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**Computational Approaches to the Study
of Reactive Flow Mixing**

JAY P. BORIS AND ELAINE S. ORAN

Laboratory for Computational Physics

February 13, 1980



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20. ABSTRACT (Continued)

for the detailed modelling and several important criteria are established which an accurate and consistent sub grid reactive flow mixing phenomenology should satisfy. One possible representation for such a generalized phenomenology is presented.

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COMPUTATIONAL APPROACHES TO THE STUDY OF REACTIVE FLOW MIXING

I. Introduction

Our understanding and eventual ability to predict the complicated interactions occurring in turbulent reactive flow problems is imperative for many combustion modelling applications. The presence of turbulence alters mixing and reaction times and heat and mass transfer rates which in turn modify the local and global dynamic properties of the system. The goal of this paper is to first describe the fundamental physical processes we must model in studying reactive flow turbulence and then to show how detailed modelling of these phenomena may be used to help construct practical phenomenological turbulence models for reactive flows.

If the full set of conservation equations for mass, momentum, and energy in multispecies flow could be solved exactly for a large enough range of time and space scales, turbulence and turbulent mixing phenomena would be contained explicitly in the solutions. Unfortunately even the fastest and largest computers are neither fast nor large enough to solve a complete problem from first principles even though the fundamental mathematical model is adequate. The basic problem in doing the computation arises from the vast disparity in time and space scales among the fundamental physical processes. For example, consider a system in which the mean free path λ , the characteristic scale length of diffusive mixing in reacting shocks, is six orders of magnitude smaller than the macroscopic convection length, L . A three-dimensional model resolving both scales would need $\sim 10^6$ computational cells in each spatial dimension, or a total of $\sim 10^{18}$ grid points. Perhaps it might be possible to use 10^6 grid points, but certainly not twelve orders of magnitude more. In trying to represent all of the macroscopic, turbulent

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mixing, and characteristic molecular dissipation scales in a single calculation, we are confronted with perhaps the most perplexing multiple time-scale and multiple space-scale problem in the detailed modelling of reactive flows. We must develop some practical algorithm to encompass these widely disparate scales in the same calculation.

In modelling turbulence phenomena, it has been the rule to try to develop separate equations which describe the subgrid scale mixing and reactions. These are then coupled to the macroscopic coarsely resolved fluid dynamics calculations we know how to perform. Here the proper separation and recoupling procedures for subgrid turbulent mixing and macroscopic flow are not nearly as obvious as the analogous problem of coupling a detailed chemical kinetics reaction scheme to a laminar hydrodynamics calculation [1,2]. It is not even clear how to represent some of the important transient mixing phenomena qualitatively let alone arrive at quantitative estimates of their effect.

In Section II of this paper we discuss the fluid dynamic origins of turbulent mixing in order to obtain an intuitive picture of the range of phenomena which must be represented. This information is then used in Section III to develop a list of resulting requirements which we would like an ideal turbulent mixing submodel to have.

First-principle, "ab initio" calculations are discussed in Section IV. These detailed calculations provide information about the dynamic characteristics and spectral evolution at length scales smaller than can be resolved with a macroscopic fluid dynamics model. The calculations are often extremely expensive, but must be performed to provide detailed understanding of microscale processes. Phenomenological turbulence models cannot be expected to tell us anything fundamental about turbulence or turbulent mixing. The basic physical processes must be built into the phenomenology, they cannot be derived from it. Thus a series of idealized ab ini-

tio calculations may be used, for example, to delineate the hydrodynamic channels for turbulent energy reappportionment and provide a way to analyze those properties which must be built into the phenomenological models.

Section V describes four types of phenomenological turbulence models. The phenomenological modelling problem involves the representation, not the resolution, of all of the myriads of individual fluid dynamic degrees of freedom within each macroscopic cell. We seek the most efficient representation for these subgrid degrees of freedom. If the basic processes controlling a particular measurable transient or turbulent transport effect are not represented in a phenomenological model, certainly the model cannot predict the occurrence of the effect. Section V is concluded with a description of a dynamic local spectral model, which would allow us to incorporate the multiscale and transient processes appearing specifically in reactive flow environments.

II. The Origins of Turbulence

In this section we discuss three aspects of reactive flow mixing which when considered together give a consistent picture of turbulent flows. By thinking in terms of these three different aspects and their interactions, we gain an intuitive understanding of reactive turbulence and the ways in which it differs from the classical non-reactive cases. Figure 1 illustrates these aspects schematically. The first aspect, labelled hydrodynamic channels, is based on the idea that turbulence begins in a laminar macroscopic flow as the onset of a fluid instability. The energy which drives this macroscopic instability then cascades through various hydrodynamic channels and is spread convectively over a broad spectral range. By concentrating on the fluid instabilities and their evolution as a response to changing fluid conditions, turbulent mixing can be viewed as a cascade of systems of distinct instabilities [3]. The second aspect focuses on the idea that turbulent mixing is dependent on the contortion of reactive surfaces which originally separate reactive species. We must first follow and then predict the behavior of these surfaces as they move and stretch with the fluid. Steady increase of the reactive surface area enhances molecular mixing and speeds reactions. The detailed chemical kinetics and chemical energy released by these reactions is the third aspect of the reactive flow mixing problem. Energy release in gaseous flows promotes expansion and, if the flow is sufficiently exothermic, can induce buoyancy. Thus the kinetics, as shown in Fig. 1, feeds back into the hydrodynamic channels and the cycle is closed.

An extensive body of knowledge and valuable expertise has been developed in using models of turbulence and turbulent mixing in constant density non-reacting fluids [4,5,6,7]. However, in combustion systems there are interactions which modify or may even obviate these models. One such physical mechanism is the localized change in the rates of heat and mass transport due to the temperature dependence of transport coefficients. Another mechan-

ism arises from the strong density gradients occurring locally in the combustion. Non-linear phenomena such as these determine the turbulent scale lengths and eventual chemical reaction effects. The various scale lengths covered by diffusive mixing, convection, and fluid instabilities are bounded by a dissipative mean free path scale length on one hand and the macroscopic system scale on the other. This is shown schematically in Figure 2. Since energy release due to chemical reactions can only occur where the fuel and oxidizer mix molecularly, turbulent combustion is driven by an energy source which fluctuates on the scale of the turbulent mixing lengths. This situation differs markedly from the classical turbulent flows.

IIA. Dynamic Fluid Instabilities and Hydrodynamic Channels: The First Aspect

The phenomena described above are examples of possible hydrodynamic channels for turbulent energy reappportionment. Most of these channels involve transient effects for which detailed balance or steady state arguments are inapplicable [8]. They involve the quick onset of a relatively short wavelength fluid instability which results from a slow or parametric variation of the background flow. Thus the configuration changes from one of local hydrodynamic stability to one of instability. At and just beyond the transition point of marginal stability, the growth rates are very slow and the unstable wavelengths relatively long. As the background flow continues to evolve into the unstable regime, maximum growth rates increase and instability spreads over a broader band of the spectrum. The turbulence, which is the non-linear manifestation of these instabilities, arises in bursts on the macroscopic scale and is an intrinsically transient phenomenon. Thus the idea of a steady state cascade of either vorticity or turbulent energy is an artificial concept because so many of the channels underlying the turbulent process are intermittent. New concepts are needed to describe these turbulent bursts.

Marginal stability methods [9,10,11] can play a very useful role in determining the transient interactions between macroscopic flows and the microscale instabilities which they induce.

In splitter-plate experiments, for example, the Kelvin-Helmholtz instability grows initially at wavelengths characteristic of the entrance flow. For certain experimental designs the instability may be essentially two-dimensional [12,13]. A vortex street begins to develop and vortices coalesce with rapidly stretching braids of interfacial material winding up in the cores. Figure 10 shows a numerical calculation of such an instability. When the local Reynold's number is high enough, the flow in the vortices becomes Taylor unstable in the third dimension at still shorter wavelength. Thus a one-time situation occurs and then passes.

In splitter plate experiments there is a constant source of energy and a tendency toward instability. The turbulence grows up to a level where the governing flow remains near marginal stability. If the turbulence decays somewhat, the background flow becomes more unstable until the turbulence builds up again. If the turbulence becomes somewhat too strong, the background flow is broken down and smeared out with the general effect of reducing the growth of instabilities. In the smoother flow the turbulence soon starts to abate. Since there is a decay time associated with the turbulence and an induction time-lag for the instabilities, it is not surprising that intermittency and bursts of turbulence are the norm rather than the exception.

One of the major physical conditions which distinguishes reactive flow from classical turbulence is the existence of density gradients. These cause the baroclinic generation of vorticity, ξ , through the term

$$\frac{d\xi}{dt} = \frac{\nabla\rho \times \nabla P}{\rho^2} + \dots$$

where ρ and P are the multidimensional fluid density and pressure fields, respectively. Below we consider two of the hydrodynamic channels activated by density gradients. These channels are rather typical of the many multi-scale interactive effects which will have to be understood before we can claim to understand turbulence.

When the mass density ρ is constant, as is assumed in much of the classical turbulence literature, all of the effects potentially depending on the vorticity source term are absent by construction. In the classical picture, the turbulent vorticity spectrum is driven at macroscopic scales, the intermediate wavelengths are populated by cascade and vortex stretching, and the short wavelengths in the spectrum are dissipated viscously (collisionally). In combustion, the localized release of heat in molecularly mixed fuel-oxidizer pockets causes strong transient expansion of the combusting gases. The resulting low density region has scale lengths characteristic of the combustion process and interacts with pressure gradients to generate vorticity in the flow on these same characteristic scales. Vorticity on these scales is efficient at turbulent mixing and can be expected to feed back on itself. The combustion process is in turn enhanced as long as fuel and oxidizer are present. Since the spectrum seems now to be driven at short wavelengths as well as long, plateaus or even peaks might form in the spectrum altering the usual notions of cascade, scaling, and hence modelling.

There are two different channels for turbulent mixing that this fluid expansion activates in chemically reactive flows. These can be understood qualitatively in terms of localized Rayleigh-Taylor growth. The first role, an *active* one, occurs when a pocket of gas is actively expanding due to the heat released from chemical reactions. This case is shown schematically in Figure 3. The expansion occurs in a restricted volume because the fuel and oxidizer enter the reaction region separately. A time-varying acceleration accompanying this expansion is felt in the surrounding fluid. A region of strong density gradients undergoing this acceleration will be subject to the Rayleigh-Taylor instability during much of the time the energy is being released. A perturbation, whose wavelength is comparable to the distance the fluid moves while expanding, will e-fold about once from the expansion.

The second role of density gradients, depicted in Figure 4, is *passive*, but is potentially more important than the active role. In the passive role the expansion influences turbulent mixing by providing the density gradient which leads to vorticity generation. Consider a localized fluid vortex rotating at angular frequency ω . The acceleration of the fluid is $R\omega^2$ at radius R . Smaller low-density pockets in this vortex, formed by chemical reaction at an earlier time, are unstable to the Rayleigh-Taylor modes where the local centrifugal fluid acceleration points opposite to the density gradient. The acceleration is provided by the divergence-free rotational flow generated earlier or driven into the system externally.

Because the active generation of vorticity is limited in time to the expansion phase itself, it is reasonable to expect that the amount of vorticity generated by the passive interaction of existing density gradients with large scale vortices is much greater. A very simple analysis indicates that there are several growth times of the Rayleigh-Taylor mode during a single rotation of the vortex when the mode wavelength is comparable to the vortex radius. Both the active and the passive role of expansion are not described by standard incompressible fluid turbulence theories and models.

IIB. Reactive Interface Dynamics: The Second Aspect

Turbulent mixing can also be viewed as the stretching and convolution of surfaces which originally separate reactive species. These reactive interfaces or surfaces move with the fluid. As the fuel and oxidizer diffuse molecularly, these surfaces continue to lie normal to the strongest species density gradients. The situation is presented in Figure 5. In the upper left-hand panel a cube of fluid 1 cm on a side is shown at time $t = 0$. An interface between reacting species A and B divides the cube into two halves. Subsequent stretching of this reactive surface is controlled by the local fluid velocity.

Motion of the fluid elements making up the reactive surface breaks down into a component normal to the surface which can change the integrated area and components parallel to the surface which cannot. All of these components are important and complement each other in the turbulent mixing process. When nearby points on the surface separate or stretch, the fluid on opposite sides of the surface approaches the surface to keep the flow roughly divergence-free. Any species or temperature gradients normal to the initial surface are enhanced, which in turn increase the diffusive interpenetration of the reactants. This surface stretching process is independent of convective interpenetration of material which also enhances mixing. This latter process, shown on the right of Figure 6, is governed by derivatives of the normal velocity parallel to the surface. By increasing the actual area of the reactive surface, the bulk reactivity is also increased. Stretching and interpenetration usually occur simultaneously but for clarity have been illustrated separately in Figure 6.

If the turbulent spectrum is dominated by short wavelengths, an originally smooth surface will become very wrinkled at short wavelengths before larger scale convolutions have had a chance to grow. This is illustrated in the upper right hand panel of Figure 7. Because the length scale of the turbulent spectrum is close to molecular mixing lengths, the effective volume in which enhanced mixing occurs is much less than what would be calculated knowing the stretched surface area. Adjacent folds of the surface which approach within the molecular diffusion length of each other tend to merge their mixed volumes, as shown in the Figure 7. The small surface corrugations rapidly get smoothed over with diffusive "fluff" so the effect of molecular diffusion is to limit the growth of the reactive surface area.

In the opposite case, shown in the lower left hand panel of Figure 7, the dominant wavelengths are long compared to the molecular mixing length. The surface is characterized by relatively smooth, long wavelength bulges which can fill the entire cell before any of the mutual

interference effects described in the previous paragraph can occur. In fact, the area of an ideal Lagrangian surface in an isotropic, homogeneous turbulent velocity field should probably increase exponentially. Molecular mixing now occurs along convolutions which have scales longer than the diffusion length. Eventually, however, overlap of the effective mixed volume occurs as the surface becomes more convoluted. Thus, the molecularly mixed volume is again limited even though the ideal reactive surface area goes to infinity.

IIC. Detailed Chemical Kinetics: The Third Aspect

The two aspects of time-dependent turbulent mixing in reactive flows presented above, the hierarchy of instabilities and the evolution of the reactive surface, focus on the nonlinear fluid dynamic interactions and the reactant-mixing effects respectively. Thus these two aspects complement each other and a clear picture from each will be required to gain a proper perspective on turbulent mixing. The third aspect we wish to discuss closes the schematic loop of Fig. 1. The essentially one-dimensional profiles of the fuel, oxidizer, and other reactants perpendicular to the reactive surface change not only from convection and molecular diffusion but also from chemical reactions. The fluid dynamic expansion and heat release must self-consistently couple back into the excitation of hydrodynamic channels to complete the picture.

A major concern then is the range of validity of fast chemistry approximations made to simplify the analysis. In some cases the overall reaction rate is governed by the diffusion of hot fuel and oxidizer together through an expanding region of hot products and reactants. In other cases the fuel and oxidizer mix convectively and then molecularly before ignition occurs. These latter situations are generally ignited by a rapidly moving flame front which travels parallel to the reactive interface rather than perpendicular to it. Here finite chemical kinetics clearly plays a crucial role since it determines the flame speed.

Figure 1 emphasizes the feedback and interactions between the study of hydrodynamic channels, of reactive interface dynamics, and of detailed chemical kinetics. These three distinct aspects also suggest independent yet complementary approaches to ab initio computational techniques, a subject considered further in Section IV.

III. Some Properties of an "Ideal" Subgrid Mixing Model

Accurate yet compact phenomenological turbulence models must be developed to model realistic combustor systems, open flames, and other turbulent reactive flows confidently and efficiently. These computational models must asymptotically decouple the subgrid turbulence and microscopic instability mechanisms from calculations of the macroscopic flow. In this section, the important properties which we would like to see incorporated in an ideal turbulence model are listed and described. The goal is to use these desired properties to guide us in both extracting information from ab initio calculations (Section IV) and constructing phenomenological turbulence models (Section V).

IIIA. Chemistry – Hydrodynamic Coupling and Feedback

Explicit energy feedback mechanisms from the mixing and reactions to the turbulent velocity field and the macroscopic flow must be formulated. The "laminar" macroscopic flow equations contain phenomenological terms which represent averages over the macroscopic dynamics. Examples of these terms are eddy viscosity and diffusivity coefficients and average chemical heat release terms which appear as sources in the macroscopic flow equations. These modified Navier-Stokes equations are postulated to include the effects of turbulence. Besides providing these phenomenological terms, the turbulence model must make use of the information provided by the large scale flow dynamics in order to determine the energy which drives the turbulence. The model must be able to follow reactive interfaces on the macroscopic scale.

IIIB. Modelling Onset and Other Transient Turbulence Phenomena

The model should be able to predict the onset of turbulence in what was initially laminar flow since bursts and other highly transient phenomena seem to be the rule in reactive flow turbulence. The fundamental gradients in density, temperature, and velocity fields in the reacting

fluid drive the macroscopic fluid dynamic instabilities which initiate turbulence. Thus these gradients from the macroscopic calculation are bound to be key ingredients in determining the energy that is available to drive the turbulence. Density stratification in a time-dependent fluid dynamics model is essential.

III C. Complicated Reactions and Flow

The ideal turbulence model should allow for detailed calculations or suitable parameterizations of chemical kinetics, of buoyancy effects, and of the other hydrodynamic channels which the physics in a given situation might require. In particular it must be possible to deal with multiscale effects within the subgrid model. If there is a delay as velocity cascades to the short wavelength end of the spectrum, the model must be capable of representing this. Otherwise bursts and intermittency phenomena cannot be calculated.

III D. Lagrangian Framework

An ideal subgrid model should be constructed on a Lagrangian hydrodynamics framework moving with the macroscopic flow. This requirement reduces purely numerical diffusion to zero so that realistic turbulence and molecular mixing phenomena will not be masked by non-physical numerical smoothing. This requirement also removes from concern the possibility of masking purely local fluctuations by truncation errors occurring when macroscopic convective derivatives are represented numerically. The time-dependent (hyperbolic) Lagrangian framework should also generalize to three dimensions as well as resolve reactive interfaces dynamically.

III E. Scaling

As mentioned in Section II, breaking the calculation into macroscopic scales and subgrid-scales is an artifice to allow us to model turbulence. The important physics occurs continuously

over the whole spectrum from $k = 0$ to k_{diss} , which is the wave number corresponding to a mean free path of a molecule. Thus the macroscopic and subgrid scale spectra of any physical quantity must couple smoothly at k_{cell} the cell boundary wave number. If this number were to be changed, as might happen if numerical resolution were halved or doubled, the predictions of the turbulence model must not change.

IIIF. Efficiency

Of course, the model must be efficient. The number of degrees of freedom required to specify the status of turbulence in each separately resolved subgrid region has to be kept to a minimum for the model to be generally useable. The real fluid has essentially an infinite number of degrees of freedom to represent the state of the gas in each small element. We would like to be able to do the job with a minimal number of degrees of freedom.

How to choose a representation to have these ideal properties is not obvious. Several alternative approaches are mentioned in Section V of this paper. It is obvious that consideration of the dynamic aspects of instability cascade and reactive surface evolution necessitate significant departures in modelling techniques from methods found adequate when fast chemistry or steady state Eulerian models of classical turbulence are assumed.

IV. Ab Initio Calculations

In order to assess the interaction between energy release and turbulence quantitatively, it is possible to perform idealized fundamental reactive fluid dynamic calculations taking advantage of today's advanced computer systems. Available practical algorithms permit us to solve the full set of conservation equations for multi-dimensional multi-species flow on what is generally considered the hydrodynamic subgrid scale. These numerical models consider buoyancy and compressibility effects and include realistic expressions for heat and mass diffusion and chemical reactions. Thus the full spectrum of compressible fluid dynamic effects may be simulated in a small region where enough resolution is available to resolve the turbulence and the dissipation scales as well as the necessary macroscopic convective effects.

The ultimate goal of such "ab initio" calculations is to advance our basic understanding of turbulence and to provide information about the small scale mixing and energy release which can then be used to construct and calibrate phenomenological turbulence models. In constant density, idealized, incompressible turbulence, a number of these ab initio calculations have been successfully performed [14]. Such calculations could also be made for compressible reactive turbulence, but the computations are somewhat more difficult. This difficulty manifests itself in a number of ways. First, resolution of all scales is not generally possible so only very idealized and restricted questions may be asked. Second, an ab initio calculation is performed only for one specific initial condition. Thus statistical information about the "turbulence" has to be obtained in transient problems by performing a number of calculations and averaging. Finally, the cost of these detailed, first-principle fluid dynamic calculations is usually high.

The results of these detailed ab initio simulations are correspondingly valuable. Any correlation, stress term, fluctuation, or overlap integral can be determined from the computed flow without interfering with the numerical experiment. Therefore closure assumptions for the

more phenomenological decoupled turbulence models discussed in Section V may be tested directly. This calibration procedure is particularly valuable because the exact computational solution of many important large-scale reactive flow problems is far beyond present technology. It will be necessary to use intermediate phenomenological, i.e., lumped-parameter, models to incorporate all of the scales for practical engineering applications. These models must be carefully calibrated using experimental data and specific ab initio calculations.

The ab initio calculations themselves, not their parameterizations, are the only computations that can teach us something about subgrid scale turbulence. Realistic chemical models can be included on the microscopic scale if a small enough system is being treated. Therefore each fluid element, as it undergoes hydrodynamic motions which differ slightly from its neighbors, experiences a correspondingly different chemical history. The lumped-parameter subgrid model must necessarily represent an average behavior in a macroscopic fluid element. These averages can be evaluated directly in idealized situations using large detailed ab initio turbulence simulations.

The probability density functions (PDF's) currently used in multi-moment modelling of turbulence can be measured from detailed simulations as a function of time, configuration, and chemical kinetics. This can even be done in situations where the energetic feedback of the reactions on the hydrodynamics is specifically incorporated. Thus not only can phenomenological models be tested, they can be upgraded as improved phenomenologies are derived from the analyses of the ab initio calculations themselves.

Perhaps most important, ab initio calculations can be used to answer fundamental questions about the turbulent mixing process itself. In Section II, the active and passive roles of expansion in reactive flow turbulence were discussed as an illustration of nonlinear fluid dynamic phenomena which enter when sharp density variations and energy-significant reactions

characterize the flow. These phenomena are examples of many identifiable hydrodynamic channels for turbulent energy reapportionment. Ab initio calculations can be used to isolate these individual channels and study their characteristic signature in the flow. Other examples of such channels would be mixing from growth of the Kelvin-Helmholtz instability at shearing interfaces driven by the effects of buoyancy, Taylor instability arising naturally in larger vortices and vortex streets, and Rayleigh-Taylor instability mixing where the pressure gradients are gravitationally induced. Each of these channels is really a mechanism for taking relatively organized kinetic, potential, or internal energy on one scale and reapportioning it to other scales.

Results from one such ab initio calculation are shown in Figures 8 and 9. A two-dimensional version of the FCT reactive flow model [2,15] was used to solve the conservation equations for mass, momentum and energy on a square, doubly periodic domain using an ideal gas equation of state. A three species model kinetics scheme is included to represent the exothermic reaction $A + B \rightarrow C + \text{Heat}$. Each of the three species mass densities (ρ_A , ρ_B , and ρ_C) satisfies its own continuity equation with an added molecular diffusion term. Viscosity is neglected (a von Neuman-like treatment of shock heating is not needed in the FCT formalism). Figures 8 and 9 show different computer plots of the results for two fluids of different density, which interpenetrate and diffusively mix as the result of an initial velocity field. Using such calculations we hope to measure the variation of mixing rate with density difference. From this calculation we see that "ab initio" models can only be used in very idealized turbulence problems although these limited problems can be solved.

Another two-dimensional ab initio calculation performed on the Kelvin-Helmholtz instability [16] is shown in the four panels of Figure 10. Two different fluids initially in relative shear flow abut at a sharp interface at $x = 0$. The fluid on the left moving up and the fluid on

the right moving down. Solid wall boundary conditions are applied to the left and right boundaries at $x = +$ and $x = -$ respectively. The vertical boundaries are periodic to accommodate the inflow and outflow systematically. Enough cells are present in the calculation (200×360) to allow representation of relatively short scale lengths such as the interface between species A and B (shown as two contours at the levels 0.4, and 0.6 in the function $\rho_A/(\rho_A + \rho_B)$). Intermediate scale lengths such as the vortex size which develops and longer scales characteristic of the system size can thus be easily resolved. The interaction of these scale lengths can be displayed and studied explicitly in properly posed and analyzed ab initio calculations.

Two additional data curves superimposed on the contour plots of Figure 10 are the one-dimensional vertical averages of the species densities at each horizontal location in the calculation. These averages appear as solid bars at $y = 0$ and $y = \infty$ in the upper left hand panel, our initial configuration. Species A, plotted as A's, has a vertically averaged value of $\rho_A/\rho = 1$ on the left of the initial shear interface and zero on the right. Species B has just the reverse initial profile. As the fluid instability progresses, the vertically averaged density shows a gradual transition crossing the shear layer, even though the spatially varying and stretching reactive surface remains sharp. In this way, deterministic, detailed, convective effects in the ab initio calculations can be compared one-for-one with fuzzy, statistical, averaged, diffusive-like effects in a phenomenological model.

Also from Figure 10 we can see that the average density displays a rather discontinuous drop at the edge of the turbulent layer reminiscent more of erosion at the edge of a cliff than of gentle interdiffusive penetration of two species. The effective one-dimensional diffusion coefficient has to be highly variable in space and time to model the intrinsically two-dimensional mixing which occurs. Such variability may be provided by making the turbulent diffusivity a nonlinear function of the "turbulence" itself. We can also see, particularly in the lower right

hand panel, that even though both $\langle \rho_A/\rho \rangle$ and $\langle \rho_B/\rho \rangle$ are about 1/2 at $\chi = 0$, very little of the fluid is actually mixed. Rather, strips of one or the other pure fluid are interleaved. Reactions between A and B can only occur where they are molecularly mixed. Thus reactions would still be occurring as a surface phenomena even though $\langle \rho_A \rangle \sim \langle \rho_B \rangle$ in an apparently extensive volume.

This last example makes clear one of the great operational advantages of using detailed ab initio calculations in the construction of phenomenological turbulence models. A crudely resolved macroscopic flow calculation with a subgrid model for turbulence could be compared to an ab initio calculation of the same exact problem. By varying only the resolution and keeping the initial conditions, fluid dynamics algorithm, and boundary conditions identical, the transition from an ab initio to a phenomenological representation can be studied in detail.

In a complete model of reactive turbulence, all space and time scales between the macroscopic convection and the molecular dissipation scales are equally important to the fluid and must enter into the description of turbulence. There is no intermediate scale which can be ignored safely in making the asymptotic decoupling between macroscopic and statistically indistinguishable microscopic scales. However, the transition from a discrete representation on a macroscopic mesh to a phenomenological subgrid representation is necessarily discontinuous and therefore likely to be a major source of difficulty.

In the ab initio calculations, the characteristics of and interactions between the various hydrodynamic channels for turbulent reappportionment comprise a local description of the turbulent mixing problem. This local approach risks missing global interactions in and constraints on the flow. These can only be treated by using a complementary phenomenological model coupled with the large scale macroscopic flow. Various options for phenomenological modelling are discussed in the next section.

V. Options for Phenomenological Turbulence Modelling

Most of the current "phenomenological" turbulence modelling techniques are based on the idea that local fluctuations in the macroscopic mean flow decorrelate rapidly in space. Thus the local turbulence details would depend only weakly on turbulent fluctuations a small but macroscopic distance away. Within this context, a local turbulent energy density, a characteristic mixing length, and concentration fluctuations may be defined. Conversely, fluctuating coherent structures on the macroscale must be represented in the fluid dynamics; a local turbulence model cannot be expected to deal with non-local fluid dynamics.

Below we describe four kinds of phenomenological models:

1. Turbulent Energy and Scale Models,
2. Moment Equation Methods,
3. Physically Motivated Phenomenological Models
4. Localized Spectral Dynamics Model.

These approaches are discussed in terms of the six criteria listed in Section III. The four generic model types described below are certainly not all inclusive, but they are representative of the major approaches pursued today in reactive turbulence.

VA. Turbulent Energy and Scale Models

Based on the idea that turbulence can be described by local fluctuations, a number of authors have written down evolution equations to propagate the turbulence energy, scale lengths, species overlap integrals, etc. The equations for these subgrid quantities or combinations of them take the same form as those of the mean fluid quantities. The characteristic

source and sink terms are functions of both mean flow variables and local turbulence parameters. There is a long history of work in this area, starting with Kolmogorov [17] in 1942 and continuing to date with the three-equation model of Spalding [18].

These one-, two-, and three-equation approaches have been used most successfully for certain classical non-reactive flow problems which primarily involve shear flows with high Reynolds numbers away from boundaries and turbulent boundary layers. The results are often acceptably accurate in describing problems in which the turbulence has already developed. Various free parameters must be optimized, or calibrated against experiments. These methods are questionable for the treatment of, for example, reactive flows, high mach number flows, low Reynolds number flows, flows where gravity is important, or intermittent turbulent bursts. The presence of large coherent structures in real mixing situations casts further doubt on the authenticity of many of these models.

VB. Moment Equation Methods

In an attempt to make these turbulent energy and scale models more reliable and rigorous, mathematical approaches have attempted to generalize the intuitive models described above into more formal closure procedures [19,20,21,22]. The physical variables are decomposed into a mean part representing the macroscopic flow and a fluctuating part representing the subgrid scale turbulence. Equations for the mean and fluctuating components are derived in terms of successively higher order nonlinear correlations of the fluctuating quantities. The hierarchy of moment equations can only be closed, however, by making an assumption that the unknown higher-order terms can be written as combinations of lower-order quantities. In practice, the hierarchy of equations is closed by semi-empirical arguments which range from very simple guesses for an exchange coefficient to much more sophisticated hierarchies, in which the ultimate closure is very remote from any physical bases" [8].

These closure approximations often contain a number of non-dimensional parameters, which are hoped to be universal in the sense of being constant or nearly constant over a wide range of turbulent flows. Of course this approach also suffers the criticism that so many free parameters become potentially available, if the hierarchy is carried far enough, that any functional behavior could be fitted. Nevertheless, for certain non-reactive, incompressible, constant-density flows, satisfactory agreement between the models and selected experiments is obtained.

The extension of the moment methods to reactive flows has used the idea of a probability density function (PDF), [23,24] which attempts to relate time averaged macroscopic quantities to their instantaneous local values. Choice of the PDF is close to arbitrary, although physical significance is being attached to whether delta functions or trapezoids are used [24]. A major conceptual problem lies in the fact that many calculations are extremely sensitive to the form of the PDF.

A related problem centers around the exact order and form of closure. It was originally hoped that by going to higher and higher order models, more accuracy would be obtained. The current feeling is that the simple two- or three-equation models do as well as the five, six, or twenty-six moment models. Higher orders yield more free parameters which can be fit to data. But the resulting models are no more universal.

Another point which should be mentioned here is basically a philosophical problem. The turbulence modelling schemes currently used convert the detailed consequences of microscopic motions, which are thought of as stochastic random phenomena, into absolutely deterministic effects driving flow on the macroscopic scale. Thus in a reacting fluid system which is modelled by a set of laminar fluid equations and a prescription for the effects of turbulence, a given initial configuration will always lead to the same final state. Even though the real fluid system is

being described in the model by only a small finite number of degrees of freedom, the answers predicted by the model are completely deterministic. There are an infinite number of configurations of the real system which all would be represented in the model by the same final representation, and each of these real configurations should really lead to a different final state. The variance of these final states within a given finite model representation has to be determined, and is the subject of extensive mathematical and physical research. Distinct classes of solutions seem to exist in simplified physical problems. These solutions depend to whether the problem is ergodic, i.e., gives rise to periodic, quase-periodic, or non-periodic solutions [3]. Whether this mathematical classification bears corresponding physical significance is not determined.

It is by no means clear that increased study and development of these mathematical phenomenological approaches is the way to go. In addition to the problems described above, there are other difficulties as well. The first of these involves modelling turbulent transients (bursts) and turbulence onset. In most physical systems, turbulence arises naturally as a consequence of an unstable macroscopic flow configuration and dies out when the destabilizing situation abates. As mentioned in Section III, specific local evaluation of stability criteria should be a part of any reliable model, although it does not seem to be included in any of the moment models. In fact the description of turbulent shear flows in terms of a mean profile in at least some flows (mixing layer and boundary layer) has been shown to be the result of a superposition of nearly deterministic large-scale structures having random phases [8]. The classic experiments by Roshko and coworkers demonstrate this fact clearly [12,13].

Another aspect of these transient-vs-steady-state problems is shown in Figure 11. Typical flow streamlines in both the steady state and the transient laminar computations of flow in a simple two-dimensional combustor are illustrated. The lower panel shows realistic macroscopic

fluctuating eddies carrying pockets of relatively pure oxidizer to the top of the chamber and relatively pure fuel to the bottom. Any phenomenological turbulence models based on the steady state flow of the top panel clearly cannot convect pure fuel or oxidizer into the far corners of the chamber, for it would involve crossing streamlines. Diffusive approximations will also not be able to get the pure fuel or oxidizer there either. Therefore, suitably modified approaches to the modelling are required to correctly treat this problem.

Another technical issue arises from the overall complexity of the reactive flow problem. Current turbulence models generally include approximations developed to describe incompressible, non-reacting systems. Energy released as a result of the turbulent mixing and the subsequent chemical reactions which occur is, as described extensively in Section III, qualitatively a very different problem.

VC. A Physically Motivated Phenomenological Approach

An alternative approach to the multi-equation and multi-moment approaches involves actually modelling the probability distribution function (PDF) based on certain physical processes we know occur. The models must also provide procedures for deriving the time-averaged fluid quantities. Methods of this type have been developed, and tested by a number of authors [25,26,27,28]. Their hope is that by building some of the physics into the PDF, the computed mean quantities will be less sensitive to those of its feature which are not known.

Spalding's ESCIMO theory [28] is one example of this type of model which is currently being developed. Mixtures of different composition for interleaved folds which are born, stretch and die as a function of time. Figure 12 shows a fold, in which the two species A and B, initially have sharp gradients across their interface. The gradients are smoothed and broadened by molecular diffusion. Only the direction normal to the interface is considered, so

multidimensional effects appear as compression and dilation of the gradients in the one spatial dimension which is represented. The internal gradients and structures of the folds are only driven by the macroscopic flow but not derived from it or coupled directly to it. In terms of the reactive surface concepts introduced in Section II to describe turbulent mixing with reactions, the ESCIMO theory concentrates on the perpendicular diffusive mixing and associated detailed kinetics where the reactive flow is laminar on the small scale. The effect of mutual interference in adjacent folds of the surface are neglected.

This theory deals with the evolution of a fold after it develops. A number of PDF's are defined for a fold which are functions of its age, thickness, reactedness, etc. These PDF's may then, hopefully be used to obtain averaged fluid quantities. However, one encounters a fundamental problem here: there is no way of knowing what the size distribution is for these folds at their birth. What we have is a number of small-scale one-dimensional laminar problems, which must be related to the macroscopic flow. This has been termed the "demography" problem. Spalding has discussed launching a large number of these independent Lagrangian reactor parcels in a given steady-state flow and then performing statistical analyses on the ensemble of these parcels from their "birth" to their "death." Since each parcel launched this way is an independent, well resolved one-dimensional reactive flow problem, the computational cost would be enormous even in simple flows. The practical cost will be even higher because the laminar large-scale flow must respond to the short scale fluctuations. Therefore, the "demography", thought of as an a posteriori averaging procedure should be performed in concert with the evolving hydrodynamics calculation to model many real applications. Again, we are faced with a situation where we hope that the end result of the calculations will not be too sensitive to the initial choice for the fold distribution.

We see, therefore, that the ESCIMO approach is both a simplified ab initio model which can teach us something about the local mixing and chemical kinetic aspects of turbulence and may be the basis of a potentially useful phenomenological model of turbulence. Studies of the time-history of a fold may include effects such as complex chemical reactions, molecular diffusion, etc. It is one way to study localized mixing in the microscale under idealized circumstances. The model is limited, however, in its predictive capability by those physical processes which have not been included, as well as by the open-ended question of how the parcels interact with the macroscale. A parameterized, coupled, dynamic model of the subcell turbulence is still required for use in detailed modelling calculations which is capable of representing and predicting multiscale phenomena such as occur in instability cascade.

VD. Local Spectral Dynamics

Suppose every computational fluid element has local subscale motions which must be described simply and accurately. Further, suppose these local motions can be described in important respects by a local spectrum of fluctuations. Then an efficient and flexible turbulence model might be developed by modelling the local spectrum,

$$E_k \equiv \left| \frac{1}{2} \rho V_k^2 \right|,$$

in each fluid element using just a few degrees of freedom. Here ρ is the mass density and V_k is the k^{th} wavelength component of the fourier transform of the fluid velocity. We further assume for now that only a scalar spectrum is needed to model the local motions and that the region which has to be modelled is limited as shown in Figure 2. For wavenumbers larger than k_{diss} , viscous dissipation, thermal conduction, and molecular diffusion effects dominate and the fluctuation spectra should be predictable given the values at k_{diss} . For wavenumbers smaller than k_{cell} , the macroscopic hydrodynamics equations resolve these scales explicitly.

In between k_{diss} and k_{cell} , some form of discrete representation of the localized turbulence short wavelength spectrum is needed. The best form has not yet been determined. In the figure three discrete values of the spectrum at k_1 , k_2 , and k_3 are shown breaking the turbulent interactions regime into three finite width cells or bins. The optimal number of such cells must also be determined. At least three bins are necessary to allow for transient instability onset, changing turbulent length scales, and multiscale phenomena. More bins will undoubtedly improve flexibility and accuracy of the model. In earlier idealized tests of this approach on the Kelvin-Helmholtz instability, it was necessary to use at least two bins per decade of characteristic scale length.

To advance E_{k_1} , E_{k_2} , E_{k_3} , the localized spectral strengths at k_1 , k_2 , k_3 , a set of ordinary differential equations is written down which are somewhat analogous to the coupled rate equations for chemical kinetics. For each macroscopic cell, there are a series of equations for the form

$$\frac{dE_k}{dt} = \sum_j (Q_k(\gamma_j) - L_k(\gamma_j))$$

where Q_k and L_k are production and loss terms for spectral cell k . The $\{\gamma_j\}$ refer to the particular processes which can act as a production (Q) or loss (L) terms and they represent the hydrodynamic channels for turbulent energy reappportionment, chemical reactions, diffusion processes, etc. These source and sink terms couple the various wavelength bins in much the same manner as specific chemical reactions or reaction types couple different chemical kinetic species. All the conservation conditions on total momentum and energy in the spectrum apply with the added complication of source and sink terms at both long and short wavelength. Energy dissipated at short wavelengths appears as localized heat in the macroscopic energy equation and as turbulent viscosity in the macroscopic momentum equation.

In preliminary studies, the obvious anisotropy of some of the hydrodynamic channels will be ignored, and it is hoped that the use of several spectra will not be necessary. Fully calibrated and theoretically understood parameterizations of the reactive surface area evolution as a function of spectral structure (Section II) will be needed if accurate chemical kinetics models are to be included. Further, the complementary results of a complete set of ESCIMO-like Lagrangian reactive flow calculations will need to be folded in. Certainly only a careful, quantitative analysis of the specific hydrodynamic channels and their interactions can point the way to valid simplifications in this miserable modelling morass. This analysis must provide a way to represent the basic fluid instabilities as source and sink terms, probably in terms of instability growth rates derived from separately performed ab initio or microscopic calculations. Considerable success with a variant of this approach has been achieved in a number of plasma physics problems where small-scale micro-instabilities affect macroscopic transport [9,10,29,30,31]. A similar approach has been postulated for nonreactive flow by Brodkey [32]. However, his source and sink terms did *not* explicitly identify individual hydrodynamic channels or a way of incorporating the effective boundary conditions of the macroscopic gradients on the subscale quantities. Studies of the effect of chemical energy release on the spectrum, E_k , have been made by Eschenroeder [33].

Currently this local spectral dynamics approach is being pursued in the Laboratory for Computational Physics at NRL. The goal is to use a combination of ab initio calculations and analytical theory to provide insight into the form of the P_k and L_k functions. This approach is appealing physically because it allows all the important aspects of the six criteria in Section III to be met. The model may include the growth and decay of the important hydrodynamic channels and thus potentially allows for onset and transient phenomena. Chemical reactions may be included, at the very least through an enhancement of the spectrum at wavelengths, between

k_{cell} and k_{diss} . Since we clearly must accept a prediction which is true only on average, the neglect of all but a few of the internal turbulent fluid degrees of freedom in each cell ensures this and provides efficiency. Scaling is ensured through a source term imposed on the equations at k_{cell} . Thus the procedure sketched out above does, at least in principle, meet the six conditions postulated earlier as a necessary if not sufficient for a reactive flow turbulence sub-model.

VI. Conclusion

Computational simulation techniques play two roles in reactive flow turbulence and turbulent mixing research. Ab initio calculations of basic turbulence processes, in which the fluid dynamic and chemical phenomena are coupled on the microscale must be performed to extend our understanding. In addition, macroscopic phenomenological models of turbulent mixing are required which are efficient enough for regular use in practical applications. These two roles complement each other and hence must be closely coupled in a comprehensive approach. Only the ab initio calculations can bring out new knowledge about turbulence itself. The phenomenological models contain no more physics than is built into them and thus are wholly dependent upon theory, experiment, and ab initio calculations for their content.

The obstacles confronting the detailed modeller who must include the effects of turbulent mixing depend on whether an ab initio or a phenomenological approach is adopted. Using ab initio calculations, the modeller deals with a straight-forward representation of the fluid dynamics, but adequate resolution of varied space scales will always be a major stumbling block. Improved computers and numerical algorithms help, but for years to come, detailed simulations will be confined to idealized problems in simplified geometries. The major hurdle to phenomenological modelling is the choice and implementation of a suitable representation. A successful separation and then asymptotic coupling of the macroscopic and microscopic scales makes the resolution problem becomes less important.

In this paper, the physical origins of turbulence and the desirable properties of a general time-dependent subgrid turbulence model have been described. The localized and transient aspects of turbulent mixing have been stressed along with the dynamics of reactive interfaces and the strong effects of chemical energy release. It is hoped that by thoroughly understanding these aspects of turbulent mixing in reactive flows a suitable phenomenological model can be built which displays the desired properties.

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REFERENCES

1. J.P. Boris and E.S. Oran, "Detailed Modelling of Reactive Flows," Reprinted in Proceedings of the GAMNI Congress, Paris, Nov 27-Dec 1, 1978.
2. E. Oran, T. Young and J. Boris, "Applications of Time-Dependent Numerical Methods to the Description of Reactive Shocks," *Seventeenth Symposium (International) on Combustion*, The Combustion Institute, Pittsburg, Pa., 1978; also NRL Memorandum Report 3889, Naval Research Laboratory, Washington, D.C., 20375, 1978.
3. Harry L. Swinney and Jerry P. Gollub, The Transition to Turbulence, *Physics Today*, 41-49, August, 1978.
4. F.H. Harlow, Turbulence Transport Modelling, AIAA Selected Reprint Series, Vol. XIV, AIAA, N. Y., 1973.
5. B.E. Launder and D.B. Spalding, *Mathematical Models of Turbulence*, Academic Press, New York, 1972.
6. W.C. Reynolds and T. Cebeci, "Calculation of Turbulent Flows," *Turbulence Topics in Applied Physics, Chapter 5*, Springer-Verlag, New York, 1978.
7. W.C. Reynolds, *Annual Reviews of Fluid Mechanics*, 8, p. 183, 1976.
8. H.W. Liepman, The Rise and Fall of Ideas in Turbulence, *American Scientist*, 67, 221-228, 1979.

9. J. Boris, J.H. Orens and J. Dawson, R.V. Roberts, "Computations on Anomalous Resistance," *Physical Review Letters* **25**(11), 14 September 1970.
10. W. Manheimer and J. Boris, "Self-Consistent Theory of a Collisionless Resistive Shock," *Physical Review Letters* **28**, 11, pp. 659-662, March 1972, also "Marginal Stability Analysis: A Simpler Approach to Anomalous Transport," *Comments on Plasma Physics and Controlled Fusion*, **3**(1), Gordon and Breach, New York, 1977.
11. M. Lessen, On the Power Laws for Turbulent Jets, Wakes, and Shearing Layers and their Relationship to the Principle of Marginal Instability, *J. Fluid Mech.*, **88**, 535-540, 1978.
12. A. Roshko, Structure of Turbulent Shear Flows: A New Look, *AIAA Journal*, **14**, 1349-57, 1976. Also, A. Roshko, Progress and Problems in Understanding Turbulent Shear Flows, *Turbulent Mixing in Nonreactive and Reactive Flows*, (ed. S.N.B. Murthy), 295-311, Plenum, 1975.
13. F.K. Browand and P.D. Weidman, Large Scales in the Developing Mixing-Layer, *J. Fluid Mech.*, **76**, 127-144, 1976. Also, F.K. Browand and J. Laufer, The Role of Large Scale Structures in the Initial Development of Circular Jets, *Proc. 4th Biennial Symp. Turbulence in Liquids*, Univ. Missouri-Rolla, 333-344, Science Press, 1975.
14. S.A. Orszag, M. Israel, *Annual Reviews of Fluid Mechanics*, **6**, p. 281 (1974). Also "Numerical Flow Simulation by Spectral Methods," in *Proc. of the Symposium in Numerical Models of Ocean Circulation*, Nat. Acad. of Sciences (U.S. G.P.O., Washington, D.C. 1972).
15. J.P. Boris and D.L. Book, "Solution of Continuity Equations by the Method of Flux-Corrected Transport," *Methods in Computational Physics*, Chapter 3, **16**, p. 85 Academic Press, New York, 1976.

16. J.P. Boris, T.P. Coffey, and S. Fisher, "The Kelvin-Helmholtz Instability and Turbulent Mixing," NRL Memorandum Report 3125, Naval Research Laboratory, Washington, D.C. 20375, September 1975.
17. A.N. Kolmogorov, Equations of Turbulent Motion of an Incompressible Fluid, *Izv. Akad. Nauk Ser. Phys.*, 6, No. 1/2, 56-58, 1942.
18. D.B. Spalding, Concentration Fluctuations in a Round Turbulent Free Jet, *Chem. Eng. Sci.*, 26, 95-107, 1971.
19. W.S. Lewellan, M.E. Teske, and Coleman duP. Donaldson, Variable Density Flows Computed by a Second Order Closure Description of Turbulence, *AIAA Journal*, 14, 382-387, 1976.
20. W.S. Lewellan, Use of Invariant Modelling, *Handbook of Turbulence*, Vol. 1, ed. by Walter Frost and Trevor H. Moulden, Plenum Pub. Co., 1977.
21. Coleman duPont Donaldson, On the Modelling of the Scalar-Correlation Necessary to Construct a Second-Order Closure Description of Turbulent Flow, *Turbulent Mixing in Nonreactive and Reactive Flows*, ed. by S.N.B. Murthy, Plenum Press, New York, 1975.
22. E.S. Fishburne, A.K. Varma and C. duP. Donaldson, Aspects of Turbulent Combustion, AIAA 15th Aerospace Sciences Meeting, January, 1977.
23. Roland Borghi and Denis Dutoya, On the Scale of the Fluctuations in Turbulent Combustion, *Seventeenth Symposium (International) on Combustion*, The Combustion Institute, Pittsburg, Pa., 1978.

24. K.N.C. Bray, The Interaction Between Turbulence and Combustion, *Seventeenth Symposium (International) on Combustion*, The Combustion Institute, Pittsburgh, Pa., 1978.
25. Frank E. Marble, the Coherent Flame Model for Turbulent Chemical Reactions, Project SQUID Technical Report TRW-9-PU, January, 1977.
26. W.B. Bush, P.S. Feldman, and F.E. Fendell, On Diffusion Flames in Turbulent Shear Flows: Modelling Reactant Consumption in a Mixing Layer, *Comb. Sci. and Tech.*, **13**, 27-56, 1976.
27. B.F. Magnussen, B.F. Hjertager, B.H. Olsen, J.G. Bhaduri, Effect of Turbulent Structure and Local Concentration on Soot Formation and Combustion in C_2H_2 Diffusion Flames, *Seventeenth Symposium (International) on Combustion*, The Combustion Institute, Pittsburgh, Pa., 1978.
28. D. Brian Spalding, A General Theory of Turbulent Combustion, *J. Energy*, **2**, 16-23, 1978.
29. P.C. Liewer and N.A. Krall, *Physics of Fluids* **16**, 1953, 1973.
30. S. Hamasaki, R.C. Davidson, N.A. Krall, and P.C. Liewer, *Nuclear Fusion* **14**, 27, 1974. Also S. Hamasaki and N.A. Krall, "Numerical Modelling of the Implosion Heating Experiment," *Physics of Fluids*, **20**(2), 1977.
31. R. Clark and D.L. Book, "Interaction of a Laser-Produced Plasma with a Ma" by R.W. Clark and D.L. Book, *Bull, APS* **17**, 1026. R. Clark and K. Papadopoulos, "Simulation of Ion Thermalization in the Earth's Bow Shock," *Trans. AGU* **57**, 995, 1976. R. Clark, W.M. Manheimer, P. Liewer, M. Lampe, K.R. Chu, *Phys. Fluids*, **19**, 1788, 1976.

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32. Robert S. Brodkey, Mixing in Turbulent Fields, in *Turbulence in Mixing Operations*, ed. by Robert S. Brodkey, Academic Press, New York, 1975.
33. Alan Q. Eschenroeder, Turbulence Spectra in a Reacting Gas, *AIAA Journal*, 3, 1839-3846, 1965.

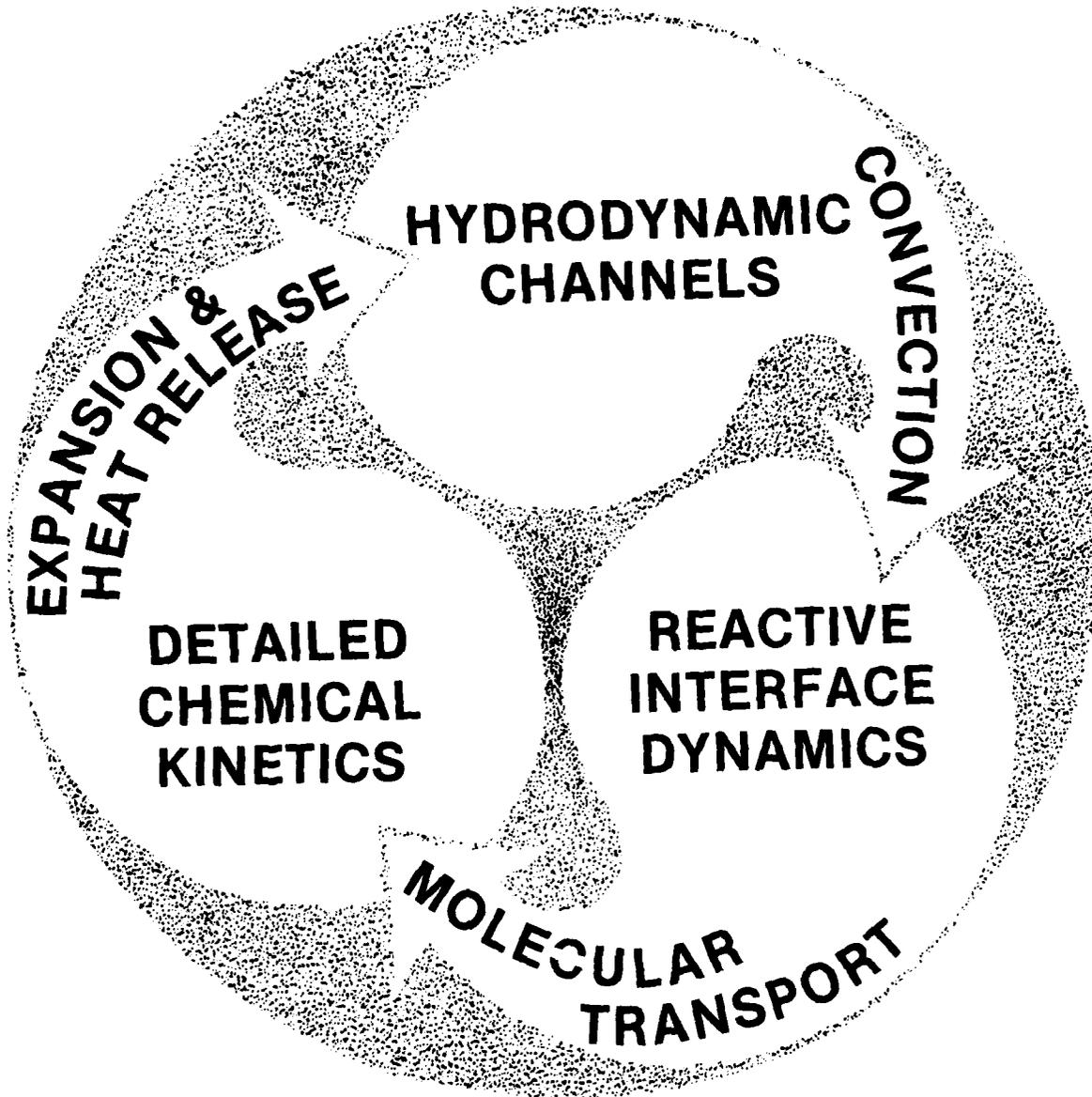


Figure 1 — A schematic diagram showing the interactions between the three different aspects of reactive flow mixing identified as: 1) hydrodynamic channels excited by velocity, density, and pressure gradients, 2) reactive interface dynamics where molecular interpenetration of reactive species is enhanced, and 3) detailed chemical kinetics whose expansion and other heat release effects feed energy back into the fluid dynamics to drive additional hydrodynamic channels.

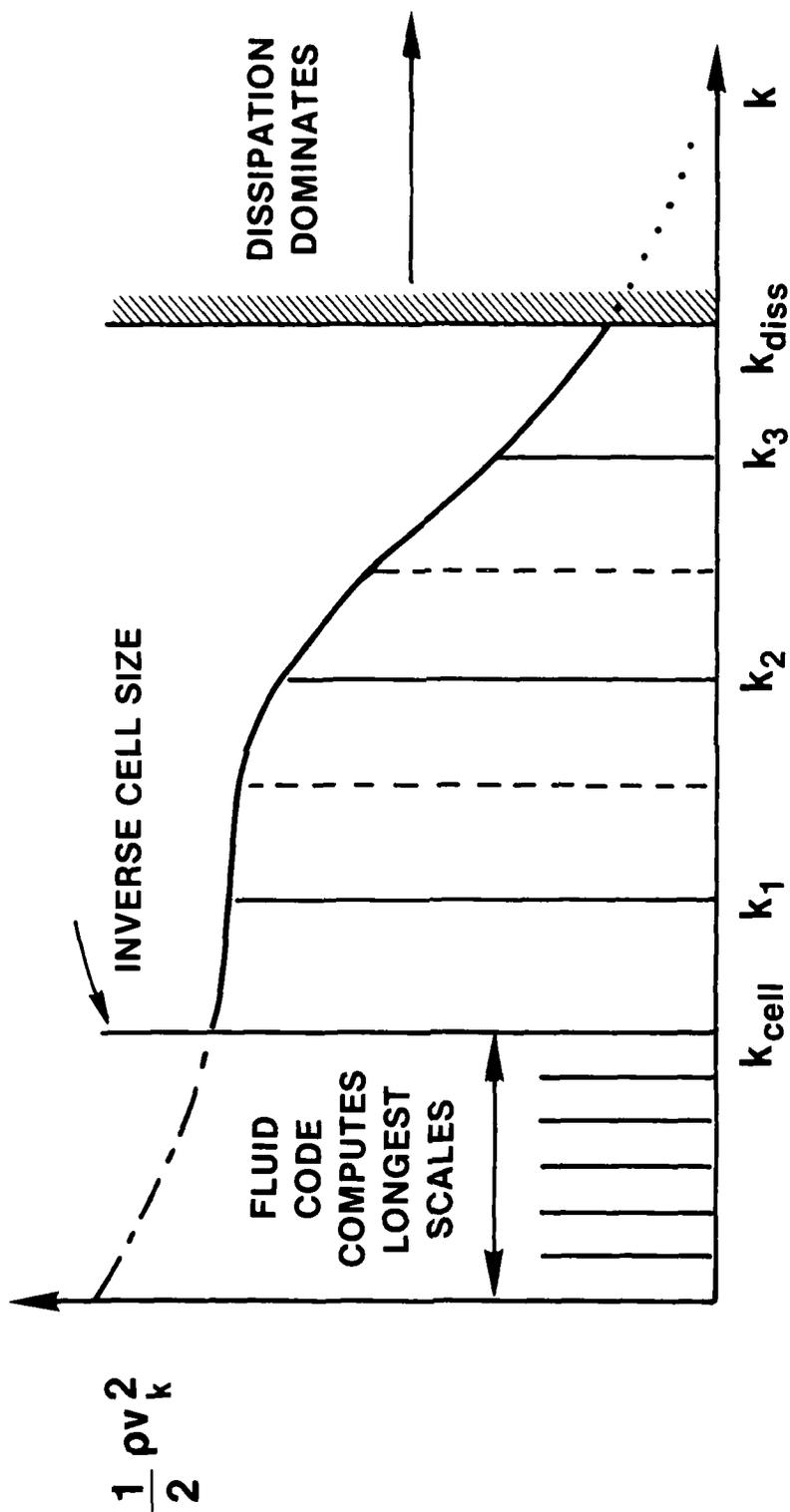


Figure 2 — Schematic of the localized spectral dynamics approach to reactive flow modelling. For long wavelengths, $k < k_{cell}$, the transient, macroscopic fluid calculation may be performed. For short wavelengths, $k > k_{diss}$, diffusion and dissipation dominate so simplified analyses suffice. The intermediate region, called inertial, subgrid, or turbulent, is broken into bins centered at discrete wavenumbers k_1 , k_2 , k_3 . The hope is that an efficient, tractable set of equations can be written down for the spectral strength of the turbulence at each wavenumber which matches suitably to the two known regions to the right and left.

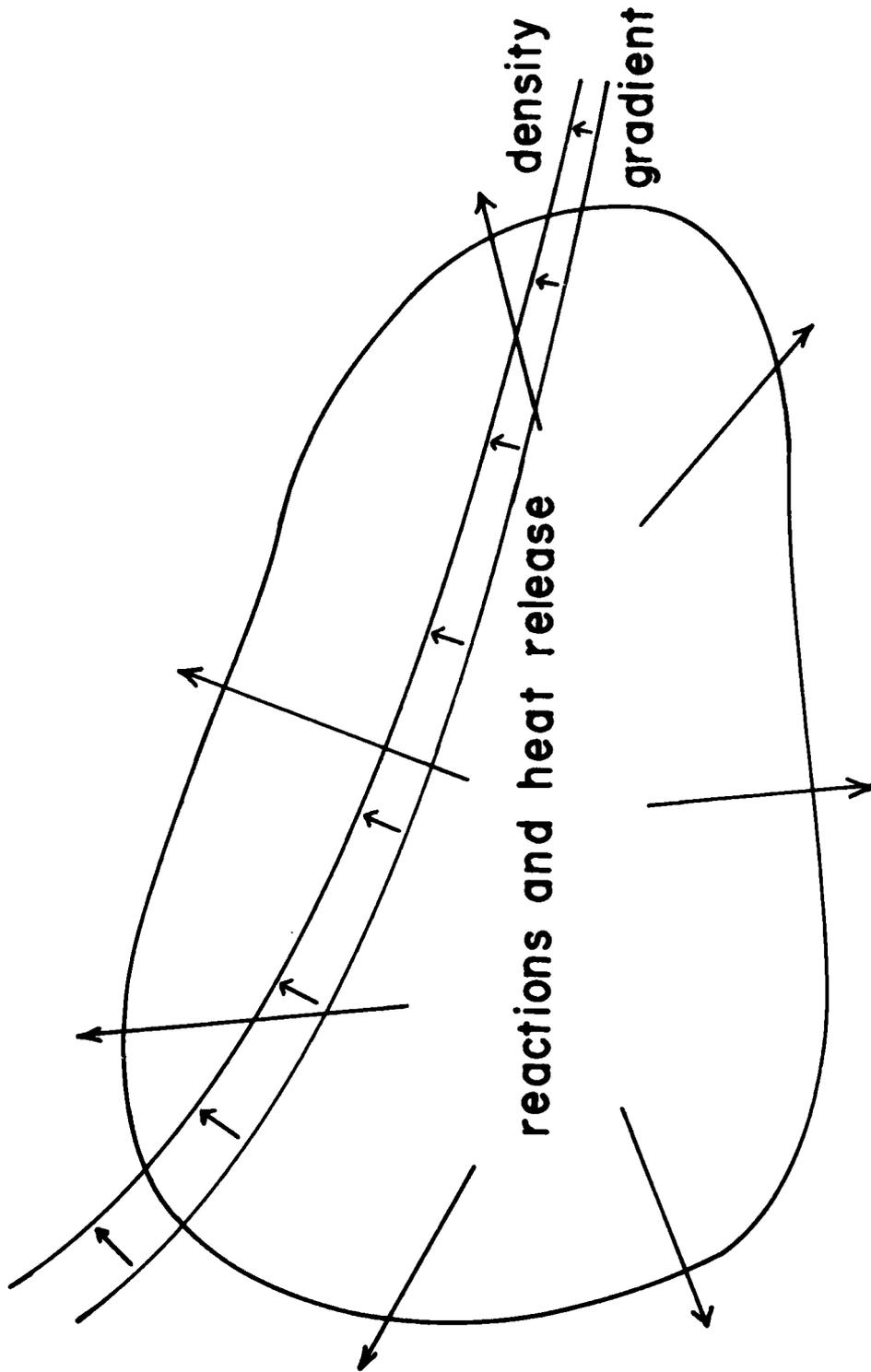


Figure 3 — The active role of expansion in the turbulence of reactive flows. A sharp density gradient is shown in the vicinity of a molecularly mixed pocket of fuel and oxidizer where reactions and heat release are occurring. The expansion induced pressure gradients interact with the density gradient to produce vorticity in the flow.

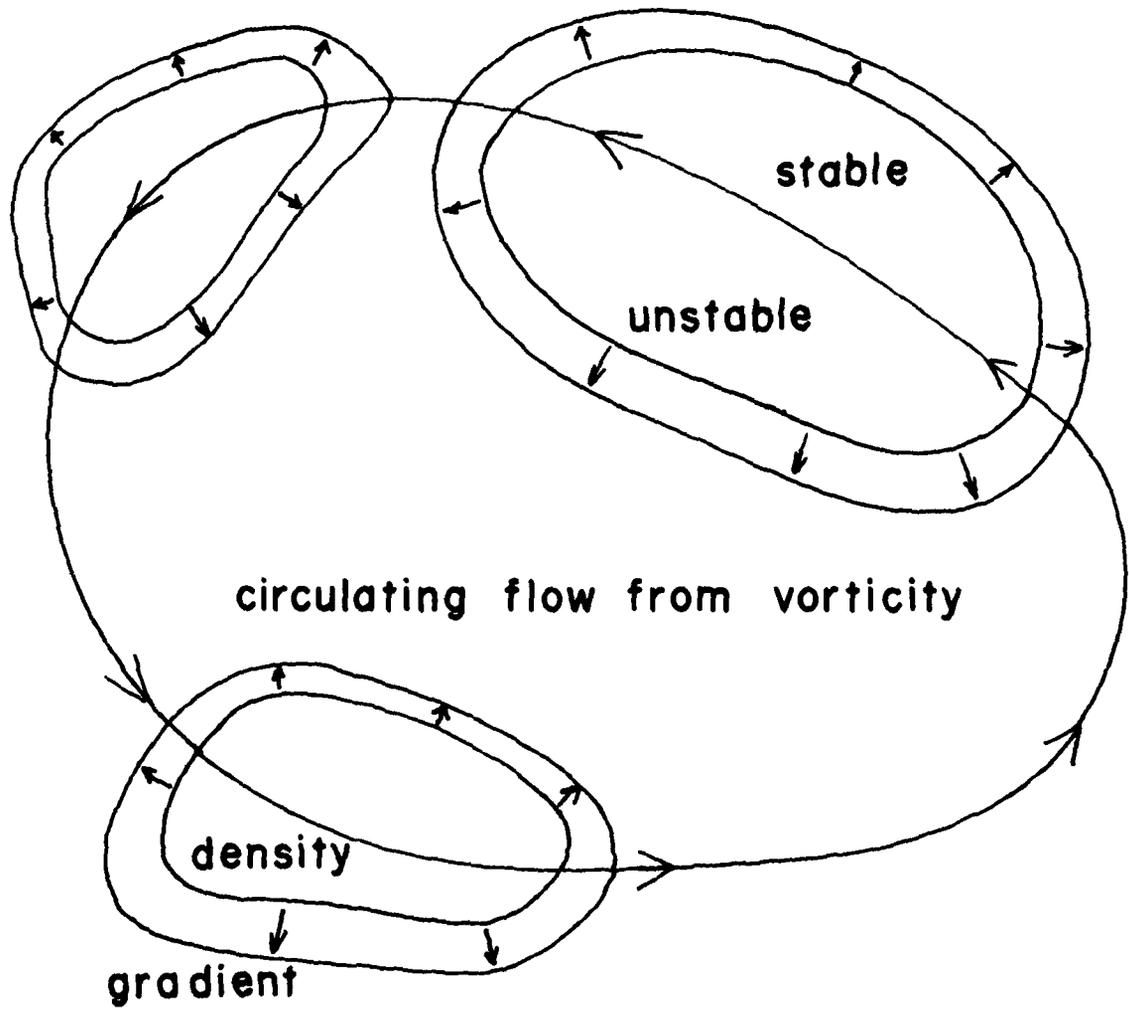


Figure 4 — The passive role of expansion in the turbulence of reactive flows. Here previously mixed pockets of fuel and oxidizer have reacted and thus expanded to low density. These density gradients again generate vorticity on a local small scale as they interact with global pressure gradients resulting from larger scale circulations of the fluid.

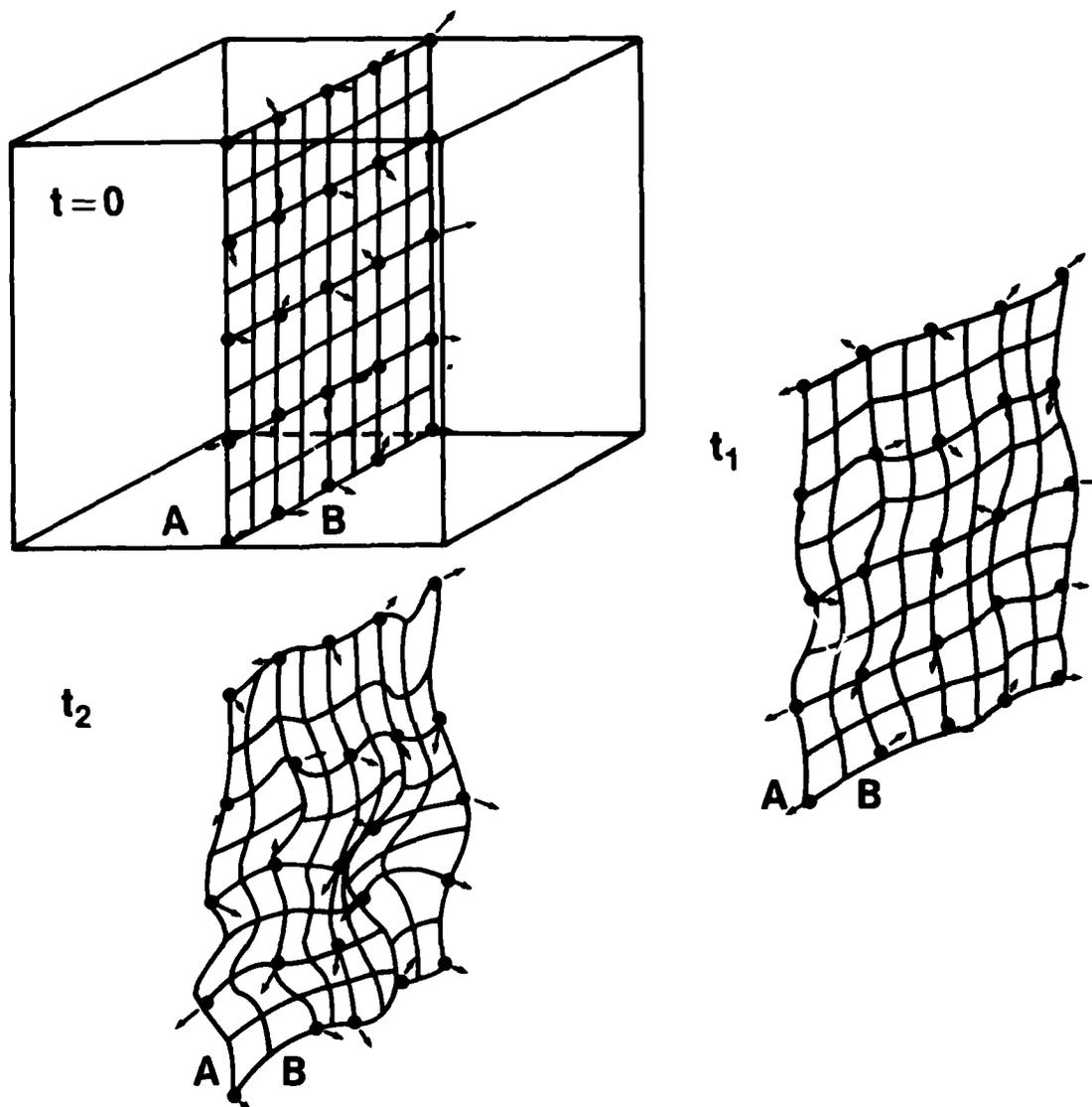
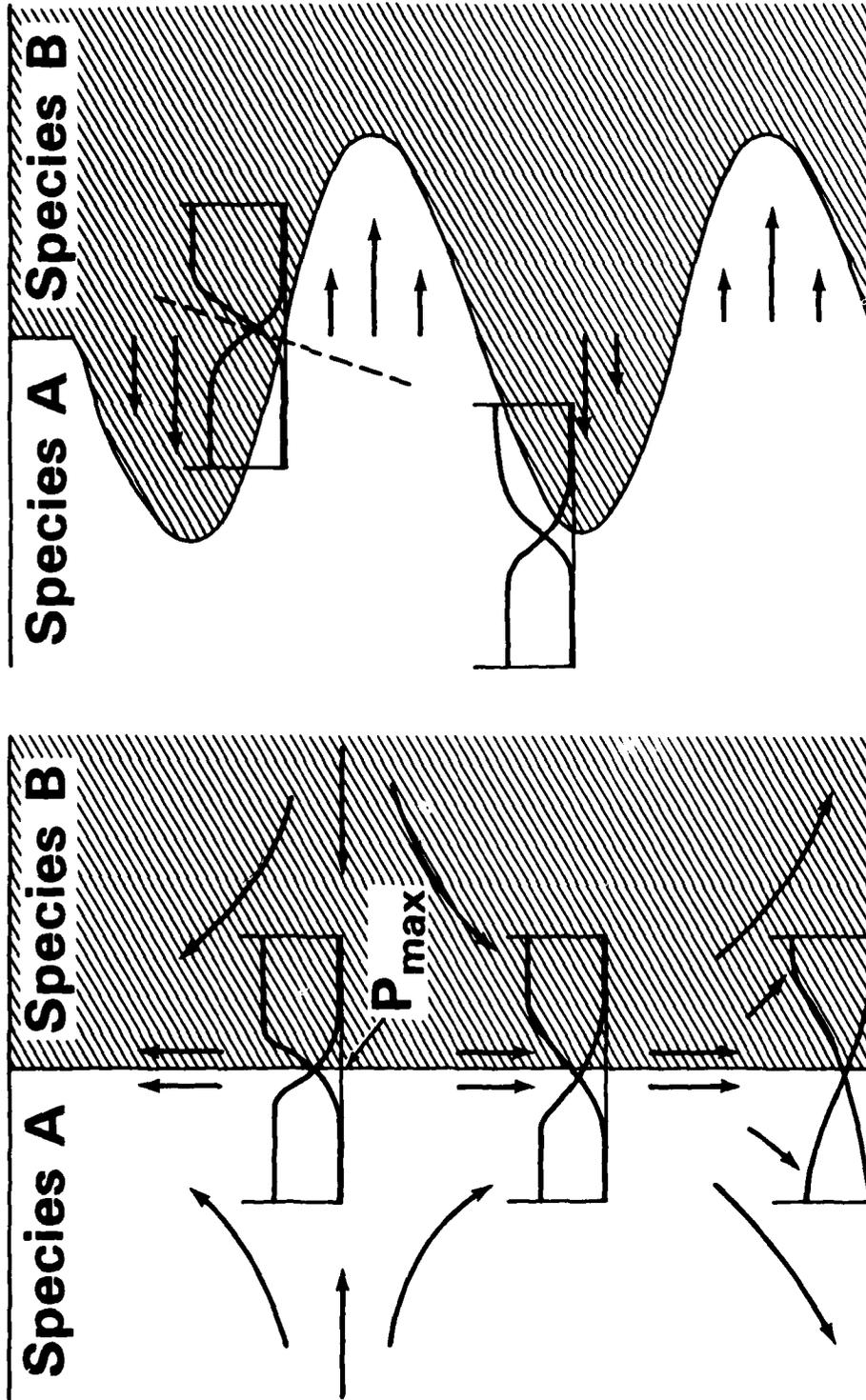


Figure 5 — Three stages during the early deformation of a reactive surface between two fluids A and B. At $t = 0$ (upper left), the surface separating A and B is shown as flat and two-dimensional in a three-dimensional volume of fluid. At later times t_1 (upper right) and t_2 (lower left), the surface progressively deforms as the result of the local Lagrangian motion of surface points shown as small arrows to indicate local direction of flow.



interpenetration stretching

Figure 6 — Interpenetration of two species A and B as influenced by local reactive interface dynamics. On the left the flow pattern indicated by the arrows corresponds to a convergence of the flow normal to the interface in the center and a divergence of the flow in the lower portion of the panel. Normal gradients are enhanced as convergence and mixing is accelerated locally even though the interface area is constant. This surface stretching is contrasted with the convective interpenetration shown in the right panel where mixing is enhanced primarily by increases in the reactive surface area.

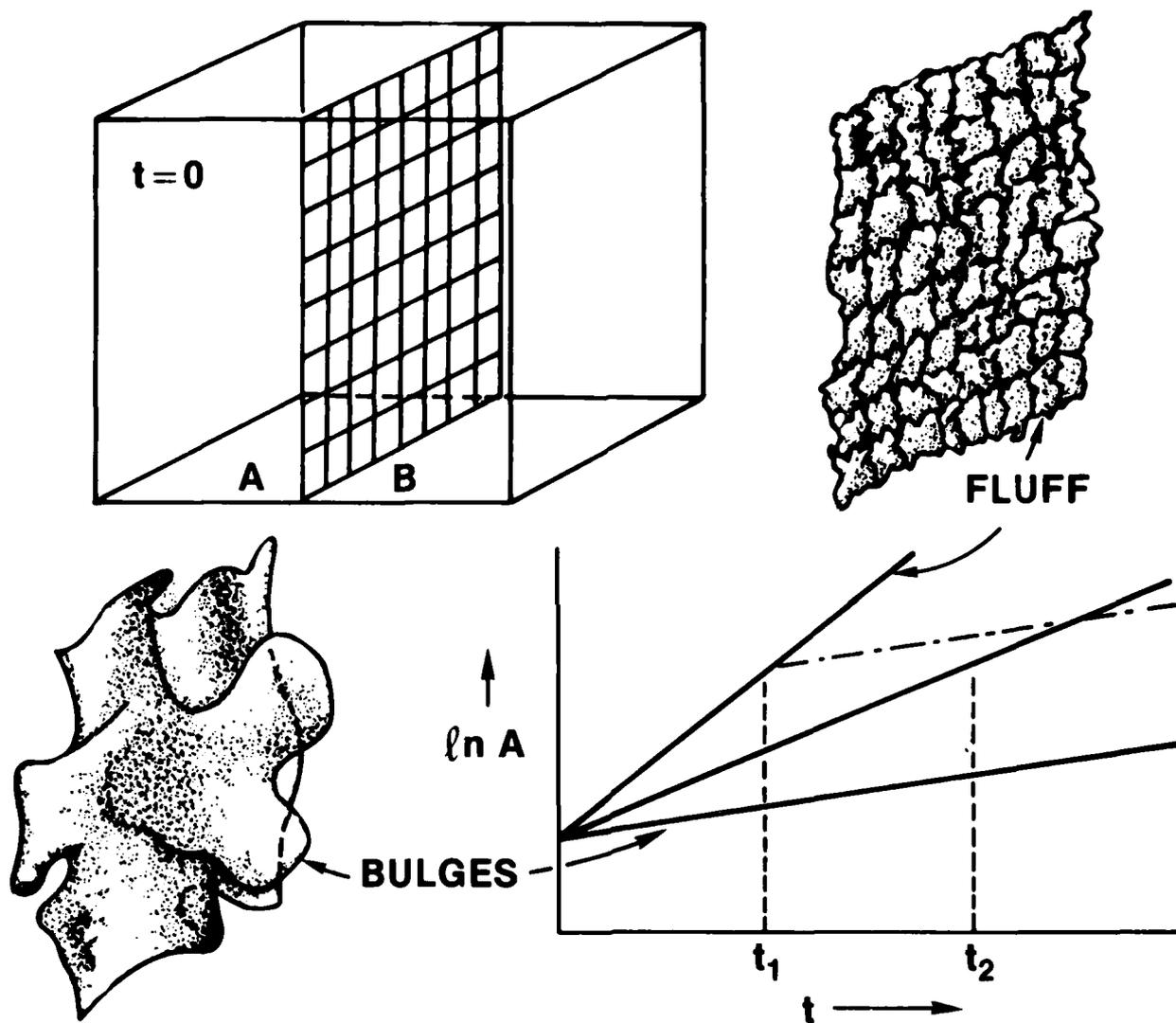
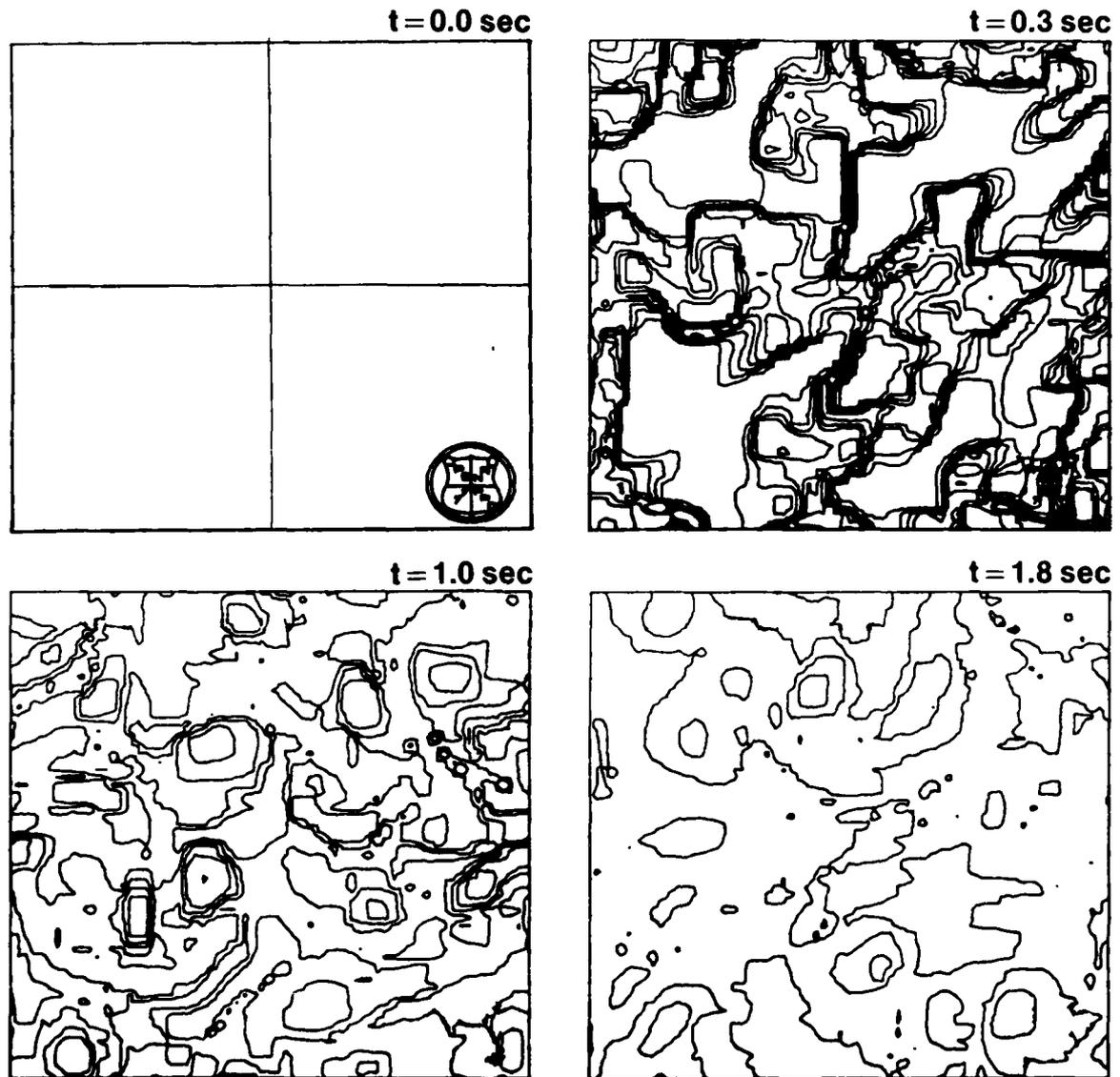


Figure 7 — Two different cases for reactive interface area increase are shown. In the upper right a relatively flat fluffy surface results from a turbulent velocity spectrum enhanced at short wavelengths where molecular diffusion is strong. Although the ideal surface area should increase exponentially as shown in the lower right, the effective surface area will increase more slowly as indicated by the — — line because diffusion can nullify small wavelength area increases. When diffusion is small and the velocity spectrum large at long wavelengths, smooth bulges result as shown in the lower left. Exponential area growth is possible but at a lower rate in this case.

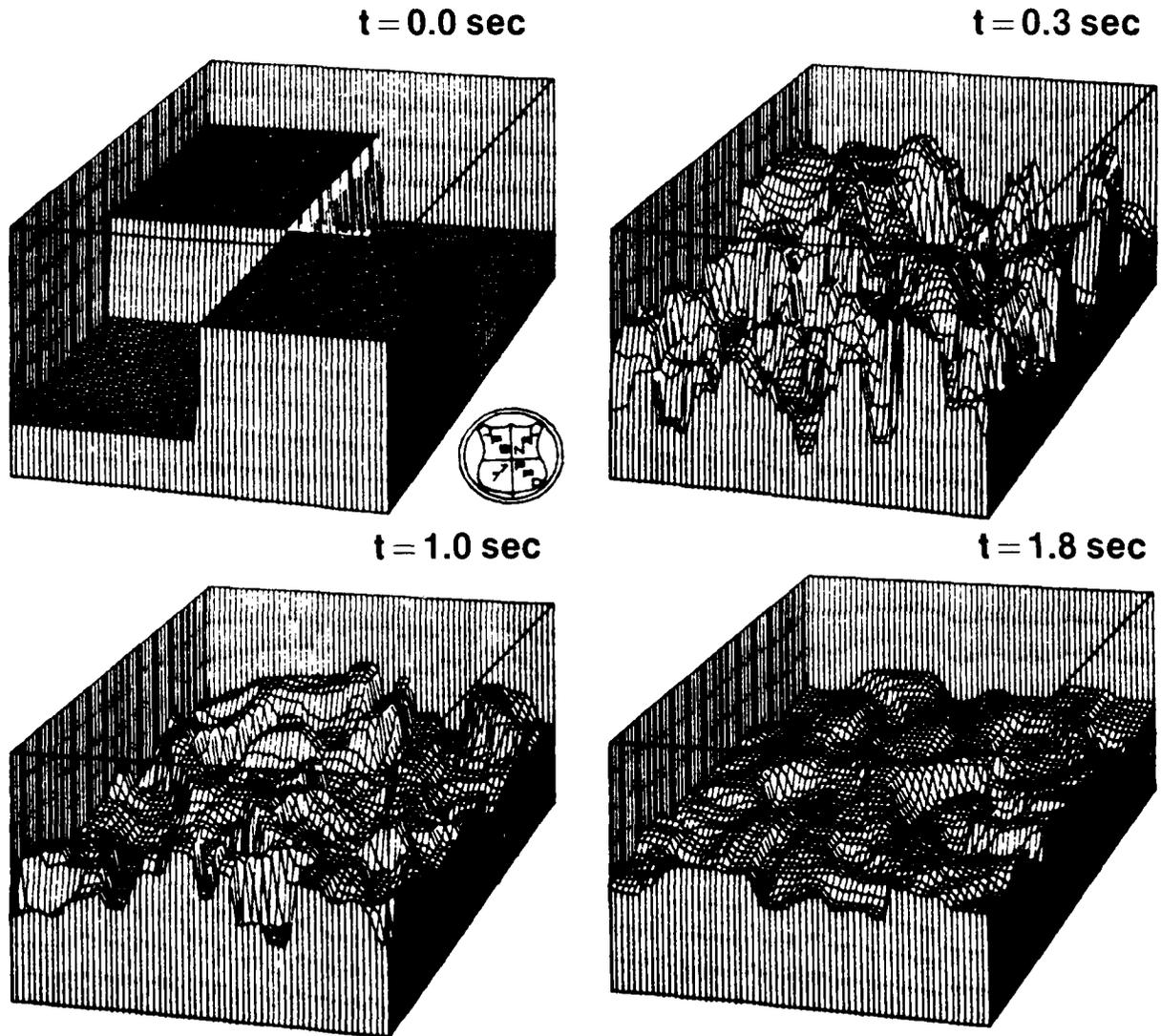
Ab Initio Simulation of Reactive Flow Mixing



density contour evolution of initial checkerboard

Figure 8 — Contour plots of density during a detailed two-dimensional reactive flow simulation designed to show the effects of density differences on the generation of short wavelength turbulence and mixing. Four regions of alternating high and low mass density are established in a checkerboard pattern at time $t = 0.0 \text{ sec}$ (see upper left panel of Fig. 9). Contours at $\rho_a + \alpha(\rho_b - \rho_a)$ are shown where $\alpha = 0.1, 0.2, \dots, 0.9$. After 0.3 seconds the beginning of convective mixing is seen due to an initially impressed random velocity field. At the two later times shown (lower panels), molecular mixing, enhanced by short wavelength convection, leaves only the contours at $\alpha = 0.4, 0.5$, and 0.5.

Ab Initio Simulation of Reactive Flow Mixing



density surface evolution of initial checkerboard

Figure 9 - Plots of density as a function of x and y at four times for the ab initio reactive flow mixing calculation of Fig. 8. As can be seen, molecular mixing rapidly smooths out the jagged interfaces which result from the short wavelength components of the "turbulence" field at the beginning of the calculations.

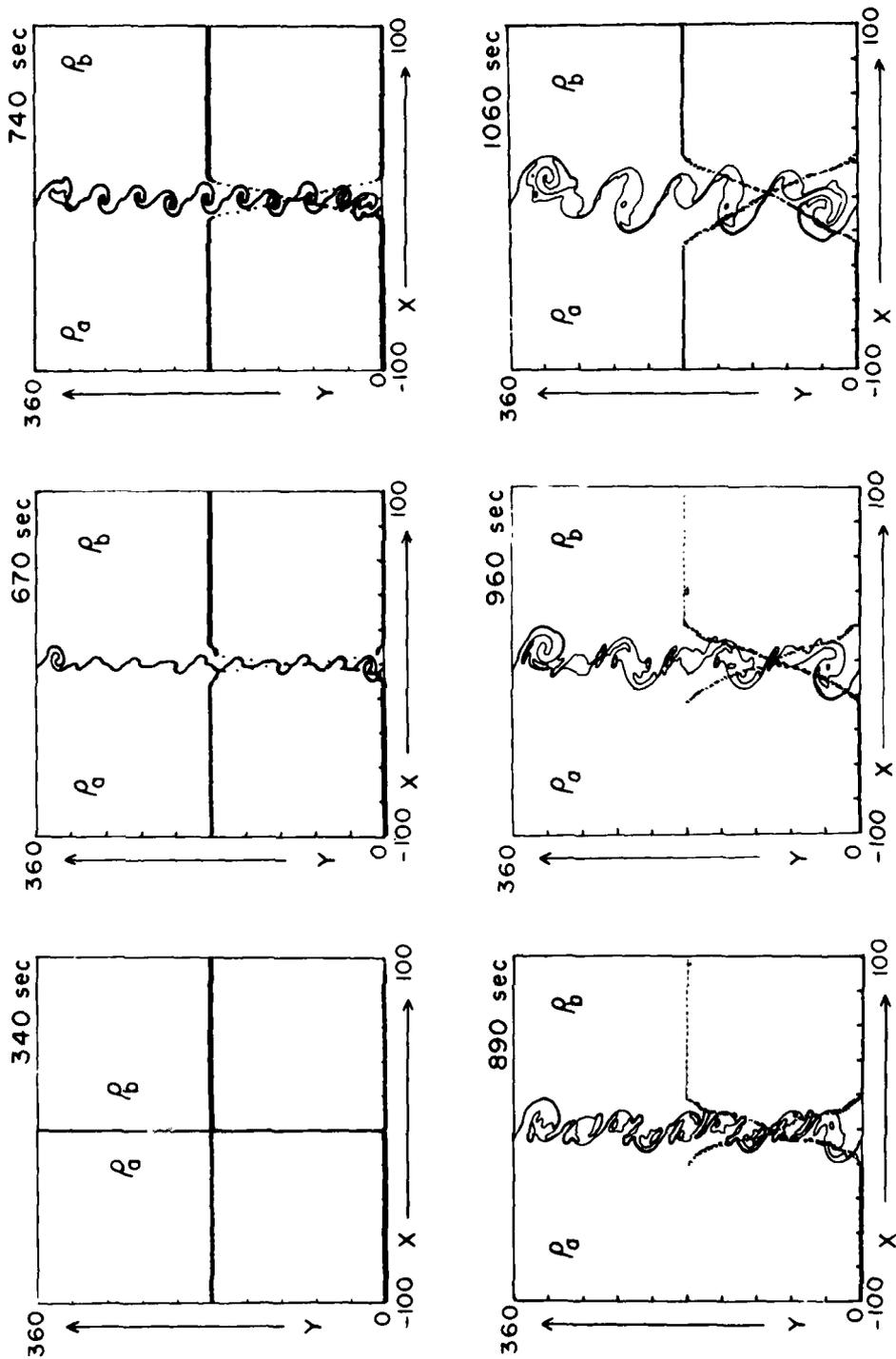


Figure 10 — Evolution of a shear mixing layer in a finely resolved two-dimensional ab initio calculation of a two species compressible fluid. The calculation was performed using flux-corrected transport algorithms on a 200×360 finite difference grid. Also plotted on top of the contours of density, which delineate the separation between species a and species b, is the vertical average at each x cell of the species densities ρ_a and ρ_b in the vertical strip from $y = 0$ to $y = 360$. Such macroscopic averages of finely resolved microscopic calculations can be extremely useful in calibrating and developing phenomenological subgrid models.

THE PROBLEM WITH STEADY FLOW APPROXIMATIONS

BORIS AND ORAN

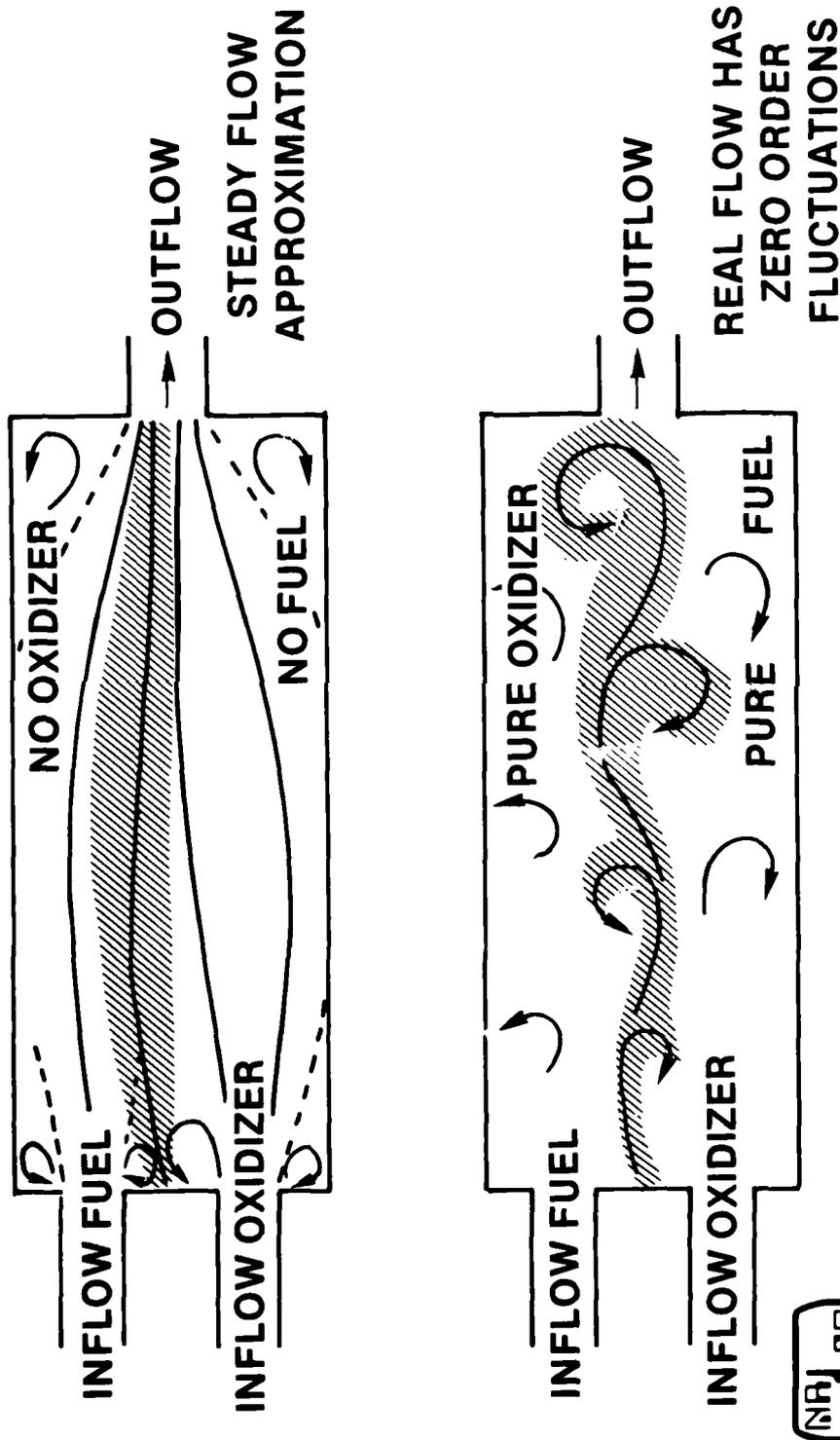


Figure 11 - A practical and philosophical problem with steady flow approximations. The upper panel shows an idealized flow assumed to be the steady state time average of a turbulent mixing flow. Pure oxidizer and pure fuel cannot cross the separating streamline so pure oxidizer in the upper right corner of the combustor or pure fuel in the lower left corner is an impossibility. In the real fluctuating flow of the lower panel, whorls and vortices ensure that there are large scale variations in flow and that fuel and oxidizer are carried intermittently to the far corners of the system.



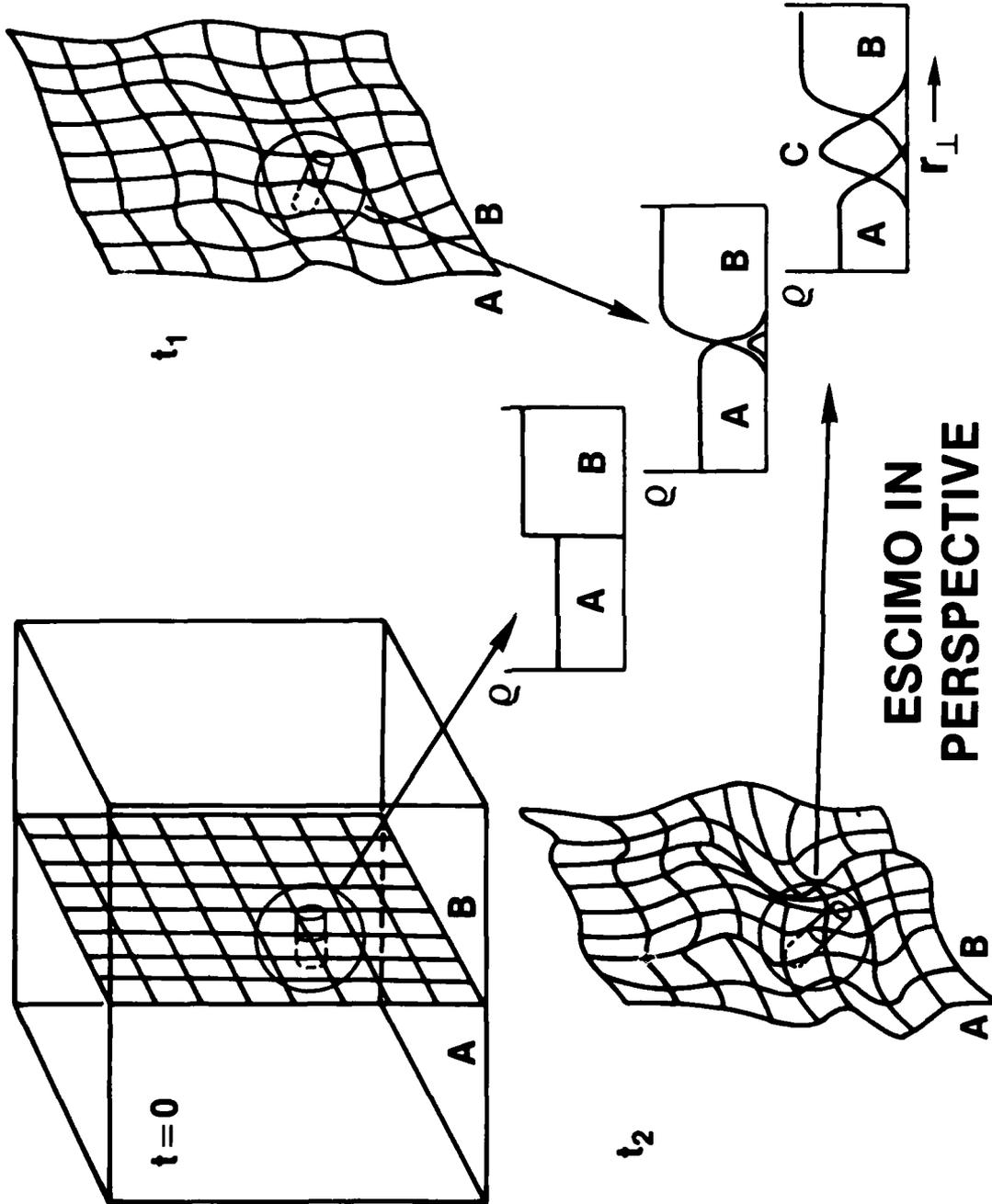


Figure 12 — A global perspective on the ESCIMO approach. Each element of the evolving reactive surface between two species can be viewed as supporting a one-dimensional reactive flow problem where only the spatial direction normal to the surface is considered. Rather than emphasizing the global dynamics of the reactive surface, this approach focuses on the complementary reaction kinetics of the diffusively interpenetrating fluids across the interface as shown in the lower right. Both approaches are crucial to extending our understanding of reactive flow mixing.