LOCAL, SMALL-SCALE INTERACTION OF TURBULENCE WITH CHEMICAL REACTIONS IN H₂-O₂ COMBUSTION

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ABSTRACT
A brief survey of commonly used techniques for simulating turbulent combustion is presented, and it is noted that, except for direct numerical simulation (which is too computationally intensive even on foreseeable supercomputers), none of the current methods is able to predict details of chemical kinetics/turbulence interactions. A new approach, based on an extension of earlier work with one-dimensional mathematical models of turbulence by McDonough and co-workers (1984a, b, 1986, 1989), is applied to study a simple, single-step forward reaction H₂-O₂ combustion problem. The method requires no averaging, or modeling, at any level due to an additive multi-scale decomposition of governing equations. Thus, like direct numerical simulation, it is completely consistent with the original, unaveraged equations; but required arithmetic is significantly reduced via consistent linking of large-scale and small-scale phenomena, resulting in the ability to focus on local regions and consistently (with respect to the full equations) simulate phenomena within these regions to a high degree of accuracy. In addition, the method is naturally parallelizable at several algorithmic levels. This technique, termed additive turbulent decomposition, is treated theoretically, and then applied to the one-dimensional, viscous, compressible Navier–Stokes and species equations. Preliminary computational results showing detailed chemical kinetics/turbulence interactions at the tip of an H₂-O₂ diffusion flame are presented and discussed for a flow with Reynolds number 6000, and thermal and mass diffusion Peclet numbers of 1000 and 3000, respectively. Computed results show a relatively long period of increase in negative amplitude of H₂ and O₂ concentrations followed by onset of chaotic oscillations simultaneously in velocity and temperature. Corresponding fluctuations then begin to appear in the concentrations via feedback from advective and species production terms.

1. INTRODUCTION
There are many fundamental, open questions concerning the physical phenomena associated with nonpremixed and premixed combustion, and one of the most interesting and important involves the interaction of hydrodynamic turbulence with the chemical kinetics of the combustion process. Current knowledge in this area is quite limited, in part because our understanding of turbulence in nonreacting flows is still very rudimentary at best (see Lumley, 1990). Nevertheless, there is much activity in the area of turbulent combustion research in general, as can be seen from recent reviews, for example by Pope (1990), Peters (1988), and the book by Libby and Williams (1980) and portions of the book by Williams (1985a). In addition, an excellent overview of turbulent combustion research up to 1985 is provided by Williams (1985b). Especially in the books, Libby and Williams (1980) and Williams (1985a), much emphasis is placed on analytical techniques, primarily perturbation analyses, to obtain either closed-form solutions or simplified equations to which numerical
methods can be easily applied. While there is much that can be contributed to the understanding of simplified models in this way, many assumptions must be made to obtain a tractable problem. In the end, this necessarily limits the applicability of the results, leading Williams (1985a,b) to caution that no one approach will likely be able to treat all problems in turbulent combustion.

Within this framework, however, it is important to note that some useful and important techniques have evolved, usually with the help of experimental results. One such approach is the conserved scalar formalism which has been quite successful in the study of laminar diffusion flames (see Bilger, 1980). Recently, efforts have been underway to extend applicability of this method to turbulent reacting flows (Bilger et al., 1990; Sivathanu and Faeth, 1990a,b). But it must be noted that there are fundamental assumptions inherent in this approach (see Williams, 1985a) that preclude its use in the analysis of many turbulent reacting flows. In particular, two main assumptions required by this technique are chemical equilibrium and Lewis number, Le, equal to unity. Furthermore, because shapes of, probability density functions (PDF's) of the conserved scalars must be assumed, and then fit to experimental data, the method is not predictive. It thus does not appear possible to employ this approach to fundamental studies of turbulence/chemical kinetics interactions.

Another, again basically perturbation expansion, approach is that of using wrinkled laminar flamelet models to simulate turbulent flames, as developed by Clavin (1985). As noted in Williams (1985a), the basic assumption underlying this method is that the laminar flame thickness is small compared with the Kolmogorov integral scale of the turbulence. It should also be mentioned that no detailed turbulent velocity fields are computed when using this approach, so we must conclude that interactions between turbulence and chemical kinetics would be difficult (impossible?) to study with this technique.

The two other main approaches to the study of turbulent combustion are experimental and computational. Many researchers are active in experimental investigations of turbulent combustion; a few recent studies pertinent to the present work include those of Magre and Dibble (1988), Drake (1986) and Mungal and O'Neill (1989). As alluded to above, such results are crucial for many modeling efforts, both in constructing the models and in checking their range of validity. Moreover, for many combustion processes, particularly those in which soot formation and radiation effects are significant (e.g., Saito et al., 1986 and Syed et al., 1990), neither perturbation techniques nor numerical modeling have yet been very successful. In such cases, experiments are needed to guide the development of computational models, as noted recently by Kennedy et al. (1990).

In recent years computational techniques have begun to receive increasing attention due to the wide availability of supercomputers, and at the same time, the tremendous improvements in numerical algorithms. Turbulence simulation in general, and calculation of flows involving turbulent combustion in particular, are at the forefront of research in computational fluid dynamics.

There is a complete range of methods now being employed for turbulence simulation, and all of these have been applied to the problem of turbulent combustion, at least on a limited basis. For practical engineering calculations, the only methods that have been widely used to date are based on the Reynolds-averaged Navier-Stokes (N.-S.), energy and species concentration equations. It is well known that these systems contain more unknowns than equations — a manifestation of the turbulence "closure" problem, arising from averaging quasilinear terms in the N.-S. equations (and bilinear, and genuinely nonlinear, terms in the energy and species equations). In particular, one must deal with averages of products of fluctuating quantities (second moments) for which there are no equations, and this is typically handled with turbulence "modeling."
The turbulence models in widest use are, not surprisingly, the simplest and least computationally intensive: mixing length and k-ε. In such models the second moments (i.e., Reynolds stresses, etc.) are expressed in terms of averaged (first moment) quantities via empirical relations, thus closing the system at first order. This simple, straightforward approach completely eliminates the ability to study turbulence/chemical kinetics interactions because all terms on the length and time scales of these interactions have been written as simple averaged quantities. Second order closures would permit simulating at least time averages of products of fluctuating quantities, but it is not clear that this is of any value for detailed analyses. In any case, correct treatment of the nonlinear chemical reaction terms is very problematic when any typical averaging method is employed. Moreover, work by McDonough and Peng (see Peng, 1990) with a simple nonlinear model problem indicates that when time averaging is used, solutions to the time-averaged equations do not equal time averages of corresponding solutions to the unaveraged equations — even when accurate Reynolds stresses have been employed to close the former. This inconsistency implies that great caution should be exercised when applying time-averaged turbulent modeling.

A somewhat different approach to turbulence modeling has been studied in recent years, beginning with work by Chung (1976), and more recently by O'Brien (1981) and Pope (1985). This approach employs PDF’s of the usual dependent variables as the problem solution variables, and by doing so is able to exactly treat averaged nonlinear terms. A thorough recent review is provided by Pope (1990). Because of the exact handling of nonlinear terms, the PDF method is particularly attractive for combustion problems, and some applied problems have already been solved using this technique (cf. Ooms et al., 1989). A concise treatment of this approach is given in Williams (1985a, b) where it is noted (as is also done by Pope, 1990) that although there is no closure problem associated with the nonlinear terms, there is a very serious difficulty with linear diffusive terms. Furthermore, even if this were not the case, in the end we obtain only averaged quantities from the PDF approach, and it is not clear that these will be of much help in understanding details of turbulence/chemical kinetics interactions.

At the next level of turbulence modeling is large eddy simulation (LES), first introduced by Deardorff (1974) for use in studies of atmospheric turbulence. The basic underlying ideas in LES are somewhat similar to those embodied in the classical, Reynolds-averaged approaches; but details of their interpretation and implementation are rather different. In particular, LES retains the decomposition of flow variables into large-scale and fluctuating (subgrid-scale, in LES terminology) parts. However, in LES averaging is spatial, rather than temporal or ensemble as in earlier approaches. This permits consistent treatment of time-dependent problems, but still leads to a closure problem, just as in the classical methods. Initially it was believed that this would not be severe because it involved subgrid-scale quantities representing motion on scales with presumably universal (and hence, easily modeled) behavior. But as reported in reviews by Ferziger (1983,1985) and Rogallo and Moin (1984), this has not proved to be the case; subgrid-scale modeling is a very weak link in the overall LES procedure. Moreover, even though the averaging is spatial, it still leads to serious difficulties in treating the nonlinear chemical reaction terms. Thus, completely independent of the large amounts of floating point arithmetic required by LES, even for simple hydrodynamic flows, it is not clear that it will ever be readily implemented for problems associated with the study of turbulence/chemical kinetic interactions. In particular, the equations have been averaged, and modeling is required, on precisely the length scales at which such interactions take place. LES is not predictive on exactly the scales we need to simulate in this problem.
The final well-known turbulence computation technique is direct numerical simulation (DNS). This method, probably first used by Orszag (1969) in studies of transition to turbulence, is conceptually the simplest. One merely numerically solves the N.–S. equations, without averaging or modeling at any level, using a spatial and temporal discretization sufficiently fine to capture all relevant behavior. Especially in light of the landmark paper by Ruelle and Takens (1971) in which it was shown that the N.–S. equations possess turbulent like, chaotic solutions, DNS would appear to always be the preferred approach to turbulence simulation. But straightforward dimensional arguments show that the required floating point arithmetic scales with the cube of the Reynolds number, Re, for simple hydrodynamic flows. Even on modern supercomputers this limits the range of computable flows to \( Re \leq O(10^6) \).

Clearly, the total arithmetic count becomes much worse when chemical reactions are considered. In the first place, if the reacting system consists of N species, then N additional equations (energy plus N-1 species concentrations) must be solved, and each of these is far more complicated than the original N.–S. equations. Furthermore, if the physical situation is such that the Damköhler number, Da, is large, then the characteristic chemical times will be far shorter than the hydrodynamic times; hence, much smaller numerical time steps will be required. It is not difficult to see from this that DNS will not be a practical tool for turbulent combustion simulations for a long time to come, as has already been noted in recent reviews, e.g., Pope (1990).

In the present paper we will describe a new approach to simulation of turbulent combustion. Development of this technique began with a study of simple 1-D models of hydrodynamic turbulence by McDonough et al. (1984a,b), and McDonough and Bywater (1986,1989). The method, which we now term additive turbulent decomposition (ATD) can be viewed as lying between LES and DNS in terms of algorithmic structure. Solution variables are decomposed somewhat as in LES (and essentially all other turbulence simulation techniques), but no averaging (or filtering) is employed to define the large-scale equations. As a consequence, there is no closure problem, and hence, no required modeling. Thus, ATD like DNS is completely consistent with the N.–S. equations (and to any other equations to which it is applied). In some respects it can be considered as simply a different implementation of DNS, but there are certain advantages to ATD that are not available in DNS. In particular, the ATD algorithm was designed to be naturally parallelizable, but at the same time it allows consistent computations over limited ranges of length and time scales, rather than requiring that all scales be computed, as in DNS. This feature can result in very significant savings of arithmetic in specific applications, and it will be exploited in the present study.

The work to be reported here consists of primarily a theoretical development of ATD applied to \( \text{H}_2\text{O}_2 \) diffusion flames in the context of a 1-D model problem. Preliminary computational results will be presented, but they should not be construed to correspond strictly to what might be observed in laboratory experiments. On the other hand, they will at least show similarities to data obtained along the centerline of axisymmetric flames. Simulations have been run with fairly high Re and very low Mach number, M. This allows neglect of buoyancy effects, and at the same time keeps the transition Mach number at a relatively low value. To achieve as much simplicity as possible in this initial study, we will consider only the forward, one-step reaction

\[
\text{H}_2 + \frac{1}{2}\text{O}_2 \rightarrow \text{H}_2\text{O}.
\]

It will be clear from the theoretical developments, however, that much more complicated chemical systems can be treated in an analogous way.

The remainder of the paper is organized as
follows. In the next section we will present the governing equations, and apply the additive turbulent decomposition to obtain the corresponding large-scale and small-scale equations. We will then focus attention on the small-scale equations, deriving the Galerkin approximations and describing the numerical solution technique. In the third section we will present and discuss some representative results that directly show the nature of the interaction between hydrodynamic turbulence and chemical kinetics on the small scale for the model problem. In the final section we will summarize what has been learned in the present study, and indicate what we believe to be fruitful directions for future research involving ATD) applied to problems in turbulent combustion.

2. THEORETICAL ANALYSES

In this section we will begin by presenting the equations that govern our model problem, the 1–D, low-Mach number, viscous, compressible N-S. and species concentration equations. We will then select scaling quantities and write the equations in dimensionless form. The additive turbulent decomposition formalism will then be introduced, and applied to obtain large- and small-scale equations. The latter of these will be approximated with a local Galerkin procedure that leads to systems of first order ordinary differential equation (ODE) initial value problems in the neighborhood of each discrete point of the large-scale approximation.

A. Governing Equations

As already noted, we will consider a 1–D model problem corresponding to combustion of H2 and O2 in a very low Mach number, relatively high Re diffusion flame. The governing equations for this situation will be taken to be

\[ \rho_u + (\rho u)_x = 0 \]  
\[ (\rho u)_t + (\rho u^2)_x - \mu u_{xx} = -p_x \]  
\[ \alpha T_t + (uT)_x - \alpha T_{xx} = - \frac{1}{\rho c_p} \sum \text{h}^0_i w_i \]

\[ (\rho Y_i)_t + (\rho u Y_i)_x - D_\text{im} (\rho Y_{i,k})_x = w_i, i = 1, 2 \]  
\[ (1d,e) \]

In these equations u is velocity; \( \rho, p, T \) are density, pressure and temperature, respectively. The transport properties dynamic viscosity, \( \mu \), thermal diffusivity, \( \alpha \), and binary molecular diffusivity, \( D_\text{im} \) are all assumed to be constant in this initial study. \( Y_i, i = 1, 2 \) are species mass fractions corresponding to H2 when \( i = 1 \), and O2 when \( i = 2 \). The \( \text{h}^0_i \) are the heats of formation for species \( i \); \( c_p \) is the specific heat (also taken to be constant), and the \( w_i \) represent rate of production of species \( i \), given as

\[ w_i = W_i \sum_k (v_{i,k} - v'_{i,k}) B_k T^\text{\alpha_k} \]  
\[ \prod_j \left( \frac{X_j p}{R^0 T} \right)^{v_{j,k}} \]  
\[ (2) \]

Here, \( W_i \) is the molecular weight of species \( i \), and \( v_{i,k} \) and \( v'_{i,k} \) are stoichiometric mole numbers corresponding to forward and backward reactions, respectively; \( B_k \) is the pre-exponential factor for reaction step \( k \), and \( E_k \) is the corresponding activation energy. \( R^0 \) is the universal gas constant, and \( \alpha_k \) is an empirically determined exponent. Finally, the \( X_j \)'s are the mole fractions. It should be noted that the temperatures appearing in the foregoing expressions are shifted by a zero-point temperature, \( T^0 \).

Because we are considering only a single-step forward reaction in the present study, the only value of \( k \) is unity, and the notation will hereafter be suppressed. Furthermore, \( v_{i,k} = v_{i,1} = 0 \) for \( i = 1, 2 \). In addition, we have chosen \( \alpha_1 = 2 \), primarily to simplify application of the Galerkin procedure to be discussed later. Also, we can express the equation of state as

\[ \frac{D}{R^0 T} = \rho \sum_i \frac{Y_i}{W_i} \]  
\[ (3) \]

and use this along with

\[ X_i = \frac{Y_i}{W_i} \]  
\[ \sum_j \frac{Y_j}{W_j} \]  
\[ (4) \]

to simplify the last factor in Eq. (2).
Although Eqs. (1) are one-dimensional, they nevertheless retain the basic form of the full N. S. and species concentration equations. Because these equations preserve the main mathematical properties of the full equations, we feel that they should provide a useful model with which to study new algorithms such as the additive turbulent decomposition to be treated herein. On the other hand, we should be cautious about attempting to too closely connect the solutions to these equations with actual physical phenomena; we should not necessarily expect solutions computed from these 1-D equations to exhibit precisely the same quantitative, or perhaps even qualitative, features found in solutions to the full 3-D system.

B. Nondimensionalization

Nondimensionalization of the compressible equations (1) leads to identification of important dimensionless parameters. For the most part we will scale dimensional quantities with reference values of the same quantity in order to derive a dimensionless form for Eqs. (1). Thus, we introduce the basic reference quantities \( \rho^0, U^0, T^0, L \) corresponding to density, velocity, temperature and length scales, respectively. We will define the time scale as \( \tau \equiv L/U^0 \), and we scale pressure with twice the dynamic pressure, \( \rho U^0 \). We also introduce the reference transport and thermodynamic properties \( \rho^0, \alpha^0, D^0, c_p^0 \). Using these, and the various simplifications described earlier, we can express Eqs. (1) in the dimensionless form

\[
\begin{align*}
\rho_t + (\rho u)_x &= 0 \quad (5a) \\
(\rho u)_t + (\rho u^2)_x - \frac{1}{Re} u_{xx} &= - p_x \quad (5b) \\
T_t + (uT)_x - \frac{1}{Pe} T_{xx} &= \frac{A\bar{T}}{\rho c_p^0} (\rho Y_1)^2 (\rho Y_2) e^{-E/\rho^0} \quad (5c) \\
(\rho Y_1)_{t} + (\rho u Y_1)_x - \frac{1}{Pe_D} (\rho Y_{1x})_x &= - C_i \bar{T}^2 (\rho Y_1)^2 (\rho Y_2) e^{-E/\rho^0}, i = 1,2 \quad (5d,e)
\end{align*}
\]

In these equations

\[
Re \equiv \frac{\rho^0 U^0 L}{\mu^0} \quad Pe_T \equiv \frac{U^0 L}{\alpha^0} \quad Pe_D \equiv \frac{U^0 L}{D^0}
\]

where Pe_T and Pe_D are, respectively, thermal and mass diffusion Peclet numbers;

\[
A \equiv \frac{L \rho^0 \alpha^2 T^B}{c_p^0 U^0} \left( \frac{2n^0}{W_1 W_2} + \frac{b_2^0}{W_1^2} \right) \quad (7)
\]

and

\[
C_1 \equiv \frac{2L(\rho^0 T_{\text{ref}})^2 B}{U^0 W_1 W_2} \quad C_2 \equiv \frac{L(\rho^0 T_{\text{ref}})^2 B}{U^0 W_1^2} \quad (8)
\]

\( T_{\text{ref}} \) is a reference temperature (different from \( T^0 \)), and \( B \) is the pre-exponential factor. \( \bar{T} \) is the dimensional, unshifted temperature, and \( \bar{T} \) is the corresponding dimensionless quantity.

Equations (5) constitute the fundamental equations for the remainder of the analyses to be performed. It is obvious that one could question some of the assumptions that have been made in obtaining them, especially constant transport and thermodynamic properties; but we believe this system still retains sufficient realism (within the 1-D framework) to provide a useful starting point for our studies of ATD applied to turbulent combustion.

C. Additive Turbulent Decomposition

In this subsection we will begin with a somewhat general, heuristic description of ATD. We will then apply the technique to the governing dimensionless equations for the 1-D combustion problem, and subsequently derive the local Galerkin ODE approximation for the small-scale equations.

The details of ATD when applied to a Burgers’ equation model have been given by McDonough et al. (1984a,b) and McDonough and Bywater (1986,1989). For the sake of completeness, however, we will repeat a significant portion of that material here, but in a somewhat more general setting.
2.1 ATD: Fundamentals

Originally, the basic goal in the development of ATD was to attempt to eliminate, or at least reduce the effects of, the two principle well-known flaws of LES: 1) subgrid-scale modeling, and 2) large-scale averaging or filtering. We have already noted that the first of these is considered to be the most serious deficiency of the LES approach; but, in fact, it would not even arise in the absence of the second. In addition, it was desired to produce an algorithm that would be highly parallelizable, and at the same time, one whose results would be completely consistent with the full, unaveraged N.–S. equations.

For any arbitrary variable, say \( u(x,t) \), a standard turbulent decomposition would yield

\[
u(x,t) = \bar{u}(x,t) + u'(x,t)
\]

where " \(-\)" denotes an averaged (or filtered) quantity, and " \( ' \)" is a fluctuating (or subgrid-scale) contribution. In ATD we begin with a similar decomposition:

\[
u(x,t) = \bar{u}(x,t) + u^*(x,t).
\]

But now \( \bar{u} \) should be viewed as the first few terms of a (possibly generalized) Fourier representation of \( u \), and \( u^* \) as the series remainder. This interpretation admits the natural generalization

\[
u(x,t) = u^{(1)}(x,t) + u^{(2)}(x,t)
+ ... + u^{(M)}(x,t), \]

where each \( u^{(m)} \), \( m = 1, ..., M \), corresponds to a certain range of temporal frequencies and spatial wavenumbers in the overall Fourier expansion. We note that, in principle, such multiscale expansions are possible for LES, but lead to extremely complicated equations (see Aldama, 1990). In the present study we will only employ the large-scale/small-scale decomposition (10), rather than the multi-scale version, (11). But, in general, when dealing with chemical systems we expect that decompositions of the form (11) with \( M \geq 3 \) will be needed. (Some evidence of this will be seen in our results to be presented below.)

Now let \( P(\partial/\partial x) \) denote a partial differential operator, and consider the evolution equation

\[
u_t = Pu.
\]

(12)

If \( P \) is linear, then substitution of (10) will give

\[
u_{t} + u_{t}^{*} = P\bar{u} + Pu^{*},
\]

(13)

which can be additively decomposed as

\[
u_{t} = P\bar{u}
\]

(14a)

\[ u_{t}^{*} = Pu^{*}.
\]

(14b)

We note that this decomposition is similar to locally one-dimensional (LOD) methods for numerically solving partial differential equations (cf. Mitchell and Griffiths, 1980), and it is closely related to projection methods first introduced by Chorin (1969) for solving the incompressible N.–S. equations. In fact, since \( u \) is assumed to possess a Fourier representation, it follows that it is an element of the separable Hilbert space \( L^2 \), and thus from a well-known result in analysis (cf. Kantorovich and Akilov, 1982) the separate solutions, \( \bar{u} \) and \( u^* \) of (14a) and (14b) when added together yield the solution \( u \) of Eq. (12). When \( P \) is nonlinear, the form of the decomposed equations must be determined on a case–by–case basis (and, in general, is not unique), and in addition there is coupling between the two (or more) equations of the decomposition. But the result stated above for the linear equation is still valid. In this regard, it is interesting to note that use has recently been made of this by Temam (1989) in constructing nonlinear Galerkin methods.

The most important aspect of this decomposition is seen by noting that the number of equations equals the number of unknown functions; hence, there is no closure problem with this particular decomposition. As a consequence, there is no modeling to be done. It should also be observed that Eqs. (14a,b), or their nonlinear counterparts, need not be solved by the same numerical algorithm. All that is necessary is that the desired degree of overall accuracy be achieved...
by each separate solution procedure. This fact is especially important in the context of treating the small-scale equations corresponding to (14b), as will be seen in our analysis to follow. Finally, we point out that solving Eqs. (14) can be advantageous from the standpoint of total required floating point arithmetic, compared with solving Eq. (12). In particular, suppose that in approximating (12) to a prescribed accuracy we obtain a discrete system containing \( N \) unknowns at each time step, and that the numerical procedure requires \( O(N^3) \), \( \beta > 1 \), floating point arithmetic operations per time step. Now assume, for definiteness, that each of the systems obtained in the discretization of Eqs. (14) contain \( N/2 \) unknowns, and that we apply the same algorithm to each separate system as was used for the complete problem. The total arithmetic per time step is in this case only \( \sim N^3/2^{\beta-1} \). Moreover, in this linear case, the separate equations of (14) can be readily parallel processed (although this is more difficult in the nonlinear case).

From the above discussions we can see that ATD provides an improvement over classical methods, and over LES, because it requires no modeling, and thus yields solutions similar to those obtained with DNS. At the same time, the total floating point arithmetic required by ATD should be significantly less than that of DNS, and ATD can be parallelized in a very natural way.

**2.2 ATD applied to 1-D N.-S. and species equations**

We will now apply the general ideas presented above to our specific problem, Eqs. (5). To simplify our subsequent analyses, we express these in terms of a slightly different set of dependent variables: namely we use \( \rho \), \( m \) \( (\equiv \rho u) \), \( T \), and \( z_i \) \( (\equiv \rho y_i) \). In terms of these, the continuity equation is linear in each of the two variables \( \rho \) and \( m \):

\[
\rho_t + m_x = 0. \tag{15}
\]

We decompose \( \rho \) and \( m \) as

\[
\rho = \bar{\rho} + \rho^*, \quad m = \bar{m} + m^*. \tag{16}
\]

Then substitution into (15), and performing an additive decomposition as done earlier, yields

\[
\bar{\rho}_t + \bar{m}_x = 0, \tag{17a}
\]

and

\[
\rho^*_t + m^*_x. \tag{17b}
\]

We remark that this decomposition implies strict mass conservation on both the large and small scales, separately.

The momentum equation can now be written as

\[
m_t + \left( \frac{1}{\rho} \frac{m^2}{x} \right)_x - \frac{1}{Re} \left( \frac{1}{\rho} \frac{m}{xx} \right) = -D \sum_{i=1}^{2} \frac{1}{W_i} \left[ (Tz_i)_x + \frac{1}{2} (T^*z_i)_x \right], \tag{18}
\]

Introducing (16), and analogous decompositions of \( T \) and the \( z_i \)'s, and again additively decomposing the resulting equation, leads to

\[
\bar{m}_t + \frac{1}{\rho} \left[ (\bar{m}^2)_x + (m^*\bar{m})_x \right] - \frac{\rho^*_t}{\rho^2} (\bar{m}^2 + m^*\bar{m})
\]

\[
- \frac{1}{Re} \left[ \frac{1}{\rho} \bar{m}_{xx} - 2 \frac{\rho^*_x}{\rho^2} \bar{m}_x + \frac{1}{\rho^3} (2(\rho^*_x)^2 - \rho_x \bar{m}) \right] = -D \sum_{i=1}^{2} \frac{1}{W_i} \left[ (T\bar{z}_i)_x + \frac{1}{2} (T^*\bar{z}_i)_x \right], \tag{19a}
\]

and

\[
m^*_t + \frac{1}{\rho} \left[ (m^2)_x + (\bar{m}m^*) \right] - \frac{\rho^{*_t}}{\rho^{*_2}} (m^2 + \bar{m}m^*)
\]

\[
- \frac{1}{Re} \left[ \frac{1}{\rho} m^{**}_{xx} - 2 \frac{\rho^{*_x}}{\rho^{*_2}} m^{*}_x + \frac{1}{\rho^{*_3}} (2(\rho^{*_x})^2 - \rho_x m^*) \right] = -D \sum_{i=1}^{2} \frac{1}{W_i} \left[ (T^*z_i)_x + \frac{1}{2} (T^*\bar{z}_i)_x \right], \tag{19b}
\]

for the large and small scales, respectively.

It should be observed that the large-scale and small-scale equations in (19) are identical in form. From the standpoint of consistency with the N.-S. equations, this is not necessary, and at present it is not known what consequences arise.
from deviating from such a formulation. We will adhere to this in the present study because of its aesthetic appeal, and because it readily lends itself to application of renormalization group techniques should that prove useful (or necessary?) in transferring information between large and small scales. We also point out that density has not been decomposed in the momentum equation. This leads to simplifications in implementing numerical procedures for the small-scale equations, but it has no effect on overall consistency. 

The energy equation is decomposed into large- and small-scale parts in a similar manner.

\[ T_t + \left( \frac{1}{\rho} m^* T^* \right)_x + \frac{1}{2} \left[ \frac{1}{\rho} \left( m^* T^* + m T^* \right) \right]_x - \frac{1}{\text{Pe}_T} T_{xx} = \frac{A}{\rho c_p} F^*, \]  

(20a)

and

\[ T_t^* + \left( \frac{1}{\rho} m^* T^* \right)_x + \frac{1}{2} \left[ \frac{1}{\rho} \left( m T^* + m^* T^* \right) \right]_x - \frac{1}{\text{Pe}_T} T_{xx}^* = \frac{A}{\rho c_p} F^*, \]  

(20b)

where

\[ \bar{F} \equiv (\bar{T}^2 + \bar{T}^* \bar{T}^*) \left( \bar{z}_2^2 \bar{z}_2 + 2 \bar{z}_1 \bar{z}_2 \bar{z}_1^* + \bar{z}_2 \bar{z}_1^2 \right) + \bar{z}_2^2 + \bar{z}_1 \bar{z}_1^* + \bar{z}_1^* \bar{z}_1 e^{-E/\text{Re}^\text{T}} \]  

(21)

with an analogous formula for \( F^* \) obtained by interchanging "-" and "*" in the above. Finally, the species concentration equations are

\[ \bar{z}_{i,t} + \frac{m_i}{\rho} \bar{z}_{i,x} + \left( \frac{m_x}{\rho} - \frac{\rho_x}{\rho^2} m \right) \bar{z}_i - \frac{1}{\text{Pe}_D} \]  

[ \bar{z}_{i,xx} - \frac{\rho x}{\rho} \bar{z}_{i,x} + \left( 1 - \frac{\rho x}{\rho} \right) \bar{z}_i ] = - C_i \bar{F}, \]  

(22a)

and

\[ \bar{z}_{i,t}^* + \frac{m_i^*}{\rho} \bar{z}_{i,x}^* + \left( \frac{m_x^*}{\rho} - \frac{\rho_x^*}{\rho^2} m \right) \bar{z}_i^* - \frac{1}{\text{Pe}_D} \]  

[ \bar{z}_{i,xx}^* - \frac{\rho x^*}{\rho} \bar{z}_{i,x}^* + \left( 1 - \frac{\rho x^*}{\rho} \right) \bar{z}_i^* ] = - C_i \bar{F}^*, \quad i = 1, 2. \]  

(22b)

There are several important aspects of these equations, and the development leading to them, that should be noted. First, as already observed for the continuity and momentum equations, the large-scale and small-scale forms are identical; one need only exchange "-" with "*" to go from one to the other. It is not difficult to see that the additive decomposition is not unique, and imposing scale invariance provides a form of uniqueness. Second, the combination of large scale plus small scale is completely consistent with the original governing equations (5), independent of the discretization method(s) or step sizes employed to solve them (provided, of course, that the methods, themselves, are consistent). This degree of consistency is not achieved by any other presently used method except DNS. Moreover, it is easily checked that the large-scale equations converge to the full N.-S. plus species equations as *-quantifies go to zero. That is, ATD \( \rightarrow \) DNS as the large-scale discretization is refined (and the small-scale contribution thus becomes negligible). This is also true for some, but not all, forms of LES. In addition, letting large-scale quantities become arbitrarily small would lead to recovery of the full equations from the small-scale equadons, by virtue of scale invariance. We remark that this is not a particularly reasonable limit to consider, in and of itself. On the other hand, it shows that the small-scale equations can be viewed as a perturbation of the full equations obtained by including large-scale information. In this sense, they can be expected to provide a tool for studying localized flow behavior in detail, as is often done with DNS. But in contrast with DNS, which incorporates almost no local large-scale information, the small-scale equations of ATD contain a wide range of large-scale quantities that can either be directly simulated, or supplied from laboratory data. It will be specifically this aspect of ATD that will be emphasized in the remainder of the present work.

### 2.3 Local Galerkin approximation of small-scale equations

We will not give attention to discretization of the large-scale equations in the present work,
except to note that this can be done in any of a variety of straightforward ways, just as in any typical solution method for the compressible N–S. equations. Here, we wish to focus on the small–scale equations. The basic approach is to consider these equations locally on subintervals of length $O(h)$, where $h$ is the large–scale discretization step size, and construct local Galerkin approximations for the dependent variables on each such subinterval. Figure 1 provides a schematic of this. Furthermore, we note that from a basic, conceptual standpoint, the technique is similar in spirit to finite element, and even more so, to spectral element (cf. Fischer et al., 1988), and domain decomposition methods (see Chan et al., 1989).

On each local interval the dependent variables will be expressed in the form

$$\rho^*(x,t) = \sum_{k=1}^{k} a_k(t) \sin(\sigma_k x)$$  \hspace{2cm} (23a)

$$m^*(x,t) = \sum_{k=1}^{k} b_k(t) \cos(\sigma_k x)$$  \hspace{2cm} (23b)

$$T^*(x,t) = \sum_{k=1}^{k} c_k(t) \sin(\sigma_k x)$$  \hspace{2cm} (23c)

$$z_1^*(x,t) = \sum_{k=1}^{k} d_k(t) \sin(\sigma_k x)$$  \hspace{2cm} (23d)

$$z_2^*(x,t) = \sum_{k=1}^{k} e_k(t) \sin(\sigma_k x)$$  \hspace{2cm} (23e)

where $\sigma = k\pi/h$, and $x^* = x - (x_i - h/2)$, with $x \in [x_i - h/2, x_i + h/2]$. It is interesting to note that the scaling (dilation) of wavenumbers by $h$ followed by translation of $x$ by (roughly) $x_i$ gives this representation features that are rather similar to those of the wavelet representations studied by Daubechies (1988,1989) and reviewed by Strang (1989), especially in the context of the multi–scale decomposition (11). However, the current approach is not identical to the use of wavelets since the basis functions employed here do not have compact support (unless identically zero, $C^0$ extensions are artificially defined on the complement of each subinterval), as required by definition of a wavelet basis.

These local representations have two distinct advantages over a global representation on the small scale. First, they lead to automatic parallelizability: all of the small–scale local approximations can be computed simultaneously if enough processors are available. Second, for a given required global accuracy on the small scale, the size of each individual local calculation is much smaller than would be the global one. In particular, suppose that it is desired to have a global small–scale representation consisting of $N$ modes on a spatial domain of length $L$. Then $N/L$ is the effective wavenumber of the highest mode. Now suppose the large–scale discretization has spacing $h \sim L/M$, where $M$ is the number of grid points (or collocation points, in a spectral method). If $N^*/h$ is the effective maximum wavenumber on each subinterval of length $h$, we have that $MN^*/L$ is the global maximum effective wavenumber on the small scale. This implies that $N^* = N/M \ll = N$ to achieve the same resolution as would be provided by the $N$ modes of the global representation. It is clear from this that even without parallel processing, considerable arithmetic can be saved by this local solution approach, following the same line of reasoning given above in the general discussion.

![Figure 1. Local Galerkin Subintervals](image-url)
of ATD.

We now substitute the solution representations (23) into the small-scale equations (17b) through (22b) and form the Galerkin inner products to obtain the following system of ODE initial value problems.

\[
\dot{a}_k = \sigma_{kh} b_k \quad \text{(24a)}
\]

\[
\dot{b}_k = \sum_{i,j=1}^{k} \left[ \frac{\pi}{\rho} jB_{ijk} + \frac{\rho_x}{2\rho^2} hC_{ijk} \right] b_i b_j - \frac{1}{Re} \left[ \frac{1}{\rho} g_{kh} + \frac{1}{\rho^2} \left( \frac{\rho_x}{\rho^2} - 2\rho_x^2 \right) \right] b_k
\]

\[
- \frac{D}{2} \left[ \sum_{i,j=1}^{k} (jD_{ijk} + iD_{ijk}) \right] \left( \frac{d_j}{W_1} + \frac{e_j}{W_2} \right) c_i + \bar{T}_x \left( \frac{d_k}{W_1} + \frac{e_k}{W_2} \right) \left( \frac{z_{1x}}{W_1} + \frac{z_{2x}}{W_2} \right) c_k \quad \text{(24b)}
\]

\[
\dot{c}_k = \sum_{i,j=1}^{k} \left[ \frac{\pi}{2\rho} (iA_{ijk} - jB_{ijk}) - \frac{\rho_x}{2\rho^2} hD_{ijk} \right] b_i c_j - \frac{1}{Pe_T} \left[ \sigma_{kh} + \frac{1}{2} \left( \frac{\rho_x}{\rho^2} + \frac{\rho_{xx}}{\rho} \right) \right] c_k + \frac{\pi}{4\rho} \frac{C_{ijk}}{\rho} + \frac{A_c}{Pe} f_k \quad \text{(24c)}
\]

\[
\dot{d}_k = \frac{\pi}{2\rho} \sum_{i,j=1}^{k} (iA_{ijk} - jB_{ijk}) b_i d_j - \frac{1}{Pe_p} \left( \sigma_{kh} - \frac{\rho_{xx}}{\rho} - 1 \right) d_k - C_{ijk} f_k \quad \text{(24d)}
\]

\[
\dot{e}_k = \frac{\pi}{2\rho} \sum_{i,j=1}^{k} (iA_{ijk} - jB_{ijk}) b_i e_j - \frac{1}{Pe_p} \left( \sigma_{kh} - \frac{\rho_{xx}}{\rho} - 1 \right) e_k - C_{ijk} f_k, \quad k = 2, 3, ..., K \quad \text{(24e)}
\]

where

\[
f_k = \left[ z_1^2 z_2 \hat{T}_{ik} + \frac{h}{2} \sum_{i,j=1}^{k} (z_1^2 z_2 c_i + 2z_1 z_2 \hat{T} d_i)ight]
\]

\[
+ z_2^2 \hat{T} e_j c_i A_{ijk} + \sum_{i,j=1}^{k} (2z_1 z_2 d_i c_i + z_1^2 e_j c_j)
\]

\[
+ z_2 \hat{T} d_i d_j + 2z_1 \hat{T} e_j c_i c_j + \hat{T} d_i e_j d_i c_m F_{ijk} + \sum_{i,j,l,m=1}^{k} d_m d_n c_i c_j G_{ijkm} \right] e^{-E/R \hat{T}}, \quad \text{(25)}
\]

\[
A_{ijk} = \int_{x_1 - \frac{h}{2}}^{x_1 + \frac{h}{2}} \sin \sigma_{nh} x' \sin \sigma_{nh} x' \sin \sigma_{nh} x' \, dx
\]

\[
B_{ijk} = \int_{x_1 - \frac{h}{2}}^{x_1 + \frac{h}{2}} \cos \sigma_{nh} x' \sin \sigma_{nh} x' \cos \sigma_{nh} x' \, dx
\]

\[
C_{ijk} = \int_{x_1 - \frac{h}{2}}^{x_1 + \frac{h}{2}} \cos \sigma_{nh} x' \cos \sigma_{nh} x' \cos \sigma_{nh} x' \, dx
\]

\[
D_{ijk} = \int_{x_1 - \frac{h}{2}}^{x_1 + \frac{h}{2}} \sin \sigma_{nh} x' \sin \sigma_{nh} x' \sin \sigma_{nh} x' \, dx
\]

\[
E_{ijk} = \int_{x_1 - \frac{h}{2}}^{x_1 + \frac{h}{2}} \sin \sigma_{nh} x' \sin \sigma_{nh} x' \sin \sigma_{nh} x' \, dx
\]

\[
F_{ijk} = \int_{x_1 - \frac{h}{2}}^{x_1 + \frac{h}{2}} \sin \sigma_{nh} x' \sin \sigma_{nh} x' \sin \sigma_{nh} x' \, dx
\]

\[
G_{ijkm} = \int_{x_1 - \frac{h}{2}}^{x_1 + \frac{h}{2}} \sin \sigma_{nh} x' \sin \sigma_{nh} x' \sin \sigma_{nh} x' \, dx
\]

In addition, we have the trivial system for $k = 1$:

\[
\begin{bmatrix}
\dot{a}_1 \\
\dot{b}_1 \\
\dot{c}_1 \\
\dot{d}_1 \\
\dot{e}_1
\end{bmatrix} = 0. \quad \text{(27)}
\]

This provides the spectral overlap needed to properly connect the large- and small-scale equations in Fourier space. There has been considerable discussion of the need for this in the LES literature (cf. Chollet, 1985, and references therein), and it has been somewhat difficult to accomplish in LES. With ATD, spectral overlap occurs naturally by requiring the lowest mode of the small scale to equal the highest mode of the large scale throughout the integration of the
small-scale equations over the large-scale time step. This is precisely the meaning of Eq. (27).

There are several other important points to be made regarding the form of Eqs. (24). We first mention that it is achieved by sifting all large-scale quantities through the Galerkin inner products in which they appear. This preserves orthogonality properties of the basis set without recourse to defining complicated weighted inner products, but it of course introduces some error. It is easily shown that the error is O(h^2), under only mild smoothness requirements; so although spectral accuracy is lost, reasonably good (typically the same order as the large-scale solution) accuracy is maintained. We also observe that except for the coefficients A_{ijk} and F_{ijlm}, all of the arrays of coefficients appearing in the convolutions of Eqs. (24) are very sparse. Hence, there is actually very little floating point arithmetic associated with constructing these convolutions. On the other hand, only one half of the A_{ijk}'s and F_{ijlm}'s are zero. Thus, terms containing these two factors lead to considerable amounts of computation. Nevertheless, it would be possible to parallelize much of this, although we have not yet done so at this time.

The qualitative structure of Eqs. (24) is also of interest. In general, these ODE's comprise a nonlinear dynamical system with dissipation, and as such may possess solutions exhibiting the chaotic behavior of a strange attractor. At this point, it is essential to notice that this system is characterized by the three dimensionless parameters Re, Pe_T and Pe_D, as well as 11 more local large-scale quantities: \( \tilde{\rho}, \tilde{\rho}_x, \tilde{\rho}_{xx}, \tilde{m}, \tilde{m}_x, \tilde{T}, \tilde{T}_x, \tilde{z}_1, \tilde{z}_{1x}, \tilde{z}_2 \) and \( \tilde{z}_{2x} \). Thus, in the context of bifurcation theory, the system could possess a quite high codimension, implying a rich variety of solution behaviors as these 14 parameters are changed in various ways. Clearly such changes occur in the large-scale solution variables in going from one spatial location to another, implying the possibility of spatio-temporal chaos. That this indeed does occur was demonstrated by McDonough and Bywater (1989) for a much simpler system. Existence of such behavior is important because it provides a different way to view the Ruelle and Takens (1971) theory of turbulence of the N.-S. equations, which is often criticized for its inability to account for the spatial chaos that is evident in most physically turbulent flows. In particular, by applying the Ruelle and Takens (or, for that matter, the Feigenbaum, 1978 or Pomeau and Manneville, 1980) theory to the N.-S. equations on local spatial domains as is done with ATD, spatio-temporal chaos is essentially guaranteed if temporal chaos exists.

Another interesting feature of Eqs. (24) is the interaction of the large-scale quantities with the dissipation terms, i.e., with the factor \( \sigma_{kh}^2 \), which basically sets the rate of decay (dissipation) of solution components. In general, one can see that at low values of k, and for specific combinations of signs on \( \tilde{\rho}_x, \tilde{\rho}_{xx}, \tilde{m} \) and \( \tilde{m}_x \), negative dissipation can occur. Because this is local in wavenumber space, it does not lead to loss of well-posedness of the overall initial value problem (assuming K is sufficiently large). Moreover, because all of the parameters responsible for these effects are local in (physical) space, we can associate this with the physical phenomenon of counter-gradient diffusion in the case of the species equations. From the mathematical standpoint it is clear that such behavior must in general produce a stretching of the characteristic time scales, and in particular, we can see that if \( \tilde{m}_x \geq 0 \) and \( \rho_{xx} \) (i.e., \( \tilde{\rho}_{xx} \)) \( \leq 0 \) hold, then the species diffusion times will be slowed. A consequence of this would be to bring chemistry time scales closer to the hydrodynamic time scale, thus invalidating the chemical equilibrium assumption (based on “fast” chemistry) often made for analyzing diffusion flames. Experimental evidence that this may actually occur has recently been reported by Magre and Dibble (1988).
2.4 Numerical solution technique

The Galerkin ODE's, Eqs. (24), are nonlinear and for large K can be expected to be stiff. Thus, one would typically expect to employ Gear's method (Gear, 1971) as the solution technique. But because we are anticipating chaotic solutions (and hence, sensitivity to initial conditions), and because Gear's method is a multi–step method (with potential for parasitic error), we have chosen to employ a modification of the A–stable, single–step trapezoidal scheme. The modification consists of treating the nonlinear terms explicitly. (via Heun's method), while maintaining implicit treatment of the linear terms, the main source of stiffness in this case. We of course do lose unconditional stability, but we also gain a significant reduction in the arithmetic that would be required to solve the linear systems that would have arisen in the application of Newton's method to the nonlinear terms had they been handled implicitly. This, in turn, reduces the round–off error, which is highly desirable when integrating dynamical systems possessing chaotic solutions, again because of sensitivity to initial conditions.

3. RESULTS

Although this paper is intended to be primarily a theoretical treatment of additive turbulent decomposition, we believe it is important to provide computational results for any new numerical algorithm. We will present a few such calculations in this section. All computations were performed in 64–bit FORTRAN 77 on an IBM 3090–600J at the University of Kentucky Computing Center (UKCC).

The simulations we will discuss are intended to locally model selected regions of an H2–O2 diffusion flame. In particular, results to be presented correspond, roughly, to the tip of the flame. As noted earlier, we are able to compute at any location provided large–scale data for that location are available. Because we have not yet performed large–scale simulations, we have used experimental data of Saito et al. (1986), and for some parameters simple estimates, for the values of the large–scale parameters. We must again caution the reader regarding the interpretation of the results. They have been obtained from a 1–D simulation, using rather crude estimates for some parameter values. We must be cognizant of this when attempting to construct physical interpretations and comparisons of these preliminary results with laboratory data.

Seven modes were retained in the small–scale representations of all dependent variables; i.e., K = 7. The dimensionless parameter values were Re = 6000, PeT = 1000 and PeD = 3000. Notice that we have not employed a Le = 1 assumption. The physical size of our small–scale region in the neighborhood of the flame tip was 0.5 mm. The dimensionless time step size employed in our numerical integrator was Δt = 5.0 × 10^-4, corresponding to a physical time step of 0.666... μsec. The simulations were run for 100 time steps.

Results for velocity, temperature and H2 and O2 concentration fluctuations are displayed in Fig. 2. These were obtained by inserting the solutions to Eqs. (24) at each time t into Eqs. (23) and summing only from k = 2 to k = K. This construction starts with k = 2 because k = 1 is actually a Fourier mode corresponding to part of the large–scale solution.

There are a number of interesting observations to be made regarding Fig. 2. To begin, the temporal behavior on the small scale corresponds to what should be termed transient chaos. Careful examination of the figures shows that oscillatory behavior first begins in the small–scale velocity and temperature almost simultaneously. But this occurs only after a relatively long period of increase in negative amplitude of the H2 and O2 small–scale concentrations, which is consistent with depletion of reactants to form products. From Eq. (24b) we see that as the negative small–scale concentration amplitudes become large, they lead to positive forcing of the momentum equation, provided the large–scale local temperature gradient is positive. We have es-
timed this to have a value of 825 K/cm from data of Saito et al. (1986). Once the oscillations in velocity and temperature begin, they feed back into the species equations through the advective terms (for velocity), and the species production terms (for temperature). It can also be seen that negative concentration fluctuations result in generally positive temperature fluctuations, as would be expected on physical grounds, since the negative concentration fluctuations imply product formation, and thus heat release. In general, these results appear to be generally consistent with expected physics.

There is another interesting point to notice with regard to Fig. 2. It is that the amplitude of the dimensionless velocity fluctuations is greater by about a factor of 10 than would be expected on the length scale being considered. This strongly suggests that (at least) a three-scale decomposition is needed to treat the diffusion flame accurately. Examination of the detailed printouts for this run showed large amplitudes in K = 2 momentum coefficients, with a rapid decay for higher values of k. This is further evidence that a separate scale is needed to handle the turbulent velocity fluctuations. Despite this, the qualitative features of these solutions show details of the chemical kinetics/hydrodynamic turbulence interactions that we feel would be essentially impossible to compute with any procedure other than ATD. As we noted in the introductory section, classical and PDF methods are unable to provide such details because they produce only averaged results. Also, modeling is required in LES at precisely the scales where the interesting interactions occur. Only DNS can provide such detail. But in the context of a full 3-D DNS of a complete diffusion flame, greater than 512^3 modes per dependent variable would be needed to achieve the resolution that we have obtained here. Of course, a 1-D DNS could certainly be performed, but clearly 3-D would not currently be possible. On the other hand, with ATD, the 3-D local calculation would require
only $O(10^3)$ Fourier modes because much of the information that would be computed in a DNS is input as local large-scale parameters in ATD).

4. SUMMARY

In this paper we have presented the theoretical analysis, and a sample calculation, for a new approach to treating chemical kinetics/turbulence interactions. This method, additive turbulent decomposition, lies between LES and DNS in terms of algorithmic structure: it retains the formal dependent variable decomposition of LES, but like DNS it does not employ averaging, or filtering, and is thus completely consistent with the N. S. equations; hence, no modeling is required. We have focused attention on the small-scale part of this algorithm in order to compute on length and time scales appropriate for the problem of $\text{H}_2\text{O}_2$ combustion considered in this work. Ability of the ATD algorithm to function in this way is, we believe, unique amongst turbulence simulation techniques, and it permits very detailed local calculations to be performed, provided local large-scale parameters can be provided by some means. In the present work, these quantities were derived mainly from experimental results, but in an implementation of the complete ATD algorithm, they would be computed directly.

It is interesting to observe that the small-scale algorithm possesses essentially all of the features discussed by Boris and Oran (1981) for an “ideal” subgrid model. In particular, they proposed that the following six properties are essential: 1) chemistry–hydrodynamic coupling and feedback, 2) ability to model onset, and other transient turbulence phenomena, 3) detailed chemical kinetics, 4) Lagrangian formulation, 5) smooth spectral overlap between scales and 6) efficiency. At the time this list was first put forth, many of its items might have seemed mutually exclusive; but the only one not found in ATD is use of a Lagrangian description of the flow field.

The results from our 1-D model problem show interaction between chemical kinetics and hydrodynamic turbulence at a level of detail that probably will not be possible to achieve by any other approach for some time to come. But we must once again caution against a too liberal association with actual physics, despite the interesting and appealing features of these results. On the other hand, it is entirely possible to simulate 3-D flow fields with finite rate chemistry using ATD, provided this is done locally in the manner described herein for one dimension. The total arithmetic requirements are easily within the realm of possibility for modern supercomputers using this technique.

The work presented here appears very encouraging; but it must be emphasized that the results are preliminary, and that much work still remains, even on the theoretical aspects of ATD. We will thus conclude this paper by mentioning some of these areas of study that we believe would be most fruitful in the development of this new method. The first pertains to the decomposition, itself. We have already noted evidence in our results that a multi-scale decomposition should have been used. In addition, we raised the question of necessity of scale invariance of the differential equations. Especially for the chemical production terms, it is not clear that maintaining this is desirable. Both of these questions deserve further attention. A second broad area is the mathematics/numerical analysis of ATD. This was discussed on a limited basis in McDonough and Bywater (1986) in the context of Burgers’ equation, and similar questions need to be addressed for the more realistic problem treated here, and even more so for 3-D problems. In particular, questions associated with grid function convergence with respect to time step size, and convergence of the Fourier representations, Eqs. (23), require careful attention. In addition, it would be of interest to investigate the bifurcation scenarios and qualitative properties of solutions as functions of dimensionless parameters, large-scale parameters and initial conditions. We comment that the variation of
large-scale parameters is equivalent to studying different regions of the flame.

At the next level of difficulty, we could consider problems with variable transport and thermodynamic properties, and more realistic models of the combustion chemistry, and of course, multi-dimensional problems. Furthermore, it is worthwhile to point out that the large-scale equations deserve study in their own right. This is because they are unaveraged, consistent perturbations of the full governing equations. Thus, if the small-scale properties can be obtained from experimental data (say, in the form of correlations involving one-dimensional maps of the interval, see Collet and Eckmann, 1980), the solutions should provide much more accurate results than can be obtained from Reynolds-averaged equations, and at essentially the same computational expense.

Finally, at the most difficult level are studies involving the complete ATD algorithm. McDonough and Bywater (1989) report results from such a calculation for Burgers' equation. Important questions needing investigation include efficient parallel processing of the local small-scale systems, and recoupling of the separately computed small-scale results. The latter is particularly important in the context of flows involving convective instabilities. Current efforts are employing ideas from domain decomposition to handle this aspect of the problem.

In closing, we note that we have discussed many interesting, and we believe, advantageous properties of the additive turbulent decomposition. But perhaps the main significance of the work reported here is that it provides an alternative way of viewing and analyzing turbulence in general, and chemical kinetics/turbulence interactions in particular. The viewpoint presented here implies that spatio-temporal chaos observed in physical turbulence may be reconciled with the purely temporal chaos of a strange attractor (i.e., the Ruelle and Takens theory of turbulence) by carrying out studies locally in space on the small scale, using equations that are parameterized by large-scale behavior. In addition to the interesting theoretical implications of this view is the practical advantage of natural parallelization, and hence automatic compatibility of ATD algorithms with the coming generations of massively parallel supercomputers.

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