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ependent Simulation of Scale Turbulent Mixing and Reaction

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ABSTRACT

A mathematical model of the local transient diffusion-controlled reaction between initially unmixed species is presented. It is intended ultimately as a computational "molecule" to be imbedded in direct simulations of larger scale reacting flows. The model consists of an interacting three-dimensional strain vortex field which exactly satisfies the Navier-Stokes equation, an analytically determined Lagrangian representation of the mixing process and convection-diffusion equations for the reacting species in Lagrangian coordinates. The length scale established by the stretching of the vorticity field is shown to be directly relatable to the Kolmogoroff scale if the local strain rate has a scale consistent with laminar boundary layer theory coordinates. Results are shown for the flow pattern and the induced mixing. An analytical solution to the convection-diffusion equation governing the diffusion-controlled reaction is derived. The solution is valid for large Schmidt number and describes the evolution of any initially two-dimensional configuration of reactants. A special two-dimensional case of this model, in which vortex strain is excluded and fuel and oxidizer initially occupy adjacent half-spaces, is also analyzed. This problem was originally formulated by F. Marble, who treated it in a very different manner from that described here.

INTRODUCTION

The numerical simulation of turbulent reacting flows has become increasingly viable in recent years. More powerful computers, advances in computational techniques, and clearer physical insight, have combined to make possible the calculation of at least some aspects of turbulent combustion directly from the governing equations.

Despite this progress, many serious problems remain unsolved. Although large scale features of turbulent flows seem amenable to computation, the prediction of local reactant consumption and energy release rates requires a description of the flow at length and time scales sufficiently small for molecular diffusion to be effective. These scales are well below the resolution limit of any finite difference simulation; particularly since the inherently three-dimensional mechanism of vortex stretching must be accounted for in the description of phenomena at this level of detail. In fact, it is the vortex stretching mechanism that is responsible for the fact that the ratio of dissipation scale to macroscopic length is proportional to $(Re)^{-3/4}$ in fully developed turbulent flow. Here Re is a Reynolds number based on macroscopic velocity and length scales. The description of flow, mixing, and diffusion of reactants at this scale is the subject of the present research.

The mathematical model presented here is intended ultimately as a computational "molecule" to be imbedded in direct simulations of larger scale reacting flows. In this spirit, it is assumed that a three-dimensional time-dependent calculation capable of resolving the largest length and time

scales of the relevant phenomena, is being performed. The resolution limits of this calculation are too coarse to directly calculate the small scale mixing and diffusion which actually control the reaction. The large-scale simulation does, however, define the environment in which the phenomena of interest evolve.

Progress made this year has been reported at the 1985 AFOSR/ONR Contractors' Meeting on Turbulent Combustion on 23-25 July in Pasadena, California in a talk entitled "Time-Dependent Simulation of Turbulent Combustion" by H. R. Baum and R. G. Rehm; and at the Eastern States Section/Combustion Institute Fall 1985 Meeting on November 4-6, 1985 in Philadelphia, Pennsylvania in a talk entitled, "Time-Dependent Simulation of Small-Scale Turbulent Mixing and Reaction", by H. R. Baum, D. M. Corley and R. G. Rehm. A paper based on this work entitled, "Time-Dependent Simulation of Small-Scale Turbulent Mixing and Reaction", by H. R. Baum, D. M. Corley and R. G. Rehm, has been submitted to The Twenty-First International Symposium on Combustion, which is to be held in Munich, West Germany on August 3-8, 1986. A copy of this paper appears as Section II. In Section III additional analytical/numerical research on the special two-dimensional case described as "the Marble problem" is presented; this is work in progress and will be published later when it is completed.

TIME-DEPENDENT SIMULATION OF SMALL SCALE

TURBULENT MIXING AND REACTION

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(9) Fire
(11) Fluid Dynamics
(18) Modeling and Scaling

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Turbulent Mixing and Reaction

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ABSTRACT

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INTRODUCTION

The numerical simulation of turbulent reacting flows has become increasingly viable in recent years. More powerful computers, advances in computational techniques, and clearer physical insight, have combined to make possible the calculation of at least some aspects of turbulent combustion directly from the governing equations. For example, finite difference simulations of inviscid turbulent mixing layers in two dimensions[1] and axially symmetric jets[2] have been performed at fairly high resolution. Less detailed calculations of simple transport by buoyant plumes in enclosures have been carried out using finite-difference and particle-tracking methods in both two and three dimensions[3,4]. Finally, the random vortex method has been combined with a flame front algorithm and finite difference techniques to produce elegant simulations of premixed turbulent combustion in two dimensions[5,6].

Despite this progress, many serious problems remain unsolved. Although large scale features of turbulent flows seem amenable to computation, the prediction of local reactant consumption and energy release rates requires a description of the flow at length and time scales sufficiently small for molecular diffusion to be effective. These scales are well below the resolution limit of any finite difference simulation; particularly since the inherently three-dimensional mechanism of vortex stretching must be accounted for in the description of phenomena at this level of detail. In fact, it is the vortex stretching mechanism that is responsible for the fact that the ratio of dissipation scale to macroscopic length is proportional to $(Re)^{-3/4}$ in fully developed turbulent flow[13]. Here Re is a Reynolds number based on macroscopic velocity and length scales. The description of flow, mixing, and diffusion of reactants at this scale is the subject of the present paper.

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The mathematical model presented below is intended ultimately as a computational "molecule" to be imbedded in direct simulations of larger scale reacting flows. In this spirit, it is assumed that a three-dimensional time-dependent calculation capable of resolving the largest length and time scales of the relevant phenomena, is being performed. The resolution limits of this calculation are too coarse to directly calculate the small scale mixing and diffusion which actually control the reaction. The large-scale simulation does, however, define the environment in which the phenomena of interest evolve. This environment can be defined as follows: Classical analyses of the kinematics of an arbitrary flow[7] show that the velocity field in the neighborhood of any point can be decomposed into a uniform translational velocity, a rigid body rotation, and a pure strain. This decomposition can be readily performed for most numerical simulations. Similarly, the thermodynamic state expressed in terms of the pressure and conserved scalar quantities, (e.g. Schvab-Zeldovich variables) are assumed known. At high Reynolds numbers, the conserved scalars are primarily convected at computationally resolveable scales. It is easy to track the coordinates of a material point moving with the computationally resolveable fluid motion[3,4]. We now choose a local coordinate system in this frame of reference.

Viewed from the moving coordinate system, the ambient velocity field consists of a linear strain field and a vorticity, with a specified pressure. There are two possibilities for the conserved scalar fields. If the nominal interface between reactants is macroscopically determined [5,6], then at the resolution limit the interface is taken to be initially planar. If it is of subgrid dimensions, then its initial shape is assumed known. Examples of both

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types are shown below. The fundamental problem can now be defined as follows: Given initial conditions for the "local ambient state" (i.e. strain rate, vorticity, pressure, and conserved scalar configuration), determine their subsequent local evolution in space and time.

This problem is broken down below into three subsidiary problems. First, the construction of the local velocity field produced by the effect of the strain on the vorticity field. Next, the calculation of a local Lagrangian coordinate system so that small scale mixing of reactants can be separated from molecular diffusion. Finally, solution of the evolution equation for conserved scalars in the Lagrangian coordinates. In each case simplifications in geometry and thermophysical properties are introduced in the interest of maintaining an essentially analytical approach yielding readily interpretable results. The consequences of these simplifications are assessed in a concluding section.

A related set of investigations has been performed by Karagozian and Marble[8],[9]. However, both the general approach and the results obtained by them are significantly different from those reported below. More detailed comments are included in subsequent sections.

THE VELOCITY FIELD

Consider a flow in which the vorticity is locally aligned in the x-direction, Fig. 1, and subjected to a uniform strain of strength α. Then, if v_x, v_r, and v_θ are respectively the axial, radial, and swirl components of velocity, the Navier Stokes equations for a constant-property incompressible fluid have

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solutions of the form:

$$v_x = \alpha x \; ; \quad v_r = -\alpha r/2$$

$$\frac{\partial v_\theta}{\partial t} - \frac{\alpha r}{2} \frac{\partial v_\theta}{\partial r} - \frac{\alpha v_\theta}{2} = \nu \left\{ \frac{1}{r} \frac{\partial}{\partial r} \left(\frac{r \partial v_\theta}{\partial r} \right) - \frac{v_\theta}{r^2} \right\} \tag{1}$$

Equation (1) is the swirl component of the momentum equation for the fluid whose kinematic viscosity is ν. The axial vorticity field $\omega(r,t)$ is defined in terms of $v_\theta(r,t)$ by the expression

$$\omega = \frac{1}{r} \frac{\partial}{\partial r} (r v_\theta). \tag{2}$$

The linearity of Eqs. (1) and (2) suggests seeking a solution satisfying the initial condition

$$\omega(r,0) = r_o \Omega \delta(r-r_o) \tag{3}$$

Here δ denotes the Dirac delta function. The resulting solution for v_θ is in effect a Greens function for Eq. (1), in that its convolution with any initial axial vorticity distribution generates the corresponding solution to the Navier-Stokes equations. As such, it contains all the phenomena implied by the equation; i.e. the convection, stretching, and diffusion of vorticity.

To proceed, it is convenient to introduce the following dimensionless variables:

$$v_\theta = \Omega \, r_o \, \hat{w}(\hat{r}, \hat{t})$$

$$r = r_o \, \hat{r} \tag{4}$$

$$t = (\alpha)^{-1} \, \hat{t}$$

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Then, define a new dependent variable v, and independent variables ρ, τ in the form

$$\rho = \hat{r} \exp(\hat{t}/2)$$

$$\tau = \varepsilon[\exp(\hat{t})-1] \qquad (5)$$

$$\hat{w} = \exp(\hat{t}/2) \, v(\rho,\tau)$$

In terms of these variables, Eqs. (1)-(3) become:

$$\frac{\partial \lambda}{\partial \tau} = \frac{1}{\rho} \frac{\partial}{\partial \rho} \left(\rho \frac{\partial \lambda}{\partial \rho} \right)$$

$$\lambda(\rho,0) = \delta(\rho-1) \qquad (6)$$

where

$$\lambda \equiv \frac{1}{\rho} \frac{\partial}{\partial \rho} (\rho v)$$

The variable ρ is the characteristic coordinate of the left hand side of Eq.(1), while λ is a reduced vorticity. The parameter $(\varepsilon)^{-1}$ is a local Reynolds number based on the strain rate and the initial radius of the vortex tube whose evolution is described by λ. Note that the first of Eqs.(6) is the heat conduction equation with cylindrical symmetry. The solution is readily obtained by taking Laplace Transforms in τ[10]. The result is:

$$\lambda = (2\tau)^{-1} \exp[-(1+\rho^2)/4\tau] \, I_0(\rho/2\tau)$$

$$v = (\rho)^{-1} \int_0^\rho \lambda \, (\rho_0,\tau) \, \rho_0 d\rho_0 \qquad (7)$$

Here, I_0 is the modified Bessel function of order zero. Equations (5) and (7) constitute the desired solution. They describe the evolution of an initial shell of vorticity concentrated at radius r_0 into the classical steady state stretched vortex, whose velocity is given by:

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$$\hat{w}(\hat{r}, \infty) = (\hat{r})^{-1}\{1 - \exp[-(\hat{r})^2/4\varepsilon]\} \qquad (8)$$

The dimensionless swirl velocity $\hat{w}$ defined by Eqs. (4), (5), and (7) is

plotted in Fig. 2 for $\varepsilon = .002$, corresponding to a local Reynolds number of

500. Note that the stretching mechanism acts to steepen the velocity

gradients with time until the viscous effects become strong enough to provide

the steady-state balance described by Eq. (8). The internal length scale ℓ in

these solutions is

$$\ell = (\nu/\alpha)^{1/2} \qquad (9)$$

Thus, $(\varepsilon)^{1/2}$ is the ratio of the internal length scale to r_o, that imposed by

the largest scale flow. The actual magnitude of ℓ depends on the imposed

strain rate α. It is interesting to observe that in a laminar boundary or

free shear layer characterized by a macroscopic length L and velocity U, the

local strain rate α can be characterized by

$$\alpha \sim U(UL/\nu)^{1/2}/L \qquad (10)$$

Inserting the estimate given by Eq. (10) in Eq. (9), the internal scale ℓ can

then be related to macroscopic parameters as:

$$\ell/L \sim (Re)^{-3/4}$$
$$Re = UL/\nu \qquad (11)$$

Equation (11) shows that under circumstances where a fragment of laminar shear

layer can stretch a vortex, the resulting flow will quickly collapse to

the Kolmogoroff or dissipation scale [13]. Thus, the solution described here

offers a concrete dynamic realization of how such a small scale local flow can

develop.

The fact that the vorticity evolution can be related to the cylindrical heat

conduction equation under the symmetry conditions implied by Eqs. (1) has been

noted by several authors [8,9,10,12]. However, when solutions investigated are restricted to Gaussian forms [8,9,12] in the τ,ρ coordinate system, a rich variety of phenomena, including the collapse process itself, is lost. This has further implications which arise in the study of mixing and diffusion, which are considered next.

REACTANT MIXING

Assume that the fluid consists of reacting species "A" and "B", which are initially separated on either the macroscopic scale L or the local scale ro, For simplicity (and consistency with the flow field) the reaction is taken to be isothermal. Let n and M be the stoichiometric coefficient and molecular mass of each species, and Y be the corresponding mass fraction. Then, if Y(0) denotes the initial unmixed mass fraction of each species, it is possible to define a normalized Shvab-Zeldovich variable Z as follows:

$$Z = 2\{(Y_A/n_A M_A)-(Y_B/n_B M_B) - (1/2)[(Y_A(0)/n_A M_A) - Y_B(0)/n_B M_B]\}$$
$$\cdot [(Y_A(0)/n_A M_A) + (Y_B(0)/n_B M_B)]^{-1} \tag{12}$$

The variable Z satisfies the following equation and initial condition:

$$\frac{\partial Z}{\partial t} + \vec{u}\cdot\nabla Z = D\Delta Z \tag{13}$$

$$\text{at } t = 0 \quad Z = +1 \quad (\text{Species A}) \tag{14}$$
$$Z = -1 \quad (\text{Species B})$$

Here $\vec{u}$ is the velocity vector defined in Eq. (1), D is the diffusivity of each species, and Δ the Laplacian operator. The initial species distributions are assumed to be independent of the axial coordinate x. This restriction is not essential to the analysis which follows, and it greatly simplifies the algebra

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required to obtain results of interest. Then, introducing the dimensionless

variables defined by Eq. (4), Eq. (13) can be written in the form:

$$\frac{\partial Z}{\partial \hat{t}} - \frac{\hat{r}}{2} \frac{\partial Z}{\partial \hat{r}} + \frac{\Omega}{\alpha} \frac{\hat{w}}{\hat{r}} \frac{\partial Z}{\partial \theta} = \frac{\varepsilon}{Sc} \left\{ \frac{\partial^2 Z}{\delta \hat{r}^2} + \frac{1}{\hat{r}} \frac{\partial Z}{\delta \hat{r}} + \frac{1}{\hat{r}^2} \frac{\partial^2 Z}{\delta \theta^2} \right\} \tag{15}$$

$$Sc = \nu/D$$

The variable θ in Eq. (15) is the azimuthal coordinate, increasing in the

direction of the swirl velocity component $\hat{w}$ (see Fig. 1), while Sc is the

Schmidt number.

The left-hand side of Eq. (15) can be thought of as governing the small-scale

mixing of the reactants by the local velocity field, while the right-hand side

controls the true molecular diffusion. It is desirable to cast the solution

in a form which illustrates these two effects explicitly. This can be

accomplished by introducing Lagrangian coordinates τ, ρ, ϕ. The variables τ and

ρ are defined in Eq. (5), while ϕ is defined as:

$$\phi = \theta - (\Omega/\alpha\varepsilon) \, \psi(\rho, \tau)$$
$$\psi(\rho, \tau) = (\rho)^{-1} \int_0^\tau v(\rho, \tau_0) \, d\tau_0 \tag{16}$$

Equation (15) in Lagrangian coordinates becomes:

$$\frac{\partial Z}{\partial \tau} = (Sc)^{-1} \left\{ \frac{\partial^2 Z}{\partial \rho^2} + \frac{1}{\rho} \frac{\partial Z}{\partial \rho} + \left[\frac{1}{\rho^2} + (\Omega/\alpha\varepsilon)^2 \left(\frac{\partial \psi}{\partial \rho} \right)^2 \right] \frac{\partial^2 Z}{\partial \phi^2} \right.$$

$$\left. - (\Omega/\alpha\varepsilon) \left[\frac{\partial \psi}{\partial \rho} \frac{\partial^2 Z}{\partial \rho \partial \phi} + \frac{\partial}{\partial \rho} \left(\frac{\partial \psi}{\partial \rho} \frac{\partial Z}{\partial \phi} \right) + \frac{1}{\rho} \frac{\partial \psi}{\partial \rho} \frac{\partial Z}{\partial \phi} \right] \right\} \tag{17}$$

Note that in this system of coordinates there is no longer any convection, as the mixing has been incorporated in the transformation from Lagrangian to Eulerian coordinates. Since the quantity $v(\rho,\tau)$ is given analytically by Eqs. (7), the transformation and any of its derivatives can be evaluated readily to arbitrary accuracy. This transformation is easily generalized to three dimensions, with little added complexity to Eq. (17).

In the absence of diffusion ($Sc \to \infty$), Eq. (17) reduces to the statement that the initial configuration of the reactants does not change in Lagrangian coordinates. Thus, the mixing process can be followed by mapping each point in the Eulerian coordinates at a given time into the Lagrangian space and determining which species occupied that point originally. This has been done for two examples, shown in Fig. 3 and Fig. 4. Figure 3 shows the mixing of two species initially occupying separate half spaces displaced one half the initial vortex radius from the vortex center. This is an example of a macroscopically resolveable interface. The mixing process in this case is seen to be a relatively large scale engulfment followed by a continuous elongation of the interface between species. Figure 4 shows a "subgrid scale" interface, a circular blob of one reactant displaced one half the vortex radius with respect to the vortex center. This time the mixing seems to tear apart the blob, with two highly distorted fragments connected by a slender filament. In each case, the local Reynolds number $(\varepsilon)^{-1}$ was taken to be 500, and the ratio of vorticity to strain (Ω/α) is 2. While the infinite Schmidt number limit is unrealistic for most fluids, it is an excellent approximation for typical smoke aerosols.

MOLECULAR DIFFUSION EFFECTS

Now consider the solution of Eq. (17) for finite values of Sc. In the Lagrangian representation, the vorticity acts to enhance the diffusivity in the azimuthal direction in Langrangian coordinates. The degree of enhancement varies greatly with ρ and τ. Fig. 5 shows the variation of $(\Omega/\alpha\epsilon)\psi$ with $\hat{r}$. At any instant of time, however, $\hat{r}$ and ρ differ only by a multiplicative constant, so each individual spatial profile has the same shape in both systems of coordinates. The analogous plot in Lagrangian space would show each profile centered at $\rho=1$. The result is that the gradient of ψ is very large in an annular ring centered about $\rho=1$. Inside this ring, ψ vanishes exponentially, while outside it decays algebraically (Fig. 6).

This distribution arises from the fact that the vorticity is confined to the annular ring. Thus, there is no angular deformation inside the annulus, while the deformation outside the ring is irrotational. The ring thickens with time under the influence of viscosity, until the inner core disappears. Soon after this ocurs; all the reactants present within the ring (now a disc) will be consumed.

Since the coefficients in Eq. (17) are independent of the angular variable ϕ, it is useful to express the solution in terms of a Fourier series.

$$Z = \sum_n Z_{nc}(\rho,\tau)\zeta_{nc}(\rho,\tau) \cos (n\phi)$$
$$+ \sum_n Z_{ns}(\rho,\tau)\zeta_{ns}(\rho,\tau)\sin (n\phi). \tag{18}$$

The quantities Z_{nc} and Z_{ns} are defined to be the Fourier coefficients that would occur in the absence of vorticity. This corresponds to the solution for diffusion in a uniform strain field, a problem which has already received attention[14,15].

$$\begin{pmatrix} Z_{nc} \\ Z_{ns} \end{pmatrix} = \frac{Sc}{2\tau} \int_0^\infty d\rho_1 \rho_1 \exp\left[-Sc(\rho^2 + \rho_1^2)/4\tau\right] I_n(Sc\rho\rho_1/2\tau) \begin{pmatrix} Z_{nc}(\rho_1, 0) \\ Z_{ns}(\rho_1, 0) \end{pmatrix} \quad (19)$$

Here, I_n are the Modified Bessel functions of order n and $Z_{nc}(\rho_1, 0)$, $Z_{ns}(\rho_1, 0)$ are the Fourier coefficients of the initial distribution of reactants.

To proceed further, it is necessary to either compute the remaining factors ζ_{nc} and ζ_{ns} numerically or make an additional assumption to obtain analytical results. In the present work, the latter choice is made and it is assumed that the Schmidt number Sc is large. Under these circumstances, the diffusion is relatively ineffective in changing the initial distribution except in the annular region. Since the whole vortex collapse process occurs in times $\hat{t}$ $0(1)$, then $\tau \ll 1$ for the times of interest. For small τ, it can be shown that ψ has the form:

$$\psi = (\rho)^{-2} \tau \, \Psi(\eta, \tau)$$
$$\eta = (\rho - 1)/2(\tau)^{1/2} \quad (20)$$

The quantity Ψ in Eq. (20) is a smooth bounded function of η which tends to unity as $\eta \to \infty$ and vanishes exponentially as $\eta \to -\infty$.

For convenience in what follows let the expansion given by Eq. (18) be temporarily recast in complex exponential form:

$$Z = \sum_n \exp(in\phi) Z_n(\rho, \tau) \zeta_n(\rho, \tau) \quad (21)$$

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Substitution of Eq. (21) into Eq. (17) yields:

$$Z_n \frac{\partial \zeta_n}{\partial \tau} = (Sc)^{-1} \left\{ Z_n \frac{\partial^2 \zeta_n}{\partial \rho^2} + \left(2 \frac{\partial Z_n}{\delta \rho} + \frac{Z_n}{\rho} \right) \frac{\partial \zeta_n}{\partial \rho} - n^2 (\Omega/\alpha\epsilon)^2 Z_n \zeta_n \left(\frac{\partial \psi}{\partial \rho} \right)^2 \right.$$

$$\left. -in(\Omega/\alpha\epsilon) \left[\frac{\partial \psi}{\partial \rho} \frac{\partial}{\partial \rho} \{Z_n\zeta_n\} + \frac{Z_n\zeta_n}{\rho} \right) + \frac{\partial}{\partial \rho} \left(Z_n\zeta_n \frac{\partial \psi}{\partial \rho} \right) \right] \right\} \tag{22}$$

The independent variables are now rescaled as follows:

$$\tau = [\alpha\epsilon(Sc)^{1/2}/\Omega]\tau*$$

$$\rho-1 = [\alpha\epsilon(Sc)^{1/2}/\Omega]\rho* \tag{23}$$

Equation (20) then implies the scaling

$$\frac{\partial \psi}{\partial \rho} \equiv q = [\alpha\epsilon(Sc)^{1/2}/\Omega]^{1/2} q*(\tau*,\rho*) \tag{24}$$

Since the reactants are initially assumed to be resolveable on a scale of order one in ρ, then Z_n and its derivatives remain $O(1)$. When the scaling laws given by Eqs. (23) and (24) are used in Eq. (22), the result is:

$$Z_n \left[\frac{\partial \zeta_n}{\partial \tau*} + n^2(q*)^2 \zeta_n \right] = O(Sc)^{-1/2} \tag{25}$$

Thus, the leading terms in the expansion for large Schmidt number can be written in terms of ρ and τ as:

$$\zeta_{nc} = \zeta_{ns} = \exp \left\{ -n^2(Sc)^{-1} (\Omega/\alpha\epsilon)^2 \int_0^\tau \left(\frac{\partial \psi}{\partial \rho} \right)^2 d\tau \right\} \tag{26}$$

Equations (18), (19), and (26) then constitute the solution to Eq. (17) in the annular region. They are in fact the large Schmidt number solution every-where. To see this, note that inside the annulus, $\partial\psi/\partial\rho$ vanishes exponen-tially and $\zeta_{nc} = \zeta_{ns} = 1$, so the vortex free solution is recovered exactly. For values of ρ in the region $1 < \rho < \infty$, Eq. (22) is properly scaled in ρ.

In order to effect a balance for times $\tau^* = O(1)$ the wave number n must be rescaled according to

$$n = [\Omega/\alpha\varepsilon(Sc)^{1/2}]n^* \qquad (27)$$

This is merely a Fourier representation of a boundary layer in the angular variable ϕ. When the rescaling is performed, the same terms are dominant.

This solution can be interpreted physically as saying that the large Schmidt number prevents significant radial diffusion in the Lagrangian coordinates. The intense vorticity sufficiently enhances the azimuthal diffusion in the annulus so that only relatively low wavenumber angular modes are required to describe the solution. In the irrotational region, the diffusion is confined to narrow regions near the interface between reactants and occurs preferentially in the azimuthal direction. The implications for the combustion of a fuel blob (see Figure (6)) are:

(1) The fuel in the annular region containing vorticity is very rapidly consumed.

(2) By the time the vortex collapses to its final steady state, the only remaining fuel is in the irrotational flow region.

(3) Any remaining fuel is consumed along the fuel-oxidizer interface in the irrotational region over a period of time determined by the extent of the fuel blob as well as the vorticity and strain rate.

CONCLUDING REMARKS

A mathematical model of the local convection, mixing, and diffusion of initially unmixed reactants in a turbulent flow has been presented. The model is based directly on solutions of the Navier-Stokes equations in limiting geometrical and parametric cases; no empirical parameters are introduced. At present, the model cannot be regarded as complete. In particular, more work is needed to extend the model to incorporate three-dimensional reactant configurations, large temperature variations, and larger molecular diffusivities. It is currently more suited to the analysis of acid-base reactions in turbulent flow than to combustion. Still, many of the phenomena are similar in both reaction systems, and the study of acid-base reactions in jets and mixing layers is an ongoing project in turbulent combustion research[1],[16]. Extended versions of this model, employed in conjunction with large-scale flow simulations, offer the potential for predicting turbulent reacting flows over a much wider range of scales than is possible with supercomputers using conventional numerical methods. This statement is likely to hold for some time to come.

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FIGURE CAPTIONS

1. Configuration of an axial vortex in an axially symmetric strain field. The streamlines of the strain field are hyperbolic in each cylindrical plane. The azimuthal velocity is in the direction of the curved arrows.

2. Swirl velocity profiles of various times $\hat{t}$ for the collapsing strained vortex. The local Reynolds number $(\varepsilon)^{-1} = 500$.

3. Mixing configuration at various times $\hat{t}$ for an initially planar interface displaced one half vortex radius from the flow symmetry axis. The local Reynolds number $(\varepsilon)^{-1} = 500$. The vorticity to strain rate ratio $\hat{\Omega} = \Omega/\alpha = 2$.

4. Mixing configuration at various times $\hat{t}$ for initially circular reactant displaced one half radius from vortex center. Same flow parameters as Fig. 3.

5. Lagrangian angular coordinate at time intervals $\hat{t}$ of 0.5 from $\hat{t} = 0.5$ to $\hat{t}=5.0$. Same flow parameters as Fig. 3.

6. Sketch of mixing and diffusing reactant configuration in Lagrangian coordinates. The shaded annulus is the region of intense vorticity, the inner region has no swirl velocity, and the outer region is irrotational.
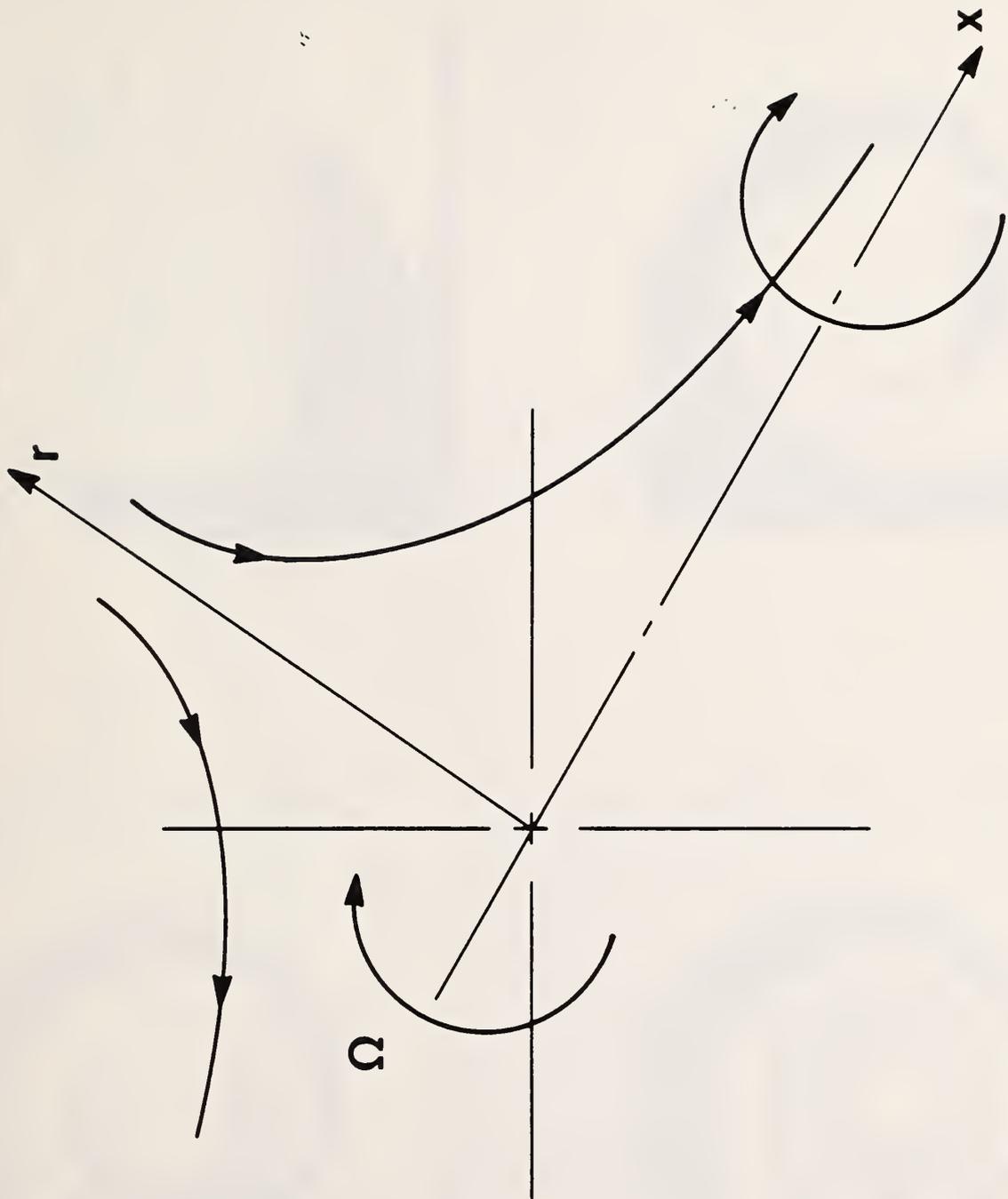
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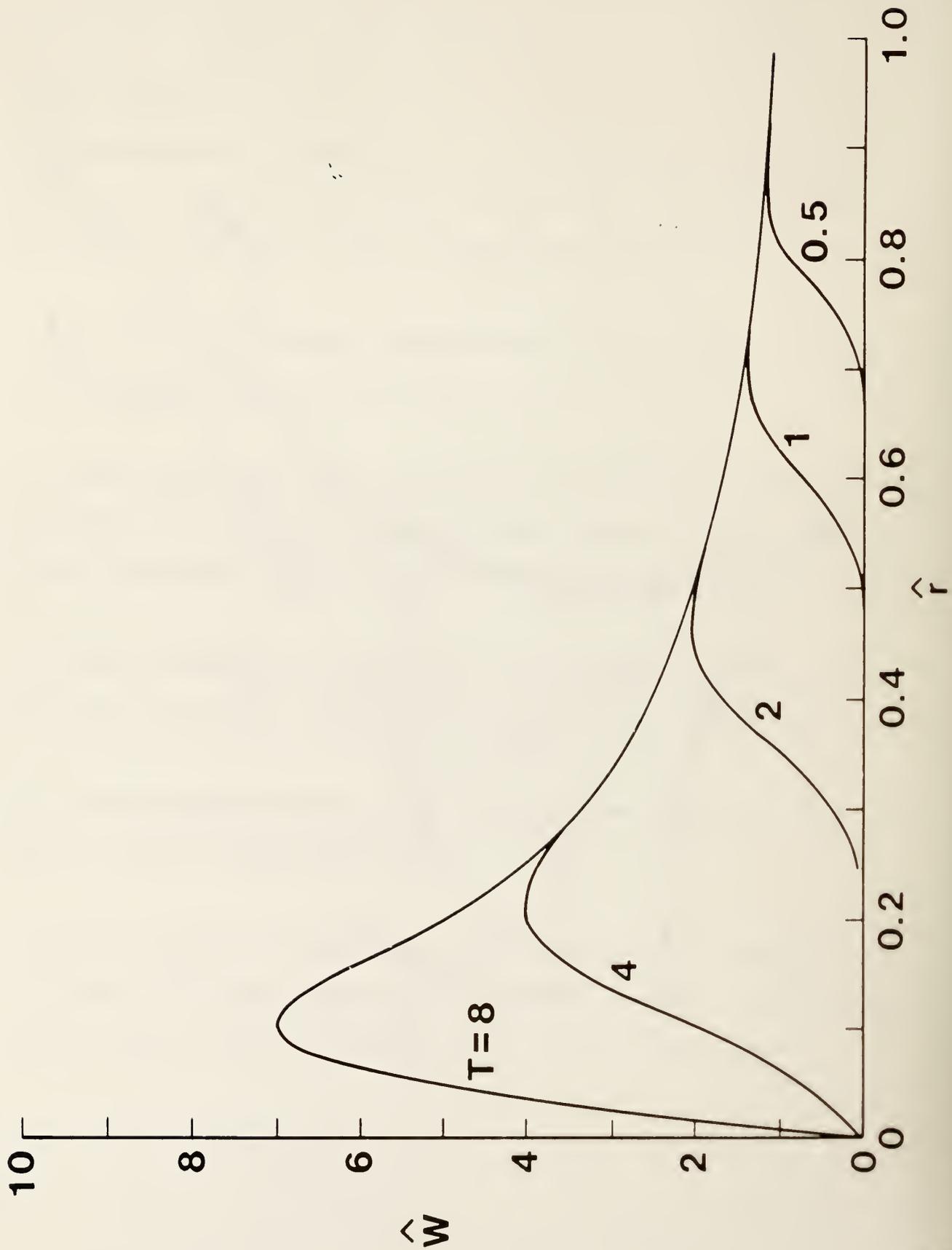
19

Figure

ε=.002 $\hat{\Omega}$= 2. TIME=0.5

ε=.002 $\hat{\Omega}$= 2. TIME=1.5

ε=.002 $\hat{\Omega}$= 2. TIME=2.0

ε=.002 $\hat{\Omega}$= 2. TIME=3.0

21

Figure 3

ε=.002 $\hat{\Omega}$= 2. TIME=0.10

ε=.002 $\hat{\Omega}$= 2. TIME=0.5

ε=.002 $\hat{\Omega}$= 2. TIME=1.0

ε=.002 $\hat{\Omega}$= 2. TIME=1.5

22

Figure

Figure 5

23

$\rho\cos\phi$

$\rho\sin\phi$

Fuel

$\dfrac{\partial\psi}{\partial\rho} \sim O(1)$

$\dfrac{\partial\psi}{\partial\rho} >> 1$

$\dfrac{\partial\psi}{\partial\rho} = 0$
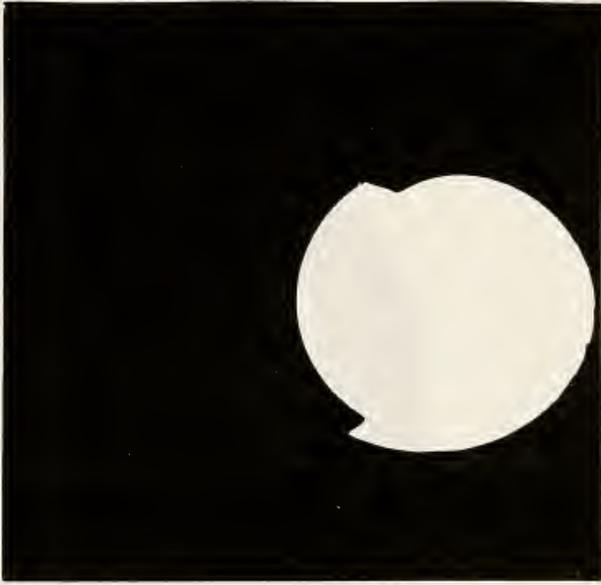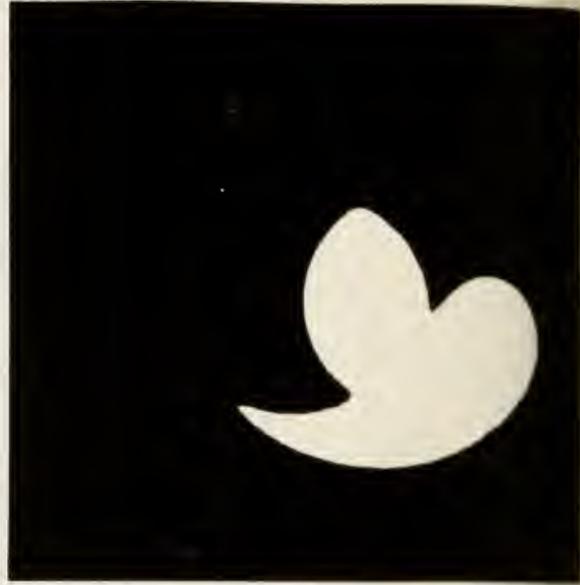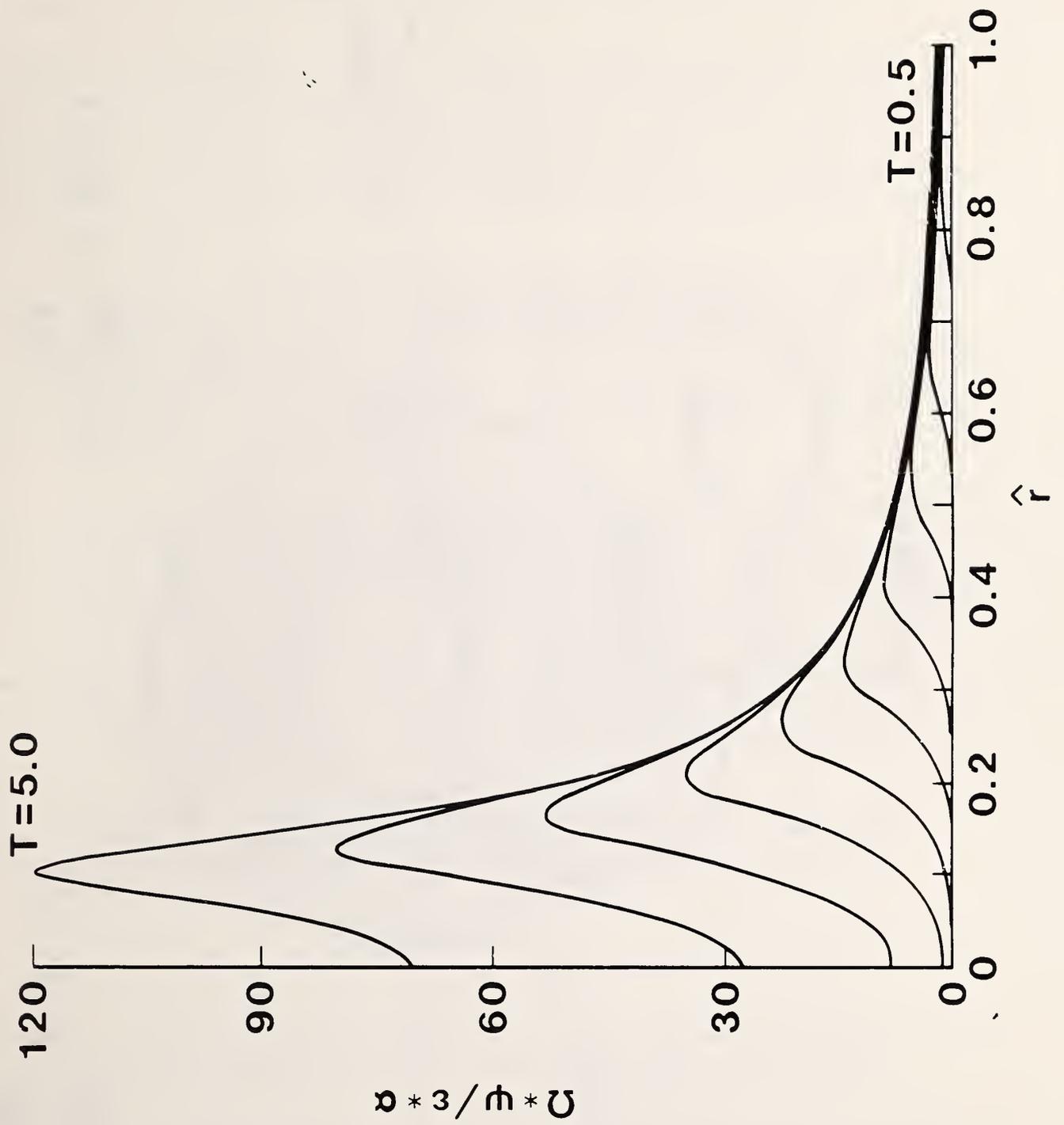
Figure
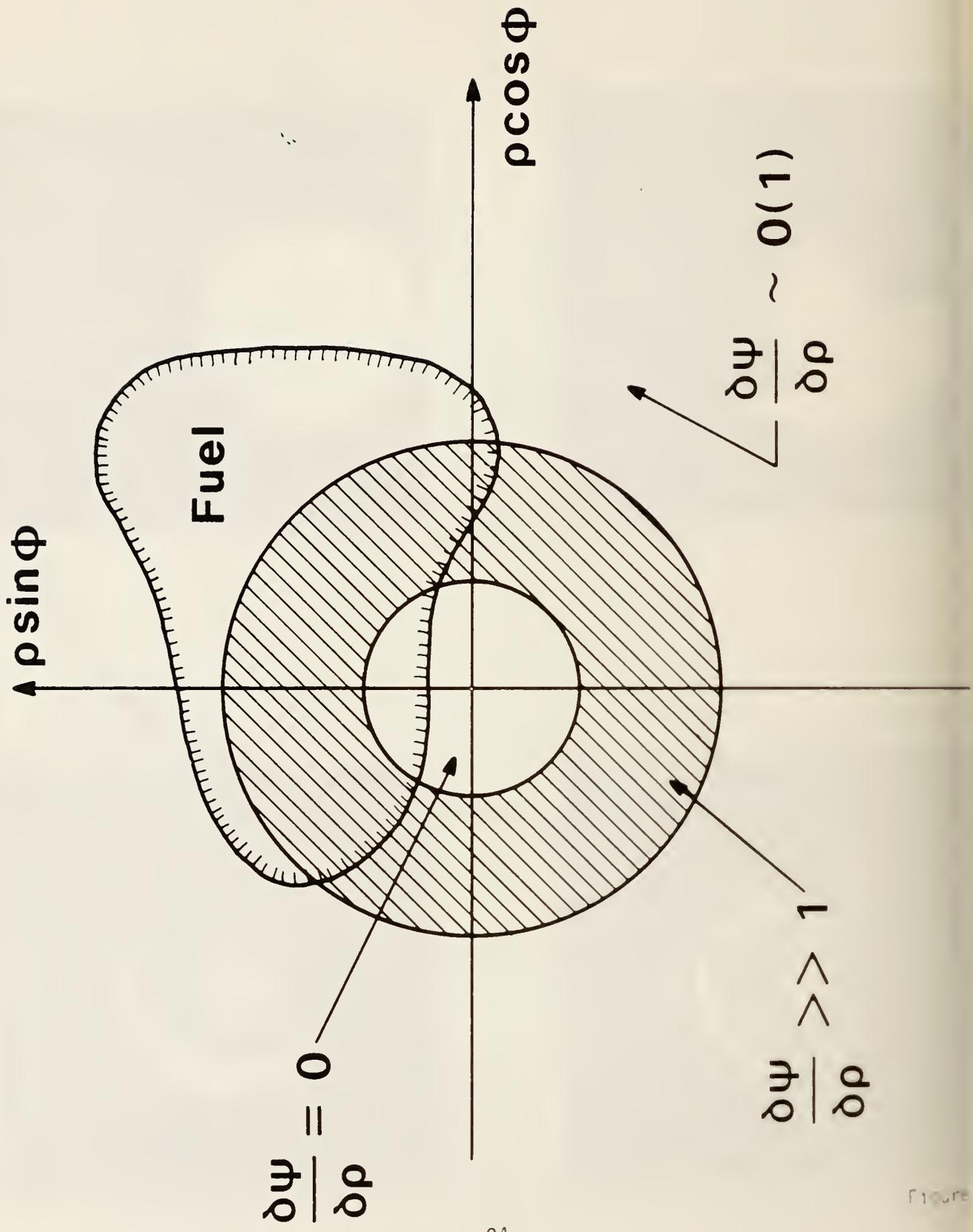
A SOLUTION FOR A TWO-DIMENSIONAL DIFFUSION FLAME IN A VORTEX FIELD

The theoretical study of chemical reactions in complex flow fields, for example turbulent reacting flows, has received increased attention recently. This attention is warranted because both numerical and analytical progress is being made in addressing the problem; discussion of some of this progress is presented in Reference 1. Also presented in Reference 1 is an outline of a rather general approach, using both analytical and numerical methods, for attacking turbulent reacting flows and an analysis of a model of small-scale mixing and reaction.

In Reference 2, a similar but more specialized model problem of small-scale mixing and reaction has been posed and analyzed locally along the flame front to provide dependencies of the solution upon dimensionless parameters. This problem has several important features; it is a diffusion-controlled reaction in a viscously spreading vorticity field which stretches the flame sheet. The problem, named the Marble problem here, allows rather detailed treatment, as seen in Reference 2 which has slight variations in detail and notation from the present write-up.

The novel features of this work compared with the analysis in Reference 2 are (i) it is observed that the convection-diffusion equation for the Shvab-Zeldovich variable permits a similarity solution, reducing the number of independent variables from three (radius, angle and time) to two (angle and similarity variable); (ii) as in Reference 1, a Lagrangian coordinate system is used to eliminate flame-sheet resolution problems induced by vortex winding; (iii) Fourier analysis in angle and a numerical treatment in the similarity variable allow one to solve the global problem. The analysis outlined below has not yet been completed. The solution to this problem should provide a special case on which to test methods for solution to the more general problems described in Referernce 1.

Initially we have fuel in the left half-plane and oxidizer in the right half-plane in arbitrary proportions (see Figure 1). At t=0, the two half spaces are brought into contact and simultaneously the line vortex with tangential velocity v_θ is imposed:

$$v_\theta \ (r,t) = r \ \frac{d\theta}{dt} = + \ \frac{\Gamma}{2\pi r} \ [1-\exp(-n)] \tag{1}$$

where Γ is the circulation of the vortex, ν is the kinematic viscosity and $n = r^2/4\nu t$. (The function $v_\theta(r,t)$ is a solution of the Navier-Stokes equations).

If the mass fraction of fuel in the left half-space initially is $Y_{f,o}$ while the mass fraction of oxidizer in the right half-space initially is $Y_{o,o}$, and if the single-step reaction occurs

$$\nu_f[Y_f] + \nu_o[Y_o] \rightarrow \nu_p[Y_p] \ ,$$
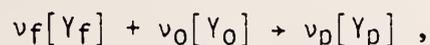
then with M_f, M_o = the molecular weight of fuel and oxidizer respectively,

$$Z \equiv \left\{ \frac{Y_f}{\nu_f M_f} - \frac{Y_o}{\nu_o M_o} + \frac{Y_{o,o}}{\nu_o M_o} \right\} / \left\{ \frac{Y_{f,o}}{\nu_f M_f} + \frac{Y_{o,o}}{\nu_o M_o} \right\} \qquad (2)$$

is the Zhvab-Zeldovich variable for which

$$Z = 1 \qquad \text{for } x < 0$$

$$Z = 0 \qquad \text{for } x > 0 \qquad @ \ t = 0 \qquad (3)$$

since

$$Y_f = Y_{f,o} \ , \qquad Y_o = 0 \qquad \text{for } x < 0$$

$$Y_f = 0 \qquad , \qquad Y_o = Y_{o,o} \qquad \text{for } x > 0 \qquad @ \ t = 0.$$

Z satisfies the convection-diffusion equation:

$$\frac{\partial Z}{\partial t} + \nabla \cdot (\vec{u} Z) = D \nabla^2 Z \qquad (4)$$

or in cylindrical coordinates

$$\frac{\partial Z}{\partial t} + \frac{v_\theta(r,t)}{r} \frac{\partial Z}{\partial \theta} = D \left\{ \frac{\partial^2 Z}{\partial r^2} + \frac{1}{r} \frac{\partial Z}{\partial r} + \frac{1}{r^2} \frac{\partial^2 Z}{\partial \theta^2} \right\} \qquad (5)$$

For the flame sheet approximation, Y_f and Y_o cannot coexist, so that

$$Z_f = \frac{Y_{o,o}}{\nu_o M_o} / \left\{ \frac{Y_{o,o}}{\nu_o M_o} + \frac{Y_{f,o}}{\nu_f M_f} \right\} \qquad (5)$$

determines the flame surface.

Integrating the tangential-velocity equation gives the angle $\theta(r,t,\theta_o)$ at t for any fluid element initially located at r,θ_o:

$$\theta(r,t) - \theta_0 = \frac{\Gamma}{2\pi r^2}\left\{t - \int_0^t \exp(-r^2/4\nu t')dt'\right\}$$

or

$$\theta(r,t) - \theta_0 = \frac{\Gamma}{2\pi\cdot 4\nu}\,\frac{1}{\eta}\,[1 - E_2(\eta)] \tag{7}$$

where

$$E_2(z) = \int_1^\infty \frac{dt}{t^2}\,\exp(-zt)$$

and

$$\eta = r^2/4\nu t$$

Change independent variables, to Lagrangian coordinates,

$$r = \rho$$
$$\theta = \theta_0 + \frac{\Gamma}{2\pi\cdot 4\nu}\,\frac{1}{\eta}\,[1-E_2(\eta)] \tag{8}$$
$$t = \tau$$

Then Eq. (5) becomes, in Lagrangian coordinates,

$$\frac{\partial Z}{\partial\tau} = D\left\{\frac{\partial^2 Z}{\partial\rho^2} + \frac{1}{\rho}\frac{\partial Z}{\partial\rho} + \left\{\left[\frac{2\Gamma}{8\pi^2}\,\frac{1}{\eta} - (1-e^{-\eta})\right]^2 + 1\right\}\frac{1}{\rho^2}\frac{\partial^2 Z}{\partial\theta_0^2}\right.$$
$$\left. + \frac{2\Gamma}{8\pi\nu}\,\frac{2}{\rho^2}\,[e^{-\eta}-(1-e^{-\eta})/\eta]\,\frac{\partial Z}{\partial\theta_0} + \frac{4\Gamma}{8\pi\nu}\,\frac{1}{\rho}\,\frac{1}{\eta}\,(1-e^{-\eta})\,\frac{\partial^2 Z}{\partial\rho\partial\theta_0}\right\} \tag{9}$$

This equation admits a similarity solution (which, in fact, exactly solves the Marble problem since neither the velocity field generated by the line vortex, nor the diffusion field produced by the two adjacent half-spaces of fuel and oxidizer have a length scale associated with them.)

Let $\eta = \rho^2/4\nu\tau$ as above, and assume $Z(\rho,\tau,\theta_0) = Z(\eta,\theta_0)$.

Then Eq. (9) becomes

$$\frac{\partial^2 Z}{\partial\eta^2} + (Sc + 1/\eta)\frac{\partial Z}{\partial\eta} + \left\{\left[\frac{2\Gamma}{8\pi\nu}\frac{1}{\eta}(1 - e^{-\eta})\right]^2 + 1\right\}\frac{1}{4\eta^2}\frac{\partial^2 Z}{\partial\theta_0^2}$$

$$+ \frac{\Gamma}{8\pi\nu}\frac{1}{\eta^2}\left[e^{-\eta} - \frac{1}{\eta}(1 - e^{-\eta})\right]\frac{\partial Z}{\partial\theta_0} + \frac{2\Gamma}{8\pi\nu}\frac{1}{\eta^2}(1 - e^{-\eta})\frac{\partial^2 Z}{\partial\eta\partial\theta_0} = 0 \qquad (10)$$

where $Sc \equiv \nu/D$ is the Schmidt number.

Fourier decomposition of Eq. (10) yields

$$\frac{d^2 Z_n}{d\eta^2} + \left[(Sc + 1/\eta) + in\frac{2\Gamma}{8\pi\nu}\frac{1}{\eta^2}(1 - e^{-\eta})\right]\frac{dZ_n}{d\eta}$$

$$+ \left\{-\left\{\left[\frac{2\Gamma}{8\pi\nu}\frac{1}{\eta}(1 - e^{-\eta})\right]^2 + 1\right\}\frac{n^2}{4\eta^2} + i\,n\frac{\Gamma}{8\pi\nu}\frac{1}{\eta^2}\left[e^{-\eta} - \frac{1}{\eta}(1 - e^{-\eta})\right]\right\}Z_n = 0$$

$$(11)$$

The fact that a similarity solution exists has reduced the number of independent variables upon which the solution depends by one. When Fourier analyzed, the mathematical problem is reduced from a one-dimensional, time-dependent partial differential equation, an initial-value problem, to an ordinary differential equation in the similarity variable, a two-point boundary-value problem. For each $Z_n(\eta)$ we have a linear ordinary differential equation for which boundary conditions are needed as $\eta\to\infty$ and as $\eta\to 0$. For fixed ρ, as $t\to 0$, $\eta=\rho^2/4\nu t\to\infty$ and $Z_n(\eta)$ must satisfy initial conditions for the Marble problem:

$$Z(\eta,\theta_0) = \sum_{n=-\infty}^{\infty} Z_n(\eta)\,\exp(in\theta_0) \qquad (12)$$

As $\eta\to\infty$ $Z(\eta\to\infty,\theta_0) = H(\theta_0-\pi/2) - H(\theta_0-3\pi/2)$

$$\text{for } 0 < \theta_0 < 2\pi$$

$$= \sum_{n=-\infty}^{\infty} A_n\exp(in\theta_0) \qquad (13)$$

Hence
$$A_0 = 1/2$$

$$A_{2j} = 0$$

$$A_{2j-1} = \frac{(-1)^j}{\pi(2j-1)} \qquad\qquad j = 1,2,3,4,\ldots$$

$$A_{-2j} = 0$$

$$A_{-(2j-1)} = \frac{(-1)^j}{\pi(2j-1)} \tag{14}$$

As $n\to0$, $Z_n(n)$ must remain finite. Examination of the indicial equation for $Z_n(n)$ as $n\to0$ shows that the two solutions behave as n^μ where $\mu = -in\Gamma/8\pi\nu \pm n/2$. Hence a change of independent variable to

$$Y_n(n) = \frac{n^{m/2}}{1+n^{m/2}} Z_n(n) \tag{15}$$

where $m = |n|$,

and requiring $Y_n(n)\to0$ as $n\to0$ implies that $Z_n(n)$ remains finite at $n=0$.
The equation for $Y_n(n)$ is

$$\frac{d^2Y_n}{dn^2} + \left[(Sc + 1/n) - \frac{m}{n(1+n^{m/2})} + i\,\frac{n\Gamma}{4\pi\nu}\,\frac{1}{n^2}(1-e^{-n}) \right]\frac{dY_n}{dn}$$

$$+ \left\{ \frac{m/2(m/2+1)}{n^2(1+n^{m/2})} - \frac{m/2(Sc+1/n)}{n(1+n^{m/2})} - \left\{ \left[\frac{\Gamma}{4\pi\nu}\,\frac{1}{n}(1-e^{-n})\right]^2 + 1 \right\}\frac{n^2}{4n^2} \right.$$

$$\left. + i\,n\,\frac{\Gamma}{8\pi\nu}\,\frac{1}{n^2}\left\{ \left[e^{-n} - \frac{1}{n}(1-e^{-n})\right] - \frac{m}{1+n^{m/2}}\,\frac{1}{n}(1-e^{-n}) \right\} \right\} Y_n = 0$$

$$\tag{16}$$

It is convenient to map the interval $0 < \eta < \infty$ into $0 < x < 1$ using the transformation

$$x = 1 - e^{-\eta} \qquad (17)$$

Then the equation for $Y_n(x)$ can be solved using boundary conditions that $Y_n(x)$ = 0 at x = 0 and $Y_n(x) = A_n$ at x = 1. Equation (16) can be discretized straightforwardly using a second-order, central difference scheme, and the resulting linear algebraic equations can be solved using a tridiagonal solver. The Fourier synthesis to obtain the complete solution can be performed using an FFT package. Location of the flame sheet and of the rate of fuel consumption must then be computed from the complete solution. Work is in progress on these tasks.

Plots of the interface, $\theta = 0$ and $\theta = \pi$, when the diffusion D = 0 for four values of the Reynold's number $\Gamma/8\pi\nu$ are shown in Figures 2-5. When the diffusion is zero, the solution depends only on this single parameter. It is important to note that this sequence of plots does not represent a time sequence; rather each plot shows the interface for that Reynold's number, the similarity variable η as a function of the angle θ. This interface is calculated from Eq. (7).

REFERENCES

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2. Marble, F.E., "Growth of a Diffusion Flame in the Field of a Vortex", Recent Advances in Aerospace Sciences (C. Casci, Ed.), p. 395, Plenum, 1985.
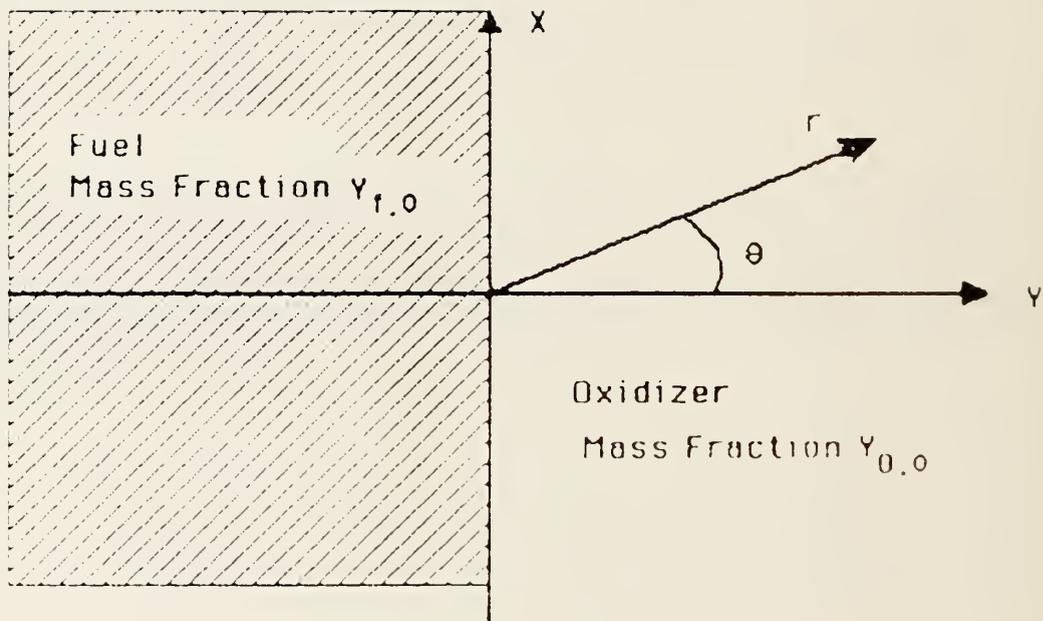
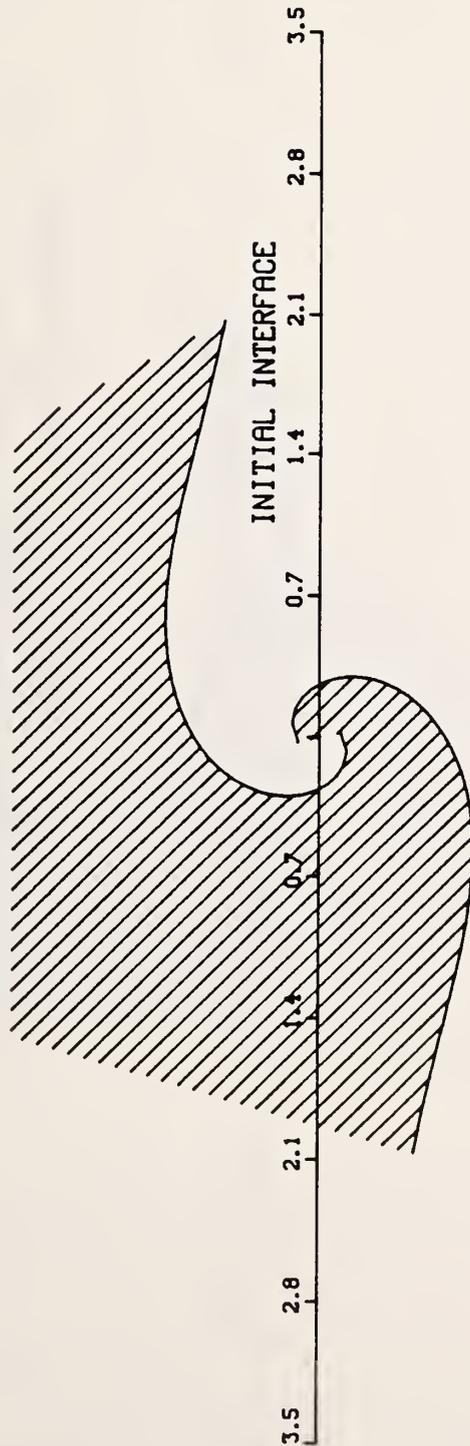Figure 1

INTERFACE SHAPE-MARBLE PROBLEM

GAM/(8*PI*NU)-1.0

INITIAL INTERFACE

Figure 2

INTERFACE SHAPE-MARBLE PROBLEM

GAM/(8×PI×NU)-2.0
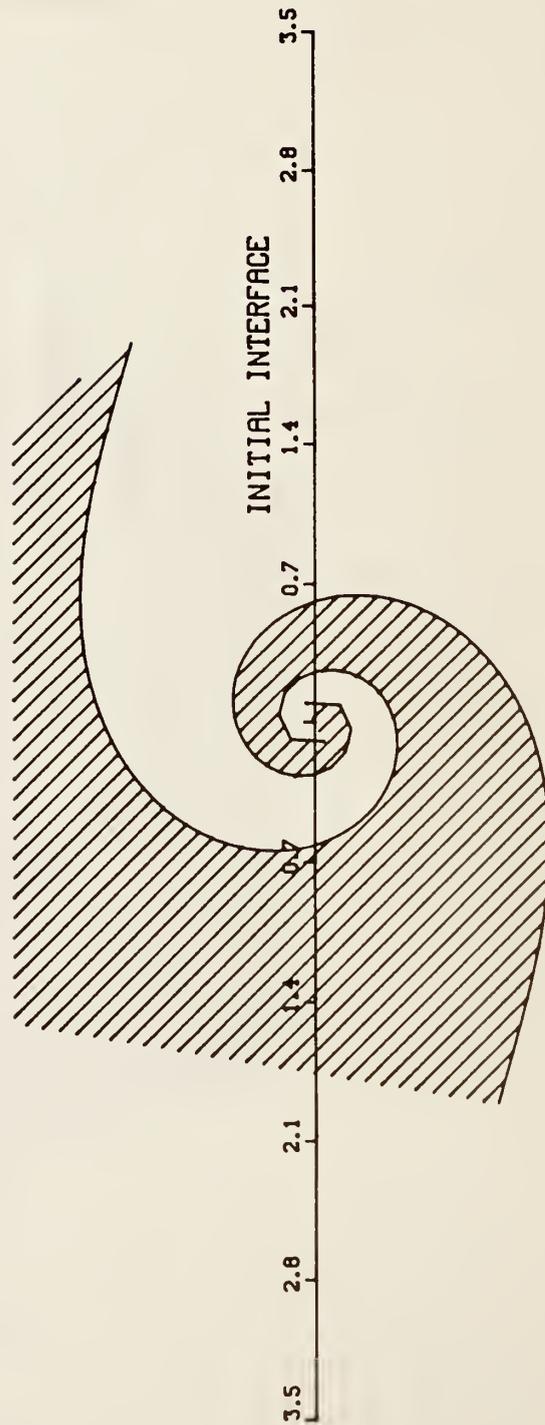
Figure 3

INTERFACE SHAPE-MARBLE PROBLEM

GAM/(8*PI*NU)-3.0

INITIAL INTERFACE
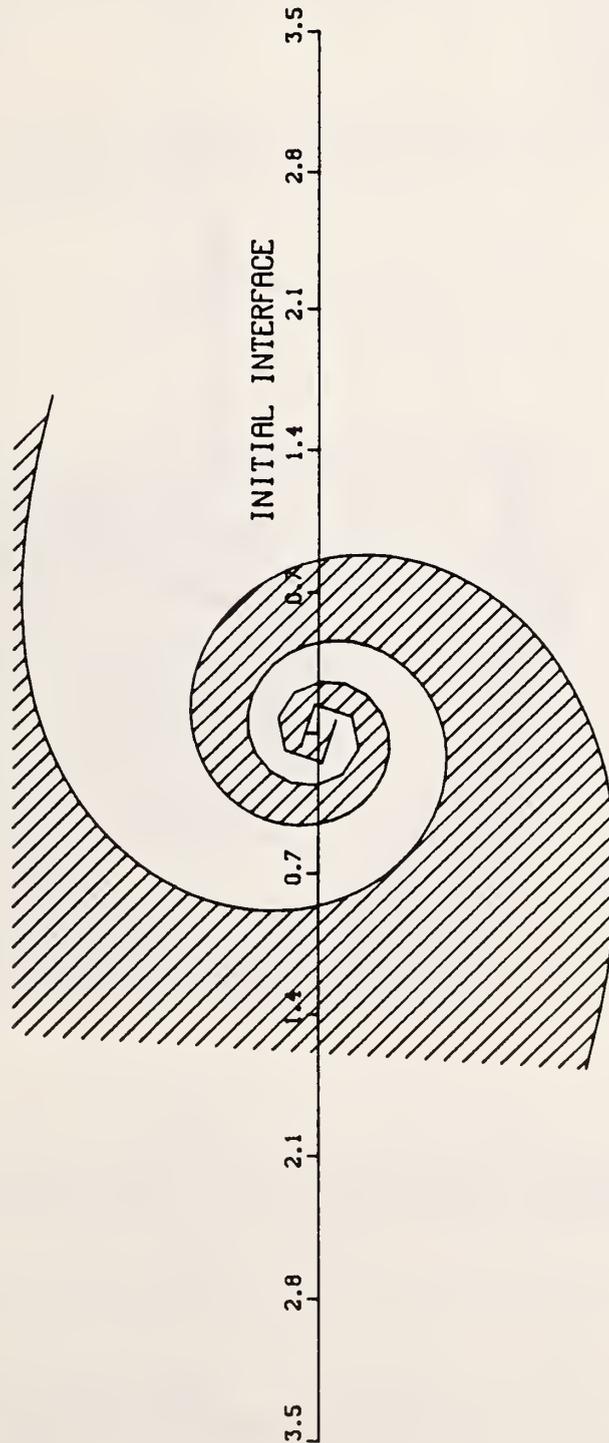
Figure 4

INTERFACE SHAPE-MARBLE PROBLEM

GAM/(8×PI×NU)-4.0

Figure 5

4. TITLE AND SUBTITLE

Time-Dependent Simulation of Small-Scale Turbulent Mixing and Reaction

5. AUTHOR(S)

H. R. Baum, R. G. Rehm, D. M. Corley, and D. W. Lozier

11. ABSTRACT (A 200-word or less factual summary of most significant information. If document includes a significant bibliography or literature survey, mention it here)

A mathematical model of the local transient diffusion-controlled reaction between initially unmixed species is presented. It is intended ultimately as a computational "molecule" to be imbedded in direct simulations of larger scale reacting flows. The model consists of an interacting three-dimensional strain vortex field which exactly satisfies the Navier-Stokes equation, an analytically determined Lagrangian representation of the mixing process and convection-diffusion equations for the reacting species in Lagrangian coordinates. The length scale established by the stretching of the vorticity field is shown to be directly relatable to the Kolmogoroff scale if the local strain rate has a scale consistent with laminar boundary layer mixing. An analytical solution to the convection-diffusion equation governing the diffusion-controlled reaction is derived. The solution is valid for large Schmidt number and describes the evolution of any initially two-dimensional configuration of reactants. A special two-dimensional case of this model, in which vortex strain is excluded and fuel and oxidizer initially occupy adjacent half-spaces, is also analyzed. This problem was originally formulated by F. Marble, who treated it in a very different manner from that described here.

12. KEY WORDS (Six to twelve entries; alphabetical order; capitalize only proper names; and separate key words by semicolons)
combustion; convection; diffusion-controlled; flame-sheet; reaction; turbulent mixing.