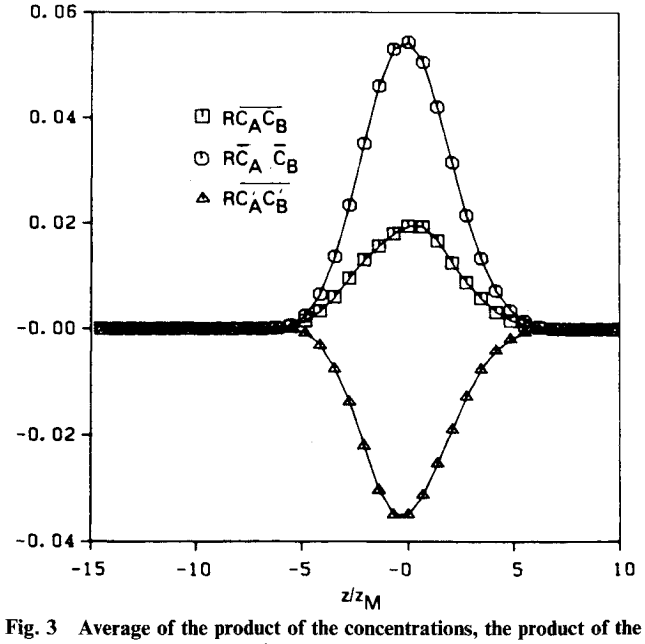

Fig. 3 Average of the product of the concentrations, the product of the averages, and the concentration correlation.

After addressing the fluid dynamical effects on chemical reaction, a logical extension of the work is to invesigate how the chemical reaction modifies the flowfield. The chemical reaction can affect the fluid dynamics through the variable density, which is caused by the thermal expansion of the fluid associated with chemical heat release. This aspect of the problem was addressed by McMurtry et al.[23,24] They assumed that the characteristic Mach number of the flow is much smaller than unity. [In practice, this was accomplished by keeping the Mach number of the ambient flow sufficiently small (< 0.3) and the chemical reaction sufficiently weak.] Starting with the fully compressible flow equations, including chemical heat release, the independent variables are formally expanded in a power series in the square of the Mach number. This results in a set of equations in which, at the lowest order, acoustic waves—a result of the elastic properties of the gas medium—are filtered out from the system, while the density variations due to heat-release effects are retained.[23,68-71] The advantage of using this set of approximate equations is that the numerical method does not need to track high-frequency acoustic waves. Thus, larger time steps can be used so that the computation is much more efficient. With the variable density of the fluid taken into consideration, the chemical reaction and the fluid dynamics are truly coupled.

McMurtry et al.[23] first developed a pseudospectral numerical scheme that solves the equations for variable density flows in two spatial dimensions. The flow under consideration is the temporally developing mixing layer as formulated by Riley et al.[22] Qualitative effects of the heat release are obtained, e.g., by comparing vorticity contour plots from these simulations to those obtained with no heat release (see Fig. 4). Vortex rollup is substantially suppressed by the heat release, as is evident from this figure.

In a two-dimensional flow, the vorticity transport equation can be written as

$$\frac{D}{Dt}\left(\frac{\omega}{\rho}\right)=\frac{1}{\rho^2}\nabla\rho\wedge\nabla p+\frac{\mu}{\rho}\nabla^2\omega \tag{7}$$

where ω is the velocity vector, ρ the density, and p the pressure. There are two principal mechanisms by which the fluid density can affect the vorticity dynamics. The first is through baroclinic torques, represented by the first term on the right-hand side. These torques, which are due to the differential acceleration of the fluid by a pressure gradient acting normal to a density gradient, are most effective in the neighborhood of the reaction surface, where the density is lowest and the density gradient highest. This surface separates two regions in which vorticities of opposite signs are produced. The ultimate effect appears to be to reduce the vorticity in the center part of the mixing layer, while increasing it at the outer edges, thus causing a more diffuse vorticity field. The second mechanism is caused directly by local fluid expansion. Without the baroclinic torques, the vorticity per unit mass ω/ρ would be conserved following the flow when viscous diffusion is neglected. Thus, decreasing the local density and, hence, increasing the local volume (e.g., through heat release) will result in a decrease in the strength of the vorticity. Again, the vorticity in the layer is made more diffuse. The combined effect is to weaken vortex rollup, causing less reactants to be entrained into the layer and, hence, resulting in lower product formation.

Based on this preliminary work in two dimensions, McMurtry et al.[24] developed a three-dimensional simulation code using the same methodology. In three-dimensional simulations, the additional effect of vortex line stretching is included, so that the simulations can more properly represent turbulence. Full turbulence simulations with typical parameter values of $Re = 500$ and $Da_I = 2$ were performed. Here $Re = \Delta U\delta/\nu$, where ΔU is the mean velocity difference across the layer, and δ is the initial vorticity thickness of the layer.

Secondary instabilities in the form of streamwise vortices

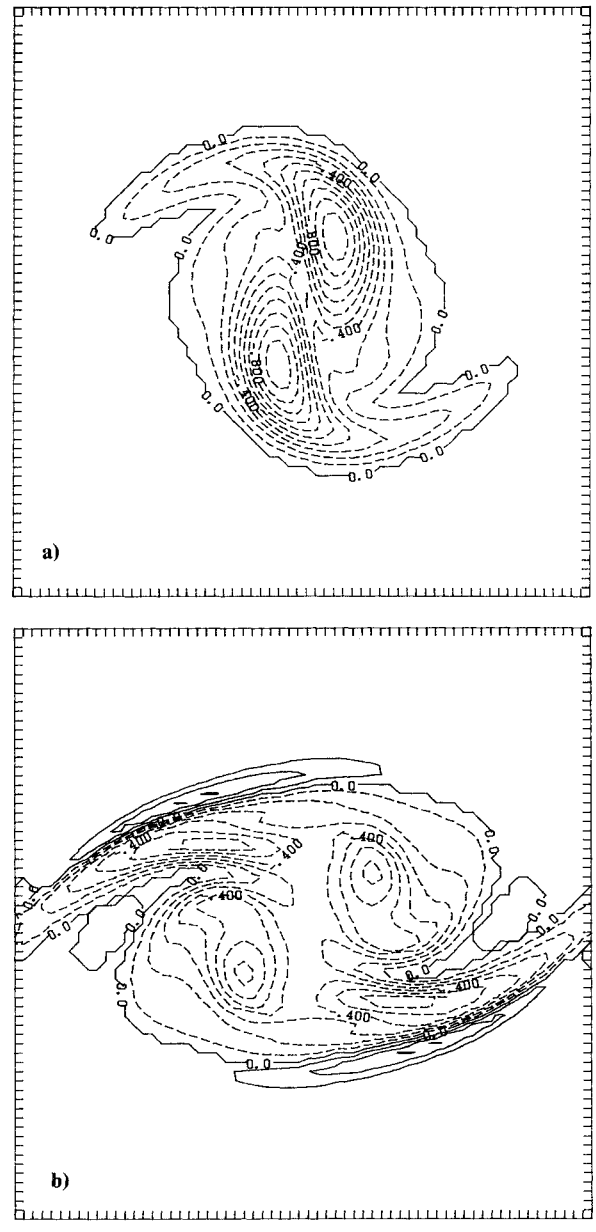

Fig. 4 Vorticity contour plots: a) without heat release; b) with heat release.

have been observed in the simulations of a constant density flow.[22] Figure 5 shows a comparison from McMurtry et al.[24] of instantaneous concentration contour plots in a cross-stream section for cases with and without heat release, revealing the three-dimensional nature of the flow. The heat release suppresses the secondary instabilities as well as the spanwise vortex rollup. The simulations generally confirmed what was observed in the two-dimensional case. In addition, the turbulent Favre-averaged kinetic-energy equation was examined, and the magnitude of each term in the case with heat release was compared to that from a constant density case in order to better understand the effects of heat release. The turbulence production resulting from the work done by turbulent stresses is shown to decrease in the case with heat release. It is interesting also to examine the left-hand side of the turbulent kinetic-energy equation:

$$\frac{\partial}{\partial t}(\bar{\rho}\tilde{q})+\nabla(\boldsymbol{U}\bar{\rho}\tilde{q})=\frac{\mathrm{D}}{\mathrm{D}t}(\bar{\rho}\tilde{q})+\bar{\rho}\tilde{q}\nabla\boldsymbol{U} \tag{8}$$

where $\bar{\rho}\tilde{q}$ is the Favre-averaged turbulent kinetic energy. Thus, the left-hand side can be written as the substantial

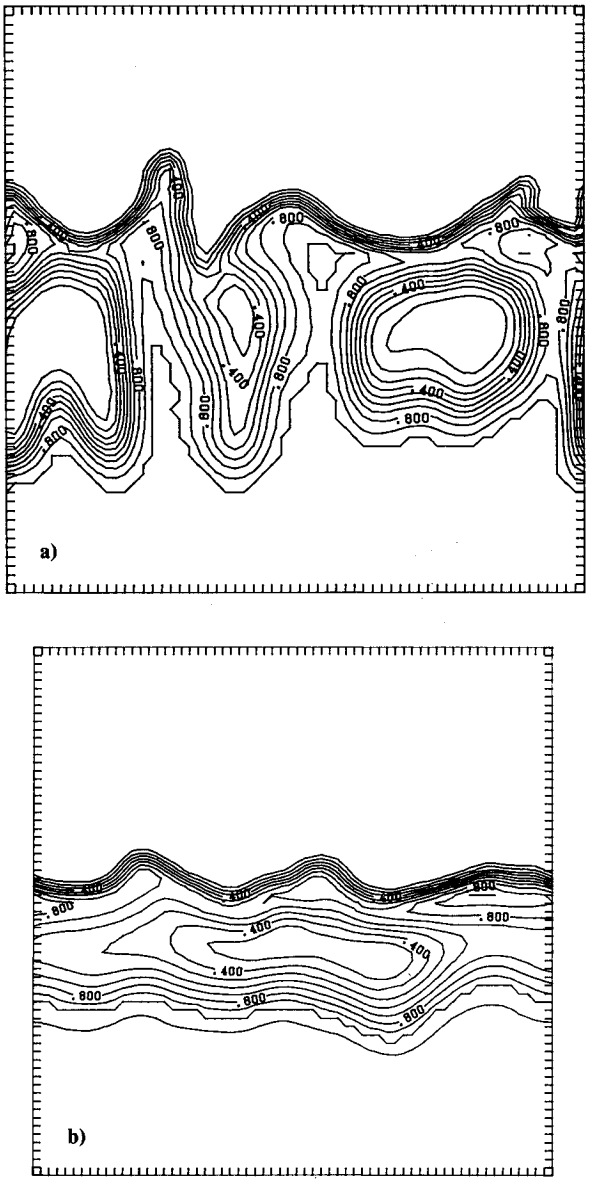

Fig. 5 Instantaneous species contour plots on a cross section x–y of a mixing layer: a) without heat release; b) with heat release.

derivative of the turbulent kinetic energy and as a term that gives the contribution from the dilatation ∇U. The dilatation field is, of course, the result of thermal expansion due to heat release. If the term with the dilatation field is moved to the right-hand side of the Favre-averaged turbulent kinetic-energy equation, it will represent destruction of turbulent kinetic energy due to thermal expansion, a conclusion consistent with that obtained by using the vorticity transport equation.

The type of methodology used in this study has significant potential in future research. In particular, the use of a conserved scalar for infinite-Damköhler-number cases, with possible artificial smoothing of the flame structure, is a potentially fruitful research direction. High-Damköhler-number simulations, with $Da_I = \mathcal{O}(30)$, may be performed to validate the infinite-Damköhler-number results using flame smoothing.

With a preliminary understanding of the heat-release effects on turbulent mixing, the next step has been to examine how a chemical reaction with a temperature-dependent reaction rate would affect the flowfield, and vice versa. According to the asymptotic analysis of ignition-extinction phenomena by Liñán,[38] a diffusion flame in a medium with given activation energy may be extinguished when the local scalar dissipation rate exceeds a certain limit. For convenience of discussion, we assume that the temperature, concentration, and all of the gas properties are the same for both the fuel and oxidizer, and that the frequency factor for chemical reaction and the gas density are both constants. The extinction limit is given by a lower bound on the local, instantaneous, reduced Damköhler number as

$$0.125 Da_{II} |\nabla Z|^{-2} (E^{-3} e^{-E}) \leq 0.315 e \tag{9}$$

where Z is an appropriately defined conserved scalar, $|\nabla Z|$ is evaluated locally at the stoichiometric surface, and Da_{II} is the second Damköhler number, defined in terms of the freestream values and a characteristic length. For more details of this extinction limit, see Ref. 35. Peters and Williams[72] argued that, in the turbulent diffusion flame of a jet, the scalar dissipation rate near the jet exit is so large that regions of local extinction (holes) in the flame sheet may become connected so that the flame sheet is ruptured. Thus, a flame cannot be sustained there. Hence, the flame lifts off and stabilizes at a location further downstream, where the local dissipation rate is smaller than the extinction limit. This explanation of flame liftoff is certainly plausible, although it is difficult to confirm experimentally. Numerical simulations of this phenomenon can be used to learn more about the structure of the flame sheet in a turbulent flow and to obtain a better understanding of the details of the rupturing mechanism of the flame sheet.

Givi et al.[39] initiated an investigation of this problem using a temporally growing mixing-layer simulation. The simulations were two-dimensional, and typical parameter values were $Re = 200$, $Da_I = 10$, and an activation energy of $E = 3$ when normalized by the adiabatic flame temperature. Figure 6 shows the contours of instantaneous rate of reaction. Along the braids of the rolled up vortex, where the strain rate is high, the temperature is reduced to a very low value and the flame becomes extinct. Givi et al. also solved the equation for a conserved scalar field. For the infinite-reaction-rate case, the surface where the scalar achieves the stoichiometric value is the flame sheet. An examination of the extinction condition given earlier, obtained from asymptotic theory, shows that, at the edge of the flame sheet in the simulation, the dissipation rate does satisfy the extinction criterion. This work is presently being extended to three dimensions.

Further interesting questions regarding flame extinction can be addressed using numerical simulations. For example, after the flame becomes extinct, the reactants diffuse toward each other to form a premixed fuel mixture. Subsequent events are not clear. For example, when the dissipation rate has decreased to a low enough level as a result of diffusion, would the flame then propagate into the mixture in the form of a premixed flame? The preliminary simulation results indicate that reignition does not occur, and the reacting sheet continues to shrink. Of course, only cases within a restricted range of parameters were simulated. Whether the conclusion can be generalized or not remains to be determined. The mechanism by which the flame is reignited is important in understanding the nature of flame liftoff. To further investigate the structure of a flame sheet, a numerical code for simulating the three-dimensional turbulent motion in a plane jet with chemical reaction is currently being developed.[73] Simulations of the flame extinction phenomenon using this code will provide a more complete picture than the previous two-dimensional simulations. As we have discussed, the activation energy in a practical system is large. The flame—when it exists—has a thickness on the order of E^{-1} compared to the diffusion scale. Therefore, numerical resolution is a serious problem. Yet a conserved scalar approach is not suitable since only part of the flowfield is in chemical equilibrium; the remainder is chemically frozen. An ingenious approach is needed that would treat the flame sheet as a discontinuity.

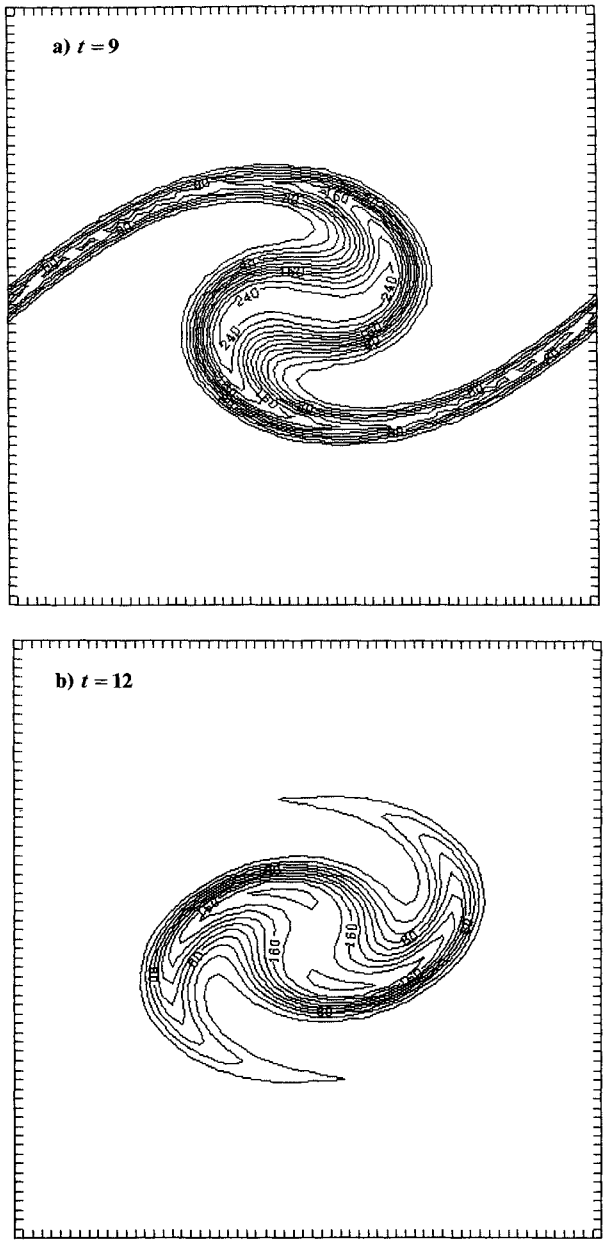

Fig. 6 Instantaneous reaction rate (with Arrhenius temperature dependence) in a mixing layer at two different times.

Other Examples

An example of the use of full turbulence simulations to test theoretical hypotheses for chemically reacting turbulent flows is given by Leonard and Hill.[40] They studied the behavior of two chemical species undergoing an irreversible, isothermal, second-order chemical reaction in a homogeneous, incompressible, decaying turbulent flow. The initial concentrations for the two species were in stoichiometric proportion and were defined as square waves that were out of phase so that the reactants were approximately segregated. In order to determine the effect of the reaction rate on various statistical properties, three calculations were performed: for Damköhler numbers of 0, 5, and 10. Pseudospectral numerical methods were used, the calculations being performed on three-dimensional $32 \times 32 \times 32$-point computational grids. The initial turbulent Reynolds number (based on the Taylor microscale) was 25, and the Schmidt numbers for both species was 0.7.

Two hypotheses were tested. The first was Toor's[74] hypothesis, which was made for reactants that are initially in stoichiometric proportion and have equal diffusivities. Based on results from certain limiting cases, Toor hypothesized that the reactant concentration covariance $\overline{C'_A C'_B}$ was independent of the reaction rate and, therefore, could be determined from a mixing experiment (without chemical reaction). Patterson[75] proposed a model for the joint probability density function (pdf) for (C_A, C_B) that does not depend explicitly on the initial stoichiometry and that enables the prediction of various terms in the moment equations for C_A and C_B, e.g., the reaction covariance term.

From the numerical simulations, Leonard and Hill computed, in particular, the reaction covariance term for the three cases for different Damköhler numbers. They found that, as hypothesized by Toor, this term was approximately independent of the reaction rate. This allowed, for example, the closure of the equations for $\overline{C_A}$ and $\overline{C_B}$, and their accurate estimation. The predictions of Patterson's model did not compare well with the simulation results. In order to explain this discrepancy, the joint of pdf C_A and C_B was computed from the simulation results and was found not to retain the form assumed by Patterson.

The results of Leonard and Hill are only preliminary. The resolution was fairly coarse, and the Reynolds number, especially toward the end of the simulations, was very low. The work gives a good example, however, of how direct numerical simulations can be used to test theoretical hypotheses regarding chemically reacting turbulent flows. We expect that this will be one of the principal uses of direct numerical simulations in the near future.

Another use of direct numerical simulations is in the prediction and study of reactant (and other parameter) pdf's. There are a number of advantages in theoretical approaches to chemically reacting turbulent flows that employ the pdf conservation equation (see, for example, Ref. 76). For example, the reaction term in the pdf equation is closed, and the conserved scalar approach can be readily used. Closure problems for other terms, e.g., the mixing terms, remain a primary difficulty, however. Another difficulty with this approach is in the solution of the resulting equations. The dimensionality of the equations is the sum of the usual dimensions (e.g., x, t) *plus* the usual dependent variables. Therefore, for reacting flows, the dimensionality of the system can become very large, obviating a solution by standard numerical methods. To circumvent this problem, Monte Carlo methods have been used to indirectly solve the pdf equation (and to obtain other statistical quantities).[77,78]

In the Monte Carlo approach, in order to solve the pdf equation, an auxiliary problem, sometimes called a Langevin problem, is often introduced. The Langevin problem is a theoretically realizable process that has, an its pdf equation, the original pdf equation of interest. To solve for the pdf or other statistics of interest, then, the auxiliary problem is solved often many times, and either ensemble, time, or spatial averages are performed. The advantage of this approach is that the Langevin problem is usually much easier to solve numerically, and the computational time increases approximately linearly as additional dependent variables are included.

When applied to chemically reacting turbulent flows, the Langevin problem for a modeled pdf equation is usually some simplified reacting flow system. As more sophistication is added to the modeled terms in the pdf equations, the Langevin problem becomes more like the original turbulent reacting flow. The realism of the pdf equation then is indicated by the sophistication of the corresponding Langevin system. As pointed out by Riley and Metcalfe,[79] direct numerical simulations can be considered as solving Langevin systems for particular pdf model equations. And, in fact, considerable physics can be incorporated into this system, making the pdf model highly realistic.

Past Langevin systems used in Monte Carlo approaches for solving the pdf equations have not directly included, for example, the physics of the large-scale structures occurring in the flow, nor of the Schmidt and Reynolds number effects on

micromixing. Those features recently were included in a study by Lin and Pratt[80] of a chemically reacting, spatially growing free shear layer. They considered a diffusion flame with an isothermal, irreversible, infinite-rate, binary chemical reaction. A two-dimensional large-eddy simulation was employed, using a modified vortex method to compute the unsteady (incompressible) velocity field. The chemical reaction was treated using the conserved scalar approach, and, in particular, molecular mixing was treated using Curl's[81] model. The mixing rate β was determined from the estimation by Broadwell and Breidenthal[82] of the time scale required to diffuse across the Kolmogorov length scale. They used

$$\beta = C|\omega(x,t)|(Re^{1/2}/Sc) \tag{10}$$

where C is an empirical constant and ω the local grid-scale vorticity. Their work can be considered one of the first where subgrid-scale models were employed in a large-eddy simulation involving a chemical reaction.

Lin and Pratt carried out simulations for three different velocity ratios ($r = U_1/U_2 = 0$, 0.3, and 0.6), and two different Schmidt numbers (0.7 and 600). The latter corresponded to values for experiments carried out by Konrad[83] and Breidenthal,[84] respectively. Their results for various velocity statistics gave reasonable agreement with laboratory data, except for the lateral rms velocity. Predictions of various concentration statistics—in particular, the dependence of the nondimensional product thickness on the Schmidt number—showed reasonable agreement with the laboratory data.

We believe that the utilization of direct numerical simulations for Langevin systems for pdf model equations has considerable potential. It allows the input of rather sophisticated models into the pdf equations. On the other hand, pdf models might suggest particualr subgrid-scale closures to be implemented in large-eddy simulations.

Eswaran and Pope[85] applied full turbulence simulations to the problem of a scalar field developing in time on a statistically homogeneous, stationary velocity field in order to obtain information regarding the pdf's of the scalar and of the scalar dissipation rate. A $64 \times 64 \times 64$-point computational grid was employed, the initial scalar field was bimodal, the turbulence was forced at low wave numbers to a statistically steady state, and only a passive scalar was considered. They found, in particular, that although the pdf starts out as a "double-delta" function, it ultimately tends to a Gaussian. Furthermore, the scalar and the scalar dissipation rate, in the early stages, were not statistically independent, contrary to the assumption of Bilger.[86] The pdf of the logarithm of the scalar dissipation rate, however, ultimately reached an approximately Gaussian self-similar state, implying that the two had finally become statistically independent.

The numerical simulation of fully compressible, turbulent, chemically reacting flows is in an embryonic state. There are specific physical phenomena in which acoustic waves are an integral component. For example, turbulent reacting flows in a ramjet combustor may interact with acoustic waves to produce large-amplitude pressure oscillations.[87] Furthermore, Kelvin-Helmholtz instabilities are much weaker in supersonic mixing layers, which may result in drastic reductions in the chemical reaction rate. Several preliminary attempts have been made to simulate these flows. For the ramjet problem, Jou and Menon[28] and Menon and Jou[29] used large-eddy simulations to address the interaction between vorticity fluctuations and acoustic waves in a combustor with no chemical reactions. Guirguis et al.[58] included chemical reaction in a similar configuration. We shall briefly review the work of Jou and Menon[28] as an example of how one can deduce acoustic information from the results.

Menon and Jou[29] considered the flow in a simplified model of a ramjet combustion chamber by solving the compressible Navier-Stokes equations in axisymmetric form using MacCormack's[50] explicit algorithm. It is expected that only the longitudinal acoustic mode will interact with the vortical disturbances to produce the low-frequency pressure oscillations prevalent in the combustor. Thus, axisymmetric vortical disturbances may be predominant.

As shown in the vorticity contour plot in Fig. 7, the shear layer behind the backward-facing step rolls up into vortices, and the merged large structures subsequently impinge on the nozzle wall downstream. To understand the physical phenomena, the acoustic field is visualized in a unique way. If one defines the acoustic component of the disturbances to be that of an unsteady potential flow,[88] the instantaneous dilatation field $\mathscr{D}$ and the acoustic potential Φ are related as follows:

$$\nabla^2\Phi = \mathscr{D} \tag{11}$$

Comparing this with the equation relating the vorticity to the stream function ($\nabla^2\psi = -\omega$), which represents the solenoidal field, it is seen that the dilatation field plays a role in acoustics analogous to that of vorticity for a solenoidal field. Since vorticity has been used successfully to visualize rotational disturbances, the dilatation field may be taken as a representative quantity for visualizing acoustic disturbances.

Figure 8 shows an instantaneous dilatation field together with the corresponding vorticity field. It was found that the near-field dilatation is dominated by the pseudosound, and the propagational aspects of acoustic waves are lost. Thus, the dilatation field gives the detailed characteristics of the acoustic sources. Around each vortex, a quadrupole dilatation field is clearly identifiable. Near the region where large vortex structures impinge on the nozzle, the structure of the dilatation field appears very complex. The acoustic sources near the vortex impingement point, however, can be considered compact. The behavior of such a compact source can be represented by its multipole expansion in terms of a distributed dilatation field. Therefore, we take the first two spatial moments of the complex dilatation field over a region to give the monopole and dipole as follows:

$$Q_1 = \int\int_V \mathscr{D}\, dV \tag{12}$$

$$Q_2 = -\int\int_V \mathscr{D}x\, dV + \frac{Q_1}{V}\int\int_V x\, dV \tag{13}$$

The time variation of the vorticity fluctuations in the same region also are determined by integration over the same volume. Figure 9 shows the time variation of the monopole, the dipole, and the vorticity. It is evident that, as the large vortical structures impinge on the nozzle wall, a strong dipole, which is approximately 180 deg out of phase with the vorticity fluctuation, is present.

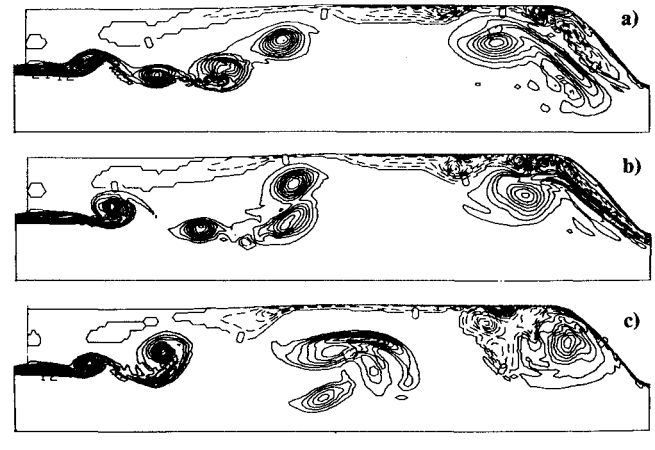

Fig. 7 Time sequence of vorticity contour plots in a ramjet nozzle; Mach number = 0.32.

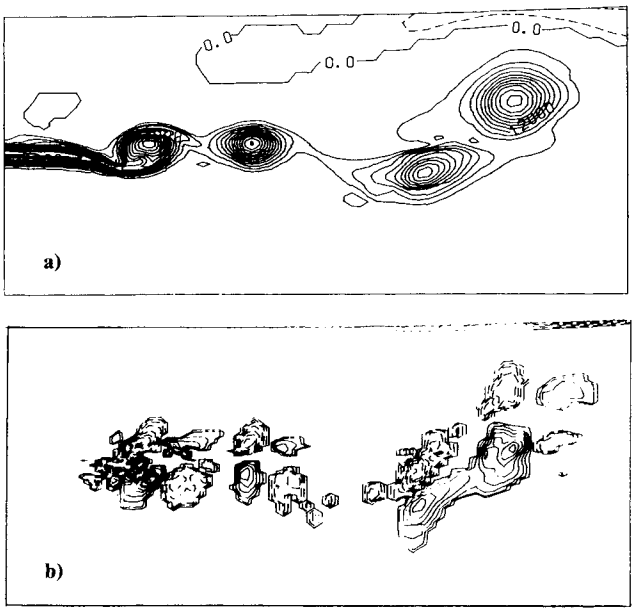

Fig. 8 Instantaneous dilatation and vorticity fields: a) vorticity contours; b) dilatation contours.

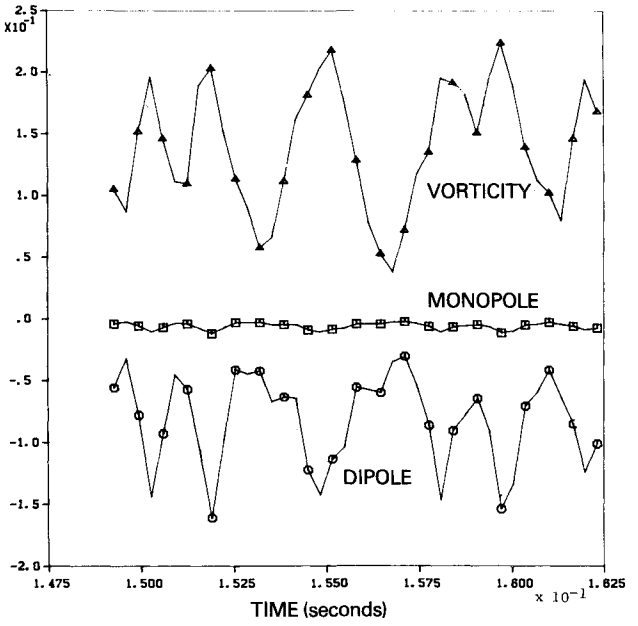

Fig. 9 Time histories of vorticity and acoustic monopole and dipole strength in a ramjet nozzle.

Jou and Menon[28] used this information to construct a model for acoustic wave/vortex interactions. This method of simulation and data analysis demonstrates the potential use of numerical simulations of compressible flow in analyzing the behavior of flow variables such as the dilatation field, which are difficult or impossible to measure experimentally. The extension of this simulation method to cases with chemical reaction, which may create strong acoustic monopoles, is currently under investigation. Preliminary simulations of the combustion and flowfield in a ramjet have been reported by Kailasanath et al.[59]

Supersonic combustion is an active area of research, partly because of the current interest in the National Aerospace Plane. Drummond[89] attempted to simulate a mixing layer with a realistic hydrogen-oxygen reaction. Some further results were presented by Zang et al.[90] The Mach number of 1.5 and Reynolds number of 3700 were chosen. The finite-thickness trailing edge of a splitter plate was suspected of playing a primary role in triggering the instabilities in a supersonic flow. The results are preliminary and require further research.

Conclusions

Direct numerical simulations of turbulent reacting flows have begun to attract interest among combustion scientists, fluid mechanicists, and numericists. This paper reviews some research on turbulent reacting flows using direct simulations, emphasizing the methodology, the kinds of results obtainable, and the strengths and limitations of the approach.

There are two implementations of direct numerical simulations: full turbulence simulations (FTS), in which all of the dynamically significant space and time scales are resolved, and large-eddy simulations (LES), in which the governing equations are filtered at the numerical grid scale and the subgrid-scale motions modeled. Because of limited numerical resolution, FTS is restricted to moderate Reynolds and Damköhler numbers (although the conserved scalar approach can, for certain cases, eliminate the latter restriction), whereas LES can be applied, at least in theory, to high-Reynolds-number, high-Damköhler-number flows. Three general classes of numerical methods have been used in the implementation of direct simulations: spectral methods, finite-difference methods, and vortex methods (and some combinations of the three). Each numerical method has its own advantages and disadvantages, with no one method the obvious choice for all problems.

The potential advantages of direct numerical simulations, when the method can be applied, are the following: the flow can be examined in detail, since all quantities are known at each point in space and time; parameters can be varied easily and experimental conditions are controlled easily; large-scale structures are directly addressed; and results are less sensitive to the models used, since, at most, only the smaller scales are modeled. The main disadvantages are the limitation in the spatial and temporal resolution available and the large amount of computer resources required, both disadvantages of which can be severe. Currently, typical applications are similar to those of laboratory experiments, i.e., understanding particular physical processes and developing and testing models.

In the foreseeable future, only two to three decades of length scale can be resolved using the most powerful computational facilities available. Full turbulence simulations require the resolution of all relevant length scales, down to the Kolmogorov scale for a nonreacting flow. Thus, only flows with moderate Reynolds numbers can be simulated. Furthermore, in chemically reacting flows, the Damköhler number and the activation energy are usually very large. An additional length scale, the thickness of the reaction zone, which can be much smaller than the Kolmogorov scale, must be resolved. Fortunately, in the limit of chemical equilibrium and for a restricted class of transport coefficients, a conserved scalar can be defined for which the governing equation is simple. Under this simplification, the reaction zone degenerates to a discontinuous sheet. Therefore, if the discontinuity can be captured, full turbulence simulations using the conserved scalar approach then will require the same resolution as the nonreacting case. This direction is one of the most promising for future research. With moderate Reynolds numbers, the simulations can be used as a research tool to provide important information on the intricate interactions between fluid dynamics and chemical reactions. The nature of these interactions, in many cases, may be approximately independent of the Reynolds number. This information can then be used to construct turbulence models for the computation of chemically reacting flows with higher Reynolds number and subgrid-scale models for large-eddy simulations.

For computations of turbulent reacting flows with parameter ranges encountered in most practical systems, large-eddy simulations are required. Thus, the development of accurate subgrid-scale models is a most urgent task. (See Ref. 91 for a

discussion of some of the difficulties in developing subgrid-scale models for chemically reacting flows and some criteria that a subgrid-scale model should meet.) Present subgrid-scale models for nonreacting flows rely on several physical hypotheses. In particular, a continuous flux of energy (or scalar variance) from low to high wave numbers is usually assumed, which implies at most a weak dependence of the larger scales of motion on the smaller scales. Furthermore, some sort of universality (e.g., a Kolmogorov spectrum) at high wave numbers is hypothesized. The validity of both of these hypotheses is probably also required for the successful application of LES to turbulent, reacting flows. For example, if the direct effects of the subgrid-scale motions on the computation scales of motion are very strong, then it is unlikely that accurate subgrid-scale models can be developed and reliable large-eddy simulations performed. If the effects of the subgrid-scale motions are weak, however, then there is reason to conclude that the LES may be employed successfully.

For large-Damköhler-number reactions, the smaller scales can be very energetic due to the chemistry at the narrow flame sheet. Hence, the small-scale behavior would be expected to be very different from that of nonreacting flows, so that the development of subgrid-scale models may be very difficult. One approach that appears to be providing useful information for nonreacting flows is renormalization group theory,[92] which can be formulated to directly address subgrid-scale issues. This approach also relies on the assumptions of energy flux and universality mentioned earlier, however, and so may have to be somewhat modified to treat chemically reacting turbulent flows.

For direct numerical simulations of compressible, chemically reacting flows, several important issues require attention. The first is the treatment of sound waves. Unlike vortical disturbances, which decay rapidly away from the source, acoustic waves may propagate great distances and, upon interacting with a boundary, be reflected and refocused into the turbulent region. A simulation of a subsonic flow using a finite domain may excite certain acoustic eigenmodes if the boundary of the computational domain is a surface that reflects sound waves. Therefore, careful formulation of the boundary conditions is required to simulate the true physical properties of the computational boundary. A second issue involves the computation of shock waves in a supersonic flow. In order to capture shock waves without spurious oscillations, most of the numerical schemes must contain some form of artificial dissipation. To resolve the dissipation scale in a full turbulence simulation, instantaneous high-gradient regions must be treated properly. Although most of the finite-difference schemes with high-gradient regions will be stable, the relative magnitudes of the artificial dissipation terms and those of the real dissipation terms must be monitored continuously to ensure accuracy.

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