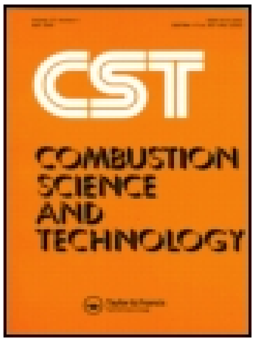

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ANDFREW MAJDA & JAMES SETHIAN

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The Derivation and Numerical Solution of the Equations for Zero Mach Number Combustion

ANDREW MAJDA *University of California at Berkeley*

JAMES SETHIAN *University of California at Berkeley and Lawrence Berkeley Laboratory, Berkeley, CA, 94720*

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Abstract—We present a limiting system of equations to describe combustion processes at low Mach number in either confined or unbounded regions and numerically solve these equations for the case of a flame propagating in a closed vessel. This system allows for large heat release, substantial temperature and density variations, and substantial interaction with the hydrodynamic flow field, including the effects of turbulence. This limiting system is much simpler than the complete system of equations of compressible reacting gas flow since the detailed effects of acoustic waves have been removed. Using a combination of random vortex techniques and flame propagation algorithms specially designed for turbulent combustion, we describe a numerical method to solve these zero Mach number equations. We use this method to analyze the competing effects of viscosity, exothermicity, boundary conditions and pressure on the rate of combustion for a flame propagating in a swirling flow inside a square.

INTRODUCTION

In this paper, we present a limiting system of equations to describe combustion processes at low Mach number in either confined or unbounded regions, and numerically solve these equations for the case of a flame propagating in a closed vessel. This limiting system allows for large heat release, substantial temperature and density variation, and substantial interaction with the hydrodynamic flow field, including the effects of turbulence. Since the detailed effects of acoustic waves have been removed, this zero Mach number limiting system is significantly simpler than the complete system of equations of compressible combustion. Under additional assumptions guaranteeing infinitely thin flame front structure, this system of combustion equations in multi-dimensions has a formal asymptotic limit which reduces to the system introduced through qualitative considerations recently (Ghoniem *et al.*, 1981) for combustion in open channels. That system was solved numerically through a combination of random vortex element techniques and flame propagation algorithms specifically designed for problems in turbulent combustion (Ghoniem *et al.*, 1981; Sethian, 1984). In this paper, the equations presented, which apply to turbulent combustion in both open and closed vessels, are solved numerically by means of an extension of the above techniques. The new algorithm, which requires only an additional fractional step involving a scalar nonlinear ordinary differential equation for the mean pressure, is used to analyze the competing effects of viscosity, exothermicity, boundary conditions and pressure on the rate of combustion for a flame propagating in a swirling flow inside a square.

A set of equations to describe large temperature and density variations in an inviscid fluid with a spatially almost constant pressure term have been developed by Rehm and Baum (1978). In that work, an equation for the mean pressure, which is solely a function of time, was presented, and the effect of a closed domain on the pressure was discussed. The driving mechanism in their set of equations was an energy source which corresponded to a localized addition of heat; the equations presented were used to simplify problems in thermally driven buoyant flow of interest in fire research. Work in combustion modelling, on the other hand, has long concentrated on obtaining simplified models of the combustion process; for example, Sivashinsky (1979) has obtained infinitely thin flame structure models from more complicated models by formally allowing the flame thickness to tend to zero. To our knowledge, the incorporation of these sets of ideas into a rigorous development of a model for zero Mach number combustion has not been previously carried out. Such a model can be regarded as existing between the full compressible Navier–Stokes equations plus combustion and constant density models where the fluid mechanics essentially decouples from the combustion process (van Harten and Matkowsky, 1982; Matkowsky and Sivashinsky, 1979). The point of this paper is to present such a model in a compact form and perform numerical experiments based on this model to analyze the various components. Our equations and numerical investigations are by no means complete; we ignore such aspects of combustion as diffusion flames, thermal boundary layers and flame speed dependence on curvature. Our hope is that this derivation and numerical investigation will provide a next step in understanding turbulent combustion.

This paper is divided into three sections. In Section One, we derive the equations of zero Mach number combustion in both bounded and unbounded regions for both inviscid and viscous flow under the simplest ideal assumptions for the chemical reaction. In Section Two, we take formal limits to derive infinitely thin flame structure models. In Section Three, we briefly describe the numerical method used in Sethian (1984) for solving the equations for open channel combustion using random vortex element techniques and flame propagation algorithms, and describe the modification and extension of this algorithm to confined volume calculations using the equations of zero Mach number combustion presented here. This numerical method is used to analyze the effects of viscosity, exothermicity, pressure and boundary conditions on a flame propagating in a swirling fluid inside a closed square. The results detail the interaction of turbulent eddies with the flame, corner effects, and the persistence of pockets of unburnt fuel within a turbulent combustion regime. The zero Mach number equations for a general chemically reacting fluid and additional aspects of the model described in Sections One and Two may be found in an earlier report (Majda, 1982).

SECTION ONE DERIVATION OF THE ZERO MACH NUMBER COMBUSTION EQUATIONS

We begin with the derivation of the equations of zero Mach number combustion under the simplest ideal assumptions for the chemical reaction. We concentrate on the case of a bounded region $\bar{\Omega}$ and assume a premixed fuel. We assume that there are only two species present, unburnt and burnt gas, and we let Z denote the mass fraction of unburnt gas. With $\gamma = C_p/C_v$, the ratio of specific heats, we assume that both the unburnt and burnt gases are governed by the same γ-gas law and have the same molecular weights. We also assume that unburnt gas is converted to burnt gas by a one-step irreversible Arrhenius kinetics mechanism. With these simplifications and with suitable nondimensionalization to be explained below, the equations describing compressible combustion are the system

Pressure Equation

$$\frac{Dp}{Dt} + \gamma p \operatorname{div} v = \Pr \varepsilon\gamma(\gamma-1)M^2 \left[\sum_{i,j}\left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i}\right)^2 - \frac{2}{3}\left(\operatorname{div} v\right)^2\right] \quad (1.1)$$

$$+ \frac{\gamma q_0 K\rho Z}{\varepsilon} e^{-A/T} + \gamma\varepsilon\Delta T.$$

Momentum Equations

$$\rho\frac{Dv_i}{Dt} + (\gamma M^2)^{-1}\frac{\partial p}{\partial x_i} = \varepsilon \Pr \sum_j \frac{\partial}{\partial x_i}\left(\frac{\partial v_j}{\partial x_i} + \frac{\partial v_i}{\partial x_j} - \frac{2}{3}\delta_{ij}\operatorname{div} v\right) \quad (1.2)$$

for $i=1, 2, 3$.

Temperature Equation

$$\rho\frac{DT}{Dt} = \frac{\gamma-1}{\gamma}\frac{Dp}{Dt} + \Pr \varepsilon(\gamma-1)M^2\left[\sum_{i,j}\left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i}\right)^2 - \frac{2}{3}\left(\operatorname{div} v\right)^2\right]$$

$$+ \frac{q_0}{\varepsilon} K\rho Z e^{-A/T} + \varepsilon\Delta T. \quad (1.3)$$

Species Equation

$$\rho\frac{DZ}{Dt} = -\frac{1}{\varepsilon} K\rho Z e^{-A/T} + (\mathrm{Le})^{-1}\varepsilon \operatorname{div}(\rho\nabla Z), \quad (1.4)$$

together with the ideal gas equation of state,

$$p = \rho T. \quad (1.5)$$

Here p is the pressure, ρ is the density, T is the temperature, v_i is the ith component of the fluid velocity, and $D/Dt=\partial/\partial t + v\cdot\nabla$. The other parameters in the equations are defined via the following:

Nondimensionalization

1) The pressure p is expressed in the units of the essentially constant initial pressure P_0.

2) The temperature T is expressed in units of the largest adiabatic flame temperature for the burnt gas T_b consistent with the initial data, *i.e.*,

$$c_p T_b = \max_{x \in \bar{\Omega}}[c_p T_0(x) + \bar{q}_0 Z_0(x)],$$

where $\bar{q}_0 > 0$ is the difference in energy of formation of the burnt and unburnt gases. (With our simplifying assumptions, this does not depend on T.)

3) $q_0 = \bar{q}_0 / c_p T_b$ is the nondimensional heat release.

4) The density is given in units of ρ_b with $\rho_b = P_0/T_b$.

5) The unit length scale is a *characteristic linear dimension for the region* Ω, *denoted by diam* Ω.

6) The units for velocity are determined by $|v_b|$ where $|v_b|$ is the free-space burning velocity associated with T_b and $T_u = T_b - c_p^{-1}\bar{q}_0$.

7) The unit time scale is determined by (5) and (6), *i.e.*, *unit time is measured by diam* $\Omega/|v_b|$.

8) $\mathrm{Pr} = vc_p/k$ is the Prandtl number and $\mathrm{Le} = k/\rho_b c_p d$ is the Lewis number, where v is the viscosity, d is the species diffusion coefficient and k is the coefficient of heat conduction.

9) The parameter ε, the flame thickness factor is defined by $\varepsilon = l_T/diam\ \Omega$, where l_T is the length scale associated with the internal thermal structure of flames $l_T = k(\rho_b |v_b| c_p)^{-1}$.

10) The quantity K is the prefactor for the reaction rate:

$$K = K_0 \rho_b^{-1} c_p^{-1} |v_b|^{-2} k,$$

with K_0 the frequency factor and A the nondimensional activation energy in units of $T_b R_0$, with R_0 the universal gas constant.

11) The quantity M is the Mach number $M = |v_b|/(\gamma P_0/\rho_b)^{1/2}$.

Throughout this paper, we shall assume that the Mach number M is small, that the initial pressure P_0 is spatially uniform within terms of order M^2, and that the initial temperature, mass fraction and velocity are in *chemical-fluid balance* within terms of order M. This last assumption of chemical-fluid balance will be made clear through the course of the derivation. Furthermore, for simplicity of exposition, we have assumed that all diffusion coefficients and the frequency factor are constants, in addition, ε is typically a small parameter, but we shall not exploit this fact immediately.

Non-Viscous Reacting Gases

First, for pedagogical simplicity, we treat the fictitious case with $\mathrm{Pr}=0$ in (1.1)–(1.3)— in which viscous effects are ignored for the reacting gas. We assume adiabatic boundary conditions ($\partial T/\partial n = \partial Z/\partial n = 0$ on $\partial\Omega$) to avoid additional complications with thermal boundary layers, etc., and we impose the requirement that the normal component of the velocity be zero at solid walls, *i.e.* $v \cdot n = 0$ on $\partial\Omega$. We assume asymptotic expansions in terms of the Mach number, given by

$$\begin{aligned} p &= P_0(x, t) + MP_1 + \gamma M^2 P_2 + O(M^3) \\ v &= v_0(x, t) + Mv_1 + O(M^2) \\ T &= T_0(x, t) + MT_1 + O(M^2) \\ Z &= Z_0(x, t) + MZ_1 + O(M^2). \end{aligned} \tag{1.6}$$

We substitute (1.6) into (1.1)–(1.4) and equate powers of M.

The terms of order M^{-2} and M^{-1} in the momentum equation imply, respectively

$$\begin{aligned} \nabla P_0(x, t) &= 0, \\ \nabla P_1(x, t) &= 0. \end{aligned} \tag{1.7}$$

To study the zero order term in the momentum equation, we shall make use of the following fact: every vector field v has a unique decomposition $v = w + \nabla\psi$, where w is divergence-free ($\nabla \cdot w = 0$). We let $Qv = w$ and observe that $Q(\nabla\psi) = 0$. Applying Q to the zero order expansion in the momentum equation, we have that $Q(\nabla\psi) = 0$ and thus

$$Q\left(\frac{P_0}{T_0} \frac{Dv_0}{Dt}\right) = 0, \tag{1.8}$$

where $D/Dt = \partial/\partial t + (v_0 \cdot \nabla)$. From the equations in (1.7) and (1.8), we conclude that

$$P_0 \equiv P_0(t), \tag{1.9}$$

and there exists a scalar pressure p^∞ with

$$\frac{P_0}{T_0} \frac{Dv_0}{Dt} = -\nabla p^\infty. \tag{1.10}$$

The zero order equations for temperature and mass fraction from (1.3) and (1.4) are straightforward and are given by

$$\frac{P_0}{T_0} \frac{DT_0}{Dt} = \frac{\gamma - 1}{\gamma} \frac{dP_0}{dt} + \frac{q_0}{\varepsilon} K\rho_0 Z_0 e^{-A/T_0} + \varepsilon \Delta T_0, \tag{1.11}$$

$$\frac{P_0}{T_0} \frac{DZ_0}{Dt} = -\frac{K}{\varepsilon} \frac{P_0}{T_0} Z_0 e^{-A/T_0} + (\mathrm{Le})^{-1} \varepsilon \operatorname{div}\left(\frac{P_0}{T_0} \nabla Z_0\right). \tag{1.12}$$

Our use of the pressure equation (1.1) rather than the conservation of mass is a significant difference in our formulation when compared with the one used by Sivashinsky (1979), and is more in line with the derivation presented by Rehm and Bahm (1978). Conservation of mass is a consequence of the two separate equations to be derived below. Using (1.9) in (1.1), we compute that the order zero terms in the pressure equation are given by

$$\frac{dP_0}{dt} = -\gamma P_0 \operatorname{div} v_0 + \gamma \frac{q_0}{\varepsilon} K\rho_0 Z_0 e^{-A/T_0} + \gamma\varepsilon\Delta T_0. \tag{1.13}$$

The self-consistency of the perturbation expansion in (1.6) requires that the order zero equation in (1.13) is satisfied. The left-hand side of (1.13) is a scalar function of time alone, while the right-hand side of (1.13) involves functions of both space and time. Therefore, there must exist a scalar function $\mathbf{H}(t)$ of time alone, so that simultaneously

$$\frac{dP_0}{dt} = \mathbf{H}(t), \tag{1.14}$$

$$\mathbf{H}(t) = -\gamma P_0 \operatorname{div} v_0 + \gamma \frac{q_0}{\varepsilon} K\rho_0 Z_0 e^{-A/T_0} + \gamma\varepsilon\Delta T_0. \tag{1.15}$$

How should $\mathbf{H}(t)$ be chosen? Since v_0 can be decomposed as $v_0 = w_0 + \nabla\phi_0$ as stated earlier, we may rewrite (1.15) as an equation for ϕ_0, namely

$$(\Delta\phi_0) = (\gamma P_0)^{-1}\left[-\mathbf{H}(t) + \frac{\gamma}{\varepsilon} q_0 K\rho Z_0 e^{-A/T_0} + \gamma\varepsilon\Delta T_0\right] \tag{1.16}$$

$$\left.\frac{\partial\phi_0}{\partial n}\right|_{\partial\Omega} = 0.$$

By the Neumann compatibility condition (Chorin and Marsden, 1979), this elliptic equation has a solution with $\nabla\phi_0$ uniquely determined if and only if the integral of the right-hand side of (1.16) over Ω vanishes; this uniquely determines $\mathbf{H}(t)$ by the equation

$$-\mathbf{H}(t) \int_\Omega dx + \frac{1}{\varepsilon} \int_\Omega \gamma q_0 K\rho_0 Z\rho_0 e^{-A/T_0} + \varepsilon \int_\Omega \gamma\Delta T_0 = 0,$$

i.e.

$$\mathbf{H}(t) = \frac{\frac{1}{\varepsilon}\int_\Omega \gamma q_0 K\rho_0 Z_0 e^{-A/T_0}}{\mathrm{Vol}(\Omega)}. \tag{1.17}$$

Here we have used our boundary condition to integrate to zero the contribution from heat conduction. This choice of $\mathbf{H}(t)$ allows us to satisfy (1.15) with a unique choice of $\nabla\phi_0$ and simultaneously to obtain an evolution equation for the mean pressure $P_0(t)$. With $\mathbf{H}(t)$ from (1.17), the equations from (1.10) to (1.12), (1.14) and (1.15) yield the:

Equations for Zero Mach Number Non-Viscous Combustion

Nonlinear O.D.E. for Mean Pressure

$$\frac{dP_0}{dt} = \frac{\dfrac{1}{\varepsilon}\displaystyle\int_\Omega \gamma q_0 K \rho_0 Z_0\, e^{-A/T_0}}{\mathrm{Vol}(\Omega)}. \tag{1.18a}$$

Elliptic Equation

$$\begin{aligned}(\Delta\phi_0) &= (\gamma P_0)^{-1}\left(-\frac{dP_0}{dt} + \frac{\gamma}{\varepsilon} q_0 K \rho Z_0\, e^{-A/T_0} + \gamma\varepsilon\Delta T_0\right),\\ \left.\frac{\partial\phi_0}{\partial n}\right|_{\partial\Omega} &= 0.\end{aligned} \tag{1.18b}$$

Nonhomogeneous Incompressible Fluid Equation

$$\begin{aligned}\rho(P_0, T_0)\frac{D}{Dt} w_0 &= -\rho(P_0, T_0)\frac{D}{Dt}\nabla\phi_0 - \nabla p^\infty,\\ \operatorname{div} w_0 = 0 \qquad & w_0\cdot n|_{\partial\Omega} = 0.\end{aligned} \tag{1.18c}$$

Reaction-Diffusion Equations

$$\begin{aligned}\rho(P_0, T_0)\frac{DT_0}{Dt} &= \frac{\gamma-1}{\gamma}\frac{dP_0}{dt} + \frac{q_0}{\varepsilon} K\rho Z_0\, e^{-A/T_0} + \varepsilon\Delta T_0,\\ \rho(P_0, T_0)\frac{DZ_0}{Dt} &= -\frac{K}{\varepsilon}\rho Z_0\, e^{-A/T_0} + (\mathrm{Le})^{-1}\varepsilon\,\operatorname{div}(\rho\nabla Z_0),\\ \frac{\partial T_0}{\partial n} = \frac{\partial Z_0}{\partial n} &= 0 \quad \text{on} \quad \partial\Omega.\end{aligned} \tag{1.18d}$$

where the formulae

$$\rho(P_0, T_0) = \frac{P_0}{T_0},$$

$$v_0 = w_0 + \nabla\phi_0 \qquad \operatorname{div} w_0 = 0 \qquad w_0\cdot n|_{\partial\Omega} = 0,$$

complete the description of this system. A rigorous proof that the above is a well-posed system will appear (Embid, 1984). Our assumption of initial chemical-fluid balance can now be seen as the requirement from (1.7) that $p(x,0)=1+O(M^2)$ and the fact that the elliptic equation (1.18b) must be satisfied at $t=0$; this, however, is a restraint imposed on the fluid dynamic potential $\nabla\phi_0$ at $t=0$ and not on w, $Z_0(x)$ or $T_0(x)$. It is important to point out that when the conditions of chemical-fluid balance are violated, even if the Mach number is small and initial pressure is spatially uniform, the effects of acoustic waves can be substantial; such systems can even exhibit transition to detonation.

Equations for Zero Mach Number Viscous Combustion

When $\mathrm{Pr}\neq 0$, the system of equations in (1.1)–(1.5) should satisfy the boundary conditions $v=0$ on $\partial\Omega$ (no-slip) and $\partial T/\partial n=\partial Z/\partial n=0$ on $\partial\Omega$. The no-slip condition boundary conditions together with the nonzero viscosity coefficient in the momentum equation changes the boundary conditions and the nature of the equation (1.18c). However, since the viscous stress contributions to the pressure and temperature equations are $O(M^2)$, the equations (1.18a)–(1.18c) are unchanged in the viscous case. By repeating the derivation given above, we compute that the equations for Zero Mach Number Viscous Combustion are given by

$$\begin{gathered}\text{Nonlinear O.D.E. (1.18a)},\\ \text{Elliptic Equation (1.18b)},\\ \text{Reaction-Diffusion Equations (1.18d)},\end{gathered}\tag{1.19a}$$

and the *Nonhomogeneous Incompressible Navier-Stokes Equation*

$$\rho(P_0,T_0)\frac{D}{Dt}\,\varepsilon\mathrm{Pr}\Delta w_0+\nabla\bar{p}^{\infty}=-\rho(P_0,T_0)\frac{D}{Dt}\nabla\phi_0,\tag{1.19b}$$

[actually, we have defined a reduced pressure $\bar{p}^{\infty}=p^{\infty}-4/3\,\varepsilon\mathrm{Pr}\Delta\phi_0$ to simplify the equations in (1.19b) even further] with the boundary conditions

$$\operatorname{div} w_0=0,\qquad w_0\cdot n|_{\partial\Omega}=0,\qquad w_0\times n|_{\partial\Omega}=-\nabla\phi_0\times n|_{\partial\Omega}.\tag{1.19c}$$

The linearized equations obtained from (1.19b) and (1.19c) are nonhomogeneous Stokes equations and yield a well-posed problem (see Teman, 1977)—in fact, a rigorous proof of the nonlinear well-posedness for the system in (1.19) will appear (Embid, 1984). We remark here that in this case the requirement of approximate chemical-fluid balance also imposes the condition $w_0\times n|_{\partial\Omega}=-\nabla\phi_0\times n|_{\partial\Omega}$ initially at time $t=0$.

The above derivation for both inviscid and viscous flow applies just as well to combustion in unbounded domains. In such a case, the normalizing length scale diam Ω is replaced by some typical large length scale. Since in unbounded domains the elliptic equation has a unique solution for any right hand-side that is square integrable, we may choose H(t) in (1.15) to be identically zero and thus the pressure remains constant independent of time and the elliptic equation for ϕ_0 reduces to

$$\Delta\phi_0 = (\gamma P)^{-1}\left[\gamma q_0 \frac{K}{\varepsilon}\rho Z_0 e^{-A/T_0} + (\gamma\varepsilon\Delta T_0)\right],$$
$$\frac{\partial\phi_0}{\partial n} = 0. \tag{1.20}$$

Finally, we remark that the equations presented preserve mass, *i.e.*, with $\rho = P_0(t)/T_0(x, t)$ and $v_0 = w_0 + \nabla\phi_0$, then $D\rho/Dt + \rho\, \mathrm{div} v_0 = 0$; this may be checked either by direct calculation or by noting that the given compressible system (1.1)–(1.5) conserves mass and that (1.18) and (1.19) are the limit of equations that conserve mass.

SECTION TWO ZERO MACH NUMBER EQUATIONS WITH INFINITELY THIN FLAME STRUCTURE

In this section we further simplify the equations of the last section to produce zero Mach number equations for infinitely thin flames. We make the following additional assumption:

The parameter ε which characterizes the ratio of the length of the internal flame structure to the typical external length scale (which in the case of a bounded domain is the diameter of the region) is an extremely small number and the activation energy A is large. (See Sivashinsky, 1979.)

These assumptions are satisfied for many typical combustion processes when the diam Ω is on the order of one meter. [We drop all subscript zeroes for the Eqs. (1.19) in this section].

Here we also study special initial data in chemical fluid balance with the form for mass-fraction and temperature given by

$$Z(x, 0) = \begin{Bmatrix} 1 & \phi_0(x) < 0 \\ 0 & \phi_0(x) > 0 \end{Bmatrix},$$
$$T(x, 0) = \begin{Bmatrix} T_u \equiv 1 - q_0 & \phi_0(x) < 0 \\ T_b \equiv 1 & \phi_0(x) > 0 \end{Bmatrix}. \tag{2.1}$$

This initial data including the fluid velocity has a jump discontinuity across the surface

$S_0=(x \in \Omega | \phi_0(x)=0)$ and is a stochiometric mixture composed of unburnt gas for those points $x \in \Omega$ with $\phi_0(x)<0$ and burnt gas for those points $x \in \Omega$ with $\phi_0(x)>0$. The reader can easily verify that all equations derived below remain valid with obvious modifications for general piecewise smooth initial data $[T(x), Z(x)]$ that jump across a surface S_0, provided that the nondimensional adiabatic equation expressing conservation enthalpy across S_0

$$T_b(x) = T_u(x) + q_0 Z(x) \qquad \text{for} \qquad x \in S_0 \tag{2.2}$$

is valid at all points of S_0.

As described in Sivashinsky (1979), and following the well-known ideas of Landau (1944), under the above assumption and with the special initial data for (1.19) given in (2.1), it follows that as $\varepsilon \to 0$, formally

$$\frac{1}{\varepsilon} KZ\, e^{-A/T_0} \to m(x, t)\delta_{S(t)}, \qquad x \in S(t), \tag{2.3}$$

where $S(t)$ is a surface described by $S(t)=[x|\phi(x, t)=0]$ with $\phi(x, o)=\phi_0(x)$ and $\delta_{S(t)}$ is the surface Dirac measure concentrated on $S(t)$ (see Gelfand and Shilov, 1964). Here the function $-m(x, t)$ is the mass flux across $S(t)$ and is determined by

$$\rho_b(v_b \cdot n - V) = \rho_u(v_u \cdot n - V) = -m(x, t) \;\; \text{for} \;\; x \in S(t), \;\; V = \phi_t/|\nabla\phi|, \tag{2.4}$$

where n is the outward spatial normal to $S(t)$. The equation in (2.4) expresses the conservation of mass across the surface $S(t)$ which is valid for solutions of (1.19) in the limit as $\varepsilon \to 0$. As $\varepsilon \to 0$ from (2.3), the reaction-diffusion equations in (1.19a) reduce to

$$\frac{dP}{dt} = \frac{\gamma q_0 \int_{S(t)} m(x, t)\, dA}{\mathrm{Vol}(\Omega)}, \tag{2.5a}$$

$$\rho \frac{DT}{Dt} = \frac{\gamma - 1}{\gamma} \frac{dP}{dt} \quad \text{for} \quad \phi(x, t) > 0 \quad \text{and} \quad \phi(x, t) < 0, \tag{2.5b}$$

$$\frac{DZ}{Dt} = 0 \quad \text{for} \quad \phi(x, t) > 0 \quad \text{and} \quad \phi(x, t) < 0, \tag{2.5c}$$

where (2.5b) and (2.5b) are supplemented by the jump conditions across $S(t)$ appropriate for data of the form in (2.1) given by

$$\begin{aligned} &T_b(x,t) - T_u(x,t) = q_0 \quad \text{for} \quad x \in S(t), \\ &Z_b(x,t) = 0, \quad Z_u(x,t) = 1 \quad \text{for} \quad x \in S(t), \end{aligned} \tag{2.6}$$

while the elliptic equation from (1.19a) becomes

$$\begin{aligned} &\Delta\phi = (\gamma P)^{-1}\left[-\frac{dP}{dt} + \gamma q_0 m \delta_{S(t)}\right], \\ &\left.\frac{\partial\phi}{\partial n}\right|_{\partial\Omega} = 0. \end{aligned} \tag{2.7}$$

The nonhomogeneous Navier–Stokes equations from (1.19b) become

$$\begin{aligned} &\rho\frac{Dv}{Dt} - (\varepsilon\mathrm{Pr})\Delta w - \nabla\bar{p}^{\infty} = 0 \quad \text{for} \quad \phi(x,t) > 0 \quad \text{and} \quad \phi(x,t) < 0 \\ &v|_{\partial\Omega} = 0 \end{aligned} \tag{2.8}$$

with $v = w + \nabla\phi$, $\operatorname{div} w = 0$, and $w \cdot n|_{\partial\Omega} = 0$. The equations in (2.8) are supplemented by the jump conditions from (3.4) across $S(t)$ and the density is given in the two regions by

$$\rho = \begin{Bmatrix} P(t)/T_u(x,t) \ \phi(x,t) < 0 \\ P(t)/T_b(x,t) \ \phi(x,t) > 0 \end{Bmatrix}. \tag{2.9}$$

[Alternatively, we could use the conservation form of the momentum equation in (2.8) across $\phi = 0$.] We have retained the viscosity term $(\varepsilon\mathrm{Pr})\Delta w$ in (2.8) for emphasis because the no-slip boundary conditions $v|_{\partial\Omega} = 0$ create boundary layers since $\varepsilon\mathrm{Pr} \neq 0$ even though this term can be neglected in the interior. Thus, the main consequence of the assumption made at the beginning of this section is that the flame is idealized as infinitely thin and represented by the surface $S(t)$. With the initial data in (2.1), it is very easy to solve the equations in (2.5c) to obtain

$$Z(x,t) = \begin{Bmatrix} 1 & \phi < 0 \\ 0 & \phi > 0 \end{Bmatrix}. \tag{2.10}$$

At this stage of the derivation, we have four equations for the four unknowns $P(t)$, v, however an equation for the unknown flame front $S(t)$ remains to be determined.

Following Carrier *et al.* (1980) and Kurylo *et al.* (1980), we get this equation by *postulating* that the mass flux $m(x, t)$ for $x \in S(t)$ is a prescribed function of the local quantities $T_u(x, t)$, P, *i.e.*,

$$m(x, t) = m(T_u, P) = m(\rho_u, P). \tag{2.11}$$

Landau postulated that $m(\rho_u, P)$ should be determined by the local laminar flame velocity (see Landau, 1944) and others (Carrier *et al.*, 1980; Kurylo *et al.*, 1980) have required that m might have a functional form determined empirically from experimental data—either turbulent or laminar. A typical form for m is the power law

$$m(\rho_u, P) = Q\rho_u{}^{1-\alpha}p^{\alpha}, \tag{2.12}$$

where α, $Q > 0$ are constant and $1 > \alpha \geq \frac{1}{2}$ (see Kurylo *et al.*, 1980), $\alpha = \frac{1}{2}$ corresponds to the laminar case. We will ignore variations in the flame speed due to curvature of the flame front; such effects will be studied in later work. Now, the equation in (2.11) and the conservation of mass from (3.4) determine an equation for the surface $S(t)$ described by $\phi(x, t) = 0$, given by

$$\rho_u(v_u \cdot n - \phi_t/|\nabla\phi|) = -m[\rho_u(t), P(t)],$$

or equivalently,

$$\begin{aligned} \phi_t + \frac{m[\rho_u(t), P(t)]}{\rho_u} + v_u \cdot \nabla\phi &= 0, \\ \phi(x, t) &= \phi_0(x). \end{aligned} \tag{2.13}$$

Thus, from (2.13) the points $\mathbf{r}(t)$ on $S(t)$ are described by the equation

$$\frac{d\mathbf{r}}{dt} = \frac{m[\rho_u(t), P(t)]}{\rho_u}\mathbf{n}(\mathbf{r}) = v_u(\mathbf{r}), \tag{2.14}$$

where $\mathbf{n}(\mathbf{r})$ is the outward normal to $S(t)$. With the assumption in (2.11), the equation in (3.5a) becomes

$$\frac{dP}{dt} = \frac{q_0\gamma m[\rho_u(t), P(t)]A(t)}{\mathrm{Vol}(\Omega)}, \tag{2.15}$$

with $A(t)$ the area of $S(t)$. Next, we indicate how to determine $\rho_u(t)$ from $P(t)$ [similar considerations apply to $\rho_b(t)$]. From the equations for $\phi(x, t) < 0$,

$$\rho_u T_u = P, \qquad \rho_u \frac{D}{Dt} T_u = \frac{\gamma-1}{\gamma} \frac{dP}{dt},$$

it follows that in the unburnt gas, generally

$$\frac{D}{Dt} \log(\rho_u{}^\gamma / P) = 0, \tag{2.16}$$

and therefore, for the special initial data in (2.9),

$$\rho_u(t) = P^{1/\gamma}(t)\rho_u(0) = P^{1/\gamma}(t)\rho_u{}^0. \tag{2.17}$$

In the burnt gas region, the temperature is generally nonuniform when Ω is a bounded domain. Once the above equations have been solved, $T_b(x, t)$ is determined in $\phi > 0$ by solving the linear boundary problem for the first order equation

$$\begin{aligned} &\frac{D}{Dt} T_b(x, t) = 0, \\ &T_b(x, t)|_{S(t)} = q_0 + \frac{P(t)}{\rho_u(t)} \\ &T_b(x, 0) = 1. \end{aligned} \tag{2.18}$$

It should be apparent to the reader that the more general initial data discussed above (2.2) are handled by straightforward modification.

SECTION THREE NUMERICAL SOLUTION OF THE EQUATIONS FOR ZERO MACH NUMBER COMBUSTION

In this section we describe a numerical method to solve our model for zero Mach number combustion. For initial data of the form in (2.1) and with the main additional *assumption* at the beginning of Section Two and postulate (2.11), we have derived the equations for zero Mach number combustion with infinitely thin flame structure described in (2.7), (2.8), (2.14) and (2.15) as a limiting case of the equation from (1.19). Here, we summarize these equations for *Zero Mach Number Combustion with infinitely thin flame structure* for the unknowns P, $S(t)$ and v.

a) Non-linear O.D.E. for the mean pressure

$$\frac{dP}{dt} = \frac{q_0 \gamma m[\rho_u(t), p(t)] A(t)}{\mathrm{Vol}\,(\Omega)}. \tag{3.1}$$

b) Eikonal equation for the flame front $S(t)$,

$$\frac{d\mathbf{r}}{dt} = v_u(\mathbf{r}) + \frac{m[\rho_u(t), P(t)]}{\rho_u}\mathbf{n}(\mathbf{r}). \tag{3.2}$$

c) Elliptic equation

$$\begin{aligned} \Delta\psi &= (\gamma P)^{-1}\left\{ -\frac{dP}{dt} + \frac{q_0\gamma m[\rho_u(t), P(t)]\delta_s}{\mathrm{Vol}(\Omega)} \right\} \\ \frac{\partial\psi}{\partial n} &= 0. \end{aligned} \tag{3.3}$$

d) Nonhomogeneous incompressible Navier–Stokes equation

$$\begin{gathered} \rho\frac{Dw}{Dt} - \varepsilon \Pr \Delta w - \nabla\bar{p}^{\infty} = -\rho\frac{D\nabla\psi}{Dt}, \\ \operatorname{div} w = 0, \\ w\cdot n|_{\partial\Omega} = 0 \quad w\times n|_{\partial\Omega} = -\nabla\psi\times n|_{\partial\Omega}, \end{gathered} \tag{3.4}$$

with the orthogonal decomposition $v=\nabla\psi+w$. Here, we again note that q_0 is the nondimensional heat release, $A(t)$ is the area of the flame front at time t, Vol (Ω) is the volume of the vessel under consideration, $\mathbf{r}(t)$ is a point on the flame front at time t, $v_u(\mathbf{r})$ is the velocity at the point $\mathbf{r}$ as taken as a limit from the unburnt side, $\mathbf{n}(\mathbf{r})$ is the normal to the front at $\mathbf{r}$, and δ_S is the surface Dirac measure concentrated on the flame front. In the special case when the domain is unbounded and is a channel of the form discussed by Ghoniem *et al.* (1981), the constant pressure approximation $dP/dt\equiv 0$ applies for the system in (1.19b) and therefore in our equations. In this situation, the equations (3.1)–(3.4) reduce to those introduced by Ghoniem, Chorin and Oppenheim (1981) and studied extensively by Sethian (1984). We now describe the numerical algorithm for approximating the system of equations (3.1)–(3.4).

Given that w is divergence-free and that $\nabla\phi$ is irrotational ($\nabla\times\nabla\phi=0$), we define ξ to be the vorticity ($\xi=\nabla\times w$) and take the curl of (3.4) to produce the vorticity transport equation

$$\frac{D\xi}{Dt} = \frac{1}{R}\nabla^2\xi, \tag{3.5}$$

where R is the Reynolds number. Here, the term $(\nabla\times\nabla P/\rho)$ which corresponds to vorticity production across the flame front has been ignored. We hope to address the more complex numerical issue of following sharp density discontinuities generated by the flame front in later work. The boundary conditions are that $w=0$ on $\partial\Omega$.

The form for the mass flux given in (2.12) is

$$m(\rho_u, P) = Q\rho_u{}^{1-\alpha}P^{\alpha}, \tag{3.6}$$

where again, Q is the local laminar flame velocity and α is a constant. Equation (3.17) provides, under the assumption of a γ-gas law, the unburnt fluid density as a function of the pressure through the relation

$$\rho_u(t) = (P(t))^{1/\gamma}\rho_u(0), \tag{3.7}$$

where $\rho_u(0)$ is the unburnt density initially. We shall now describe the technique for approximating the combustion model (3.1)–(3.3), (3.5)–(3.7).

The Numerical Algorithm

Typically, one might attempt to approximate the solution to the above equations through the application of finite difference schemes. Some of the problems inherent in these techniques are (1) the necessity of a fine grid in the boundary layer region near walls where sharp gradients exist; (2) the introduction of numerical diffusion, the error term associated with the approximation equation looks like a diffusion term; and (3) the intrinsic smoothing of finite difference schemes which damps out physical instabilities. The random vortex element, introduced in Chorin (1973), is specifically designed to deal with these problems. The equations of motion are written in vorticity form, and the motion of vorticity is followed by means of a collection of vorticity approximation elements. By avoiding the averaging and smoothing associated with finite difference formulations, this technique can follow the development of large-scale coherent, turbulent structures within the flow. In Sethian (1984), vortex methods and a flame propagation algorithm based on Huyghen's principle were applied to problems in turbulent combustion in open vessels. We briefly describe this algorithm below. For details, see Sethian (1984).

The vorticity ξ in (3.1) is approximated by a set of vortex "blobs", whose positions and strengths at any time yield the associated velocity field w. The distribution of vorticity is updated in two stages. First, the vortex elements are moved under the flow field w, corresponding to the advection of vorticity by the velocity field it induces. Second, viscous diffusion is simulated by a random walk imposed on the vortex motion. The normal boundary condition on w is met through the addition of a potential flow solution, and the tangential boundary "no-slip" condition is satisfied by a vorticity creation algorithm (vortex sheets).

To model the motion of the flame as given in (3.2), one is tempted to place marker particles along the boundary between the burnt and unburnt fluid and update their position and hence the location of the flame front in time. Because of the difficulty involved in determining the normal direction to the front (the direction in which the flame burns) from such an approximation, the flame front usually becomes unstable and develops wild oscillations (see Sethian, 1982). This problem is avoided by introducing a grid on the domain and assigning each cell a number (a "volume fraction", see Noh and Woodward, 1976) corresponding to the amount of burnt fluid in that cell at any given time. Each cell on the boundary of the burnt gas ignites all its

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neighbors at the prescribed rate k; this is an approximation based on Huyghen's principle, which states that the envelope of all disks centered on the front corresponds to the front displaced in a direction normal to itself (see Chorin, 1980). The motion of the flame is broken up into two stages: first, burning is modelled by allowing the flame to propagate in a direction normal to itself at the prescribed speed and second, the burned fluid is advected by the yet to be determined velocity field v. By updating these volume fractions according to the advection and burning processes, one may track the motion of the flame.

To determine the velocity field u, one must solve for the exothermic velocity field $\nabla\phi$ produced by volume expansion along the flame front. The position of the flame as determined by the Huyghen's principle construction described earlier determines the right-hand side of Eq. (3.3); a fast Poisson solver is used to solve the Neumann problem for ϕ. Straightforward finite differences on the fast solver grid provide $\nabla\phi$ and hence u. Although a finite difference formulation is used at this point, this does not conflict with our use of a grid-free vortex method to find the vorticity field, since the error associated with the grid computation of the irrotational component $\nabla\phi$ is not like a diffusion term. Again, the tangential boundary "no-slip" condition is satisfied by the creation of vortex sheets. The vortex elements are then advected under the field $\nabla\phi$, and the flame is advected by the velocity field $u=w+\nabla\phi$ to produce the new positions for the vortex blobs and flame.

In the extension of the above algorithm to combustion within a confined chamber, one must also consider the rise in pressure associated with exothermic effects [Eq, (3.1)] in computing $\nabla\phi$. To advance from one time step to the next, the position of the flame is used to calculate dP/dt using (3.1). As in the above description, a fast Poisson solver is again used to find ϕ. An additional fractional step is required to update the pressure in time; this is accomplished by numerically integrating the nonlinear ordinary differential equation (3.1). Finally, Eq. (3.7) is used to update the density of the unburnt gas used in the mass flux calculation in (3.6). We point out that the above description of vortex methods and the ensuing application applies to two-dimensional flow; the development of three-dimensional vortex methods is currently an area of active research. The flame front algorithm easily generalizes to three dimensions.

RESULTS

In previous work (Sethian, 1983b, 1984), numerical investigations were undertaken to analyze the relative effects of viscosity, exothermicity and boundary conditions on flame propagation in turbulent flow using the numerical method described in Sethian (1984) applied to open vessel configurations. It was shown that viscosity wrinkles the flame front, increasing the surface area of the flame and thus accelerating the combustion process, and that the slower the flame speed, the greater the effect of viscosity on the rate of combustion. When these investigations were continued into closed vessel experiments, exothermic effects were ignored, hence in confined vessels there was no feedback mechanism by which the flame motion could influence the hydrodynamics. Using this new model for zero Mach number combustion in closed vessels, in which exothermicity along the flame front plays a significant role in determining the hydrodynamics, a series of experiments to analyze the competing effects of exothermicity, pressure, boundary conditions and viscosity were performed. Similar calculations using this model are reported in Sethian (1983a).

In the first experiment, a motionless, inviscid fluid was ignited at the center of a closed square. A non-dimensional local laminar flame velocity of $Q=0.2$ was chosen, with $\alpha=0.5$ [Eq. (3.6)]. The initial conditions $P(0)=1$ and $\rho_u(0)=1$ were taken, and it was assumed that a fluid particle increased its volume by a factor of five upon burning; this corresponded u to $q_0=1.333$ (see Sethian, 1983b for details on these choices of values for q_0 and Q). In Figure 1, the results of this experiment are shown. An 80×80 grid of flame cells was used and the black region corresponds to burnt fluid. The velocity field is displayed on a 30×30 grid placed in the flow, where the magnitude of the vector at each point denotes the relative speed of the flow there; this grid plays

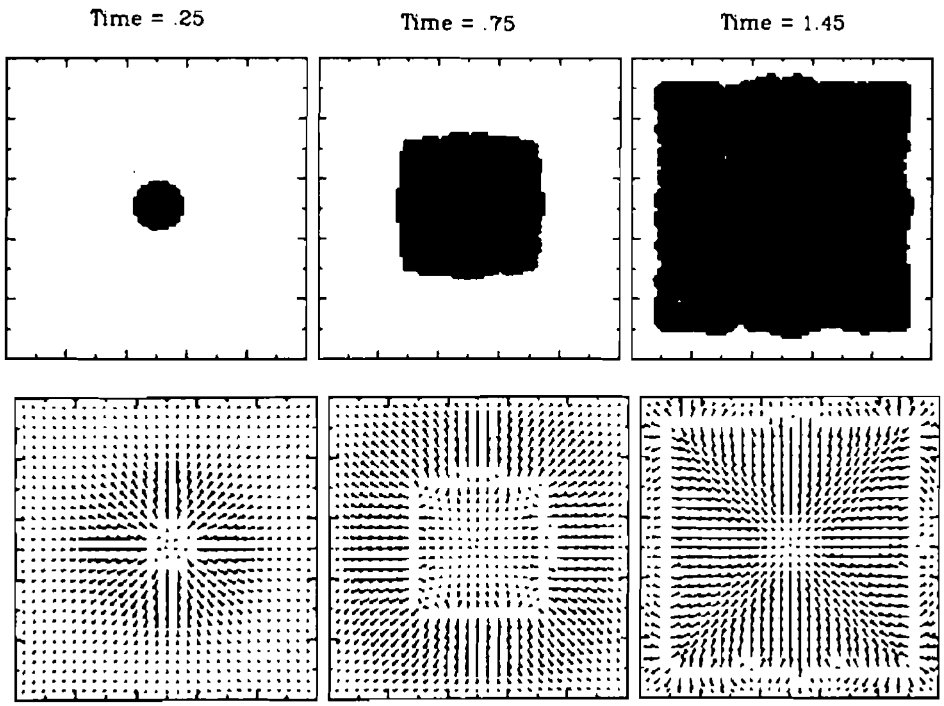

FIGURE 1 Inviscid, motionless fluid ignited in center, $q_0=1.333$.

no role whatsoever in the calculation and is purely for display purposes. The fluid motion results entirely from expansion along the flame front. One can clearly see the mechanism by which the boundary shapes the front; although the front starts off circular, it soon becomes square-like in response to the boundary conditions on the exothermic velocity field $\nabla\phi$, and thus burns into the corners. The final value ($t=1.55$) of the pressure in the vessel is 2.93 and the final value for k the propagation speed was 0.24 (compared with $k=0.2$ at $t=0$).

In the second set of experiments (Figure 2), the relative effects of viscosity and exothermicity on the rate at which combustion takes place in the vessel were investigated. In these experiments, fluid motion was generated by a vortex placed in the center of a square of sufficient strength so that the velocity tangential to each wall at its midpoint was 1. With $Q=0.14$, four different experiments were performed. The

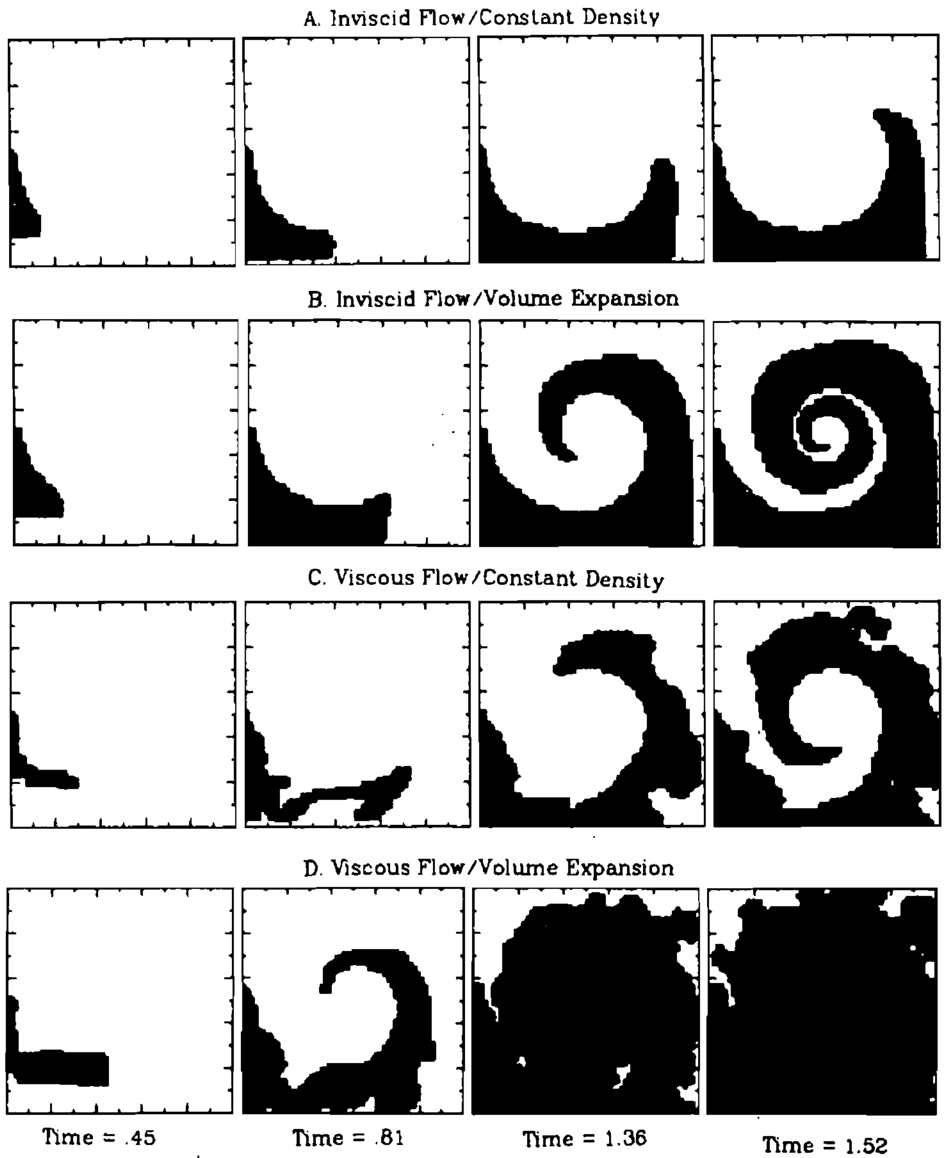

FIGURE 2 Swirling fluid.

top row corresponds to inviscid flow with $q_0=0$ (no exothermicity allowed), the next row is inviscid flow with $q_0=1.333$ (factor of five expansion), the next row is viscous flow with Reynolds number $R=1000$ and the bottom row corresponds to viscous flow, $R=1000$, $q_0=1.33$. In the two viscous runs, the flow was started two seconds before ignition so that recirculation zones would have time to develop.

The results may be summarized as follows. In the inviscid, constant density case, the flame wraps smoothly around the center, since the flow is smooth and there is no feedback mechanism from the flame to the hydrodynamics. When volume expansion effects are added, the resulting velocity field carries the flame around the center at a faster rate, in addition to the slightly higher propagation speed. In the viscous, constant density case, the flame motion is strongly influenced by the counterrotating eddies that grow in the corners as a result of vorticity production along solid walls; the flame is carried around each large eddy and then dragged backwards into the corner. These eddies are of prime importance in bringing the flame into contact with unburnt parts of the vessel. The front becomes jagged and wrinkled, increasing the surface area of the flame available for burning. In the viscous case with volume expansion, the flame is both wrinkled due to the turbulence of the flow and carried by the volume expansion velocity field, greatly decreasing the time required for complete conversion of reactants to products. This interplay between viscosity and exothermicity on the speed and shape of the burning front is the same as that obtained in Sethian (1984) for open channel calculations. In Figure 3, these comments are illustrated by plotting the percentage of the volume burnt as a function of time elapsed since ignition. All calculations were performed on a VAX 780 at the Lawrence Berkeley Laboratory. The longest calculation presented took about one hour of cpu time.

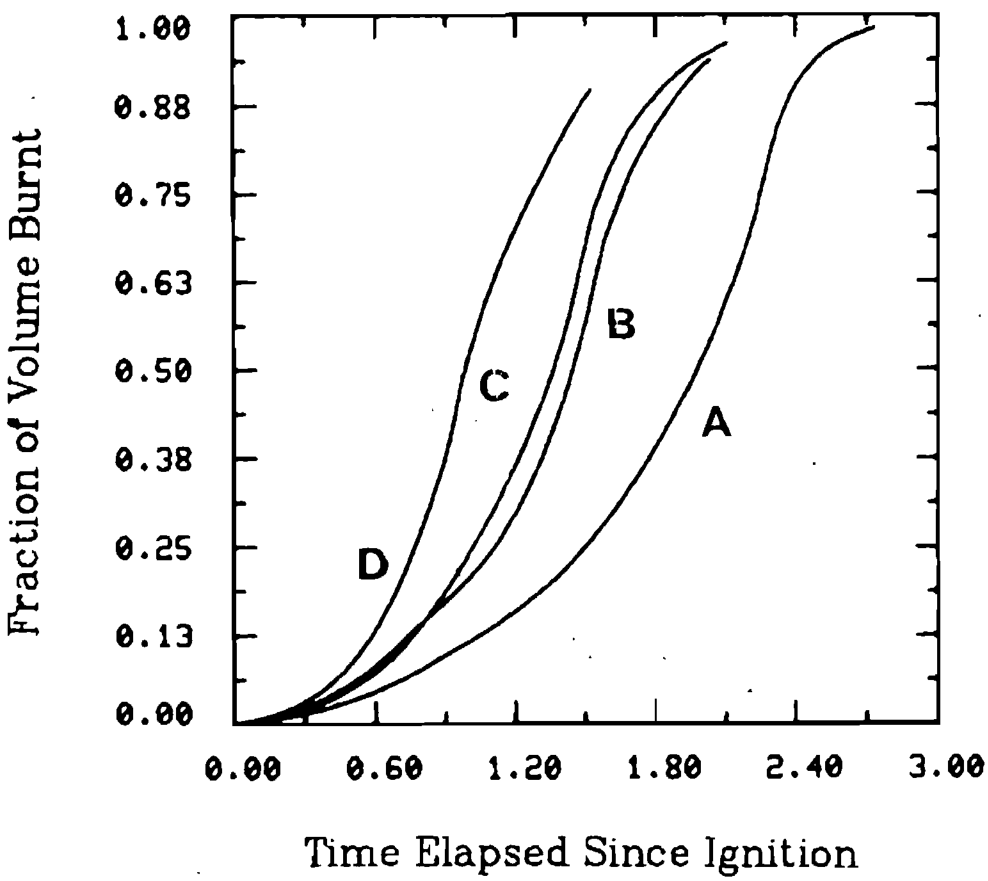

FIGURE 3 Time elapsed since ignition.

We have presented a systematic derivation of general equations for zero Mach number combustion. In Section Two, we simplified this model using the assumptions of Landau flame theory and a specific power law for flame speed. We compared numerically the effects of viscosity, exothermicity, pressure and boundary conditions on the interaction between a propagating flame and a swirling fluid. The model and numerical techniques we have presented only scratch the surface of a highly complex problem. Such issues as three-dimensional effects, thermal boundary layers, vorticity production across flame fronts and flame speed dependence on curvature must be tackled before a complete picture can begin to emerge. We hope to analyze these additional effects in the same manner as presented here.

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