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A. Majda and J. Sethian

January 1984

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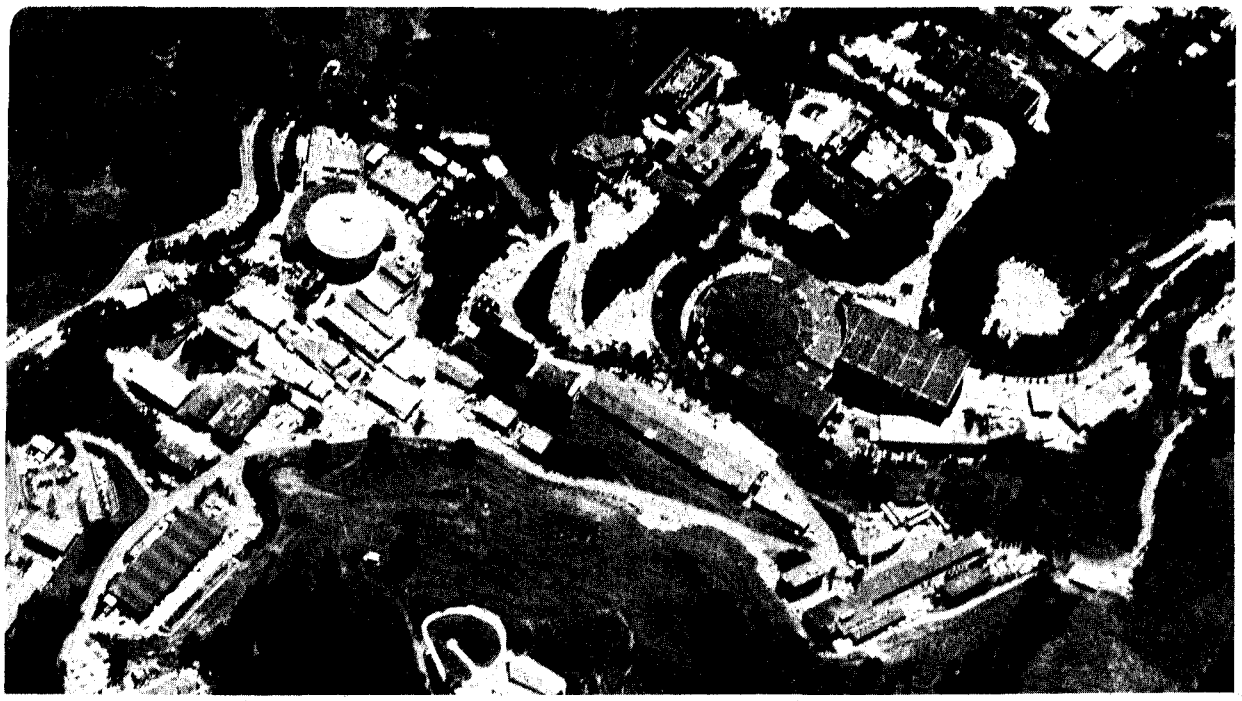

Prepared for the U.S. Department of Energy under Contract DE-AC03-76SF00098

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LBL-17289

THE DERIVATION AND NUMERICAL SOLUTION OF THE EQUATIONS FOR ZERO MACH NUMBER COMBUSTION[1]

Andrew Majda[2]

Department of Mathematics
University of California
Berkeley, California 94720

and

James Sethian[3]

Lawrence Berkeley Laboratory
and
Department of Mathematics
University of California
Berkeley, California 94720

January 1984

[1]This work was supported in part by by the Director, Office of Energy Research, Office of Basic Energy Sciences, Engineering, Mathematical, and Geosciences Division of the U.S. Department of Energy under contract DE-AC03-76SF00098.

[2]Partially supported by A.R.O. grant No. 483964-25530.

[3]National Science Foundation Mathematical Sciences Postdoctoral Fellow.

Abstract

We introduce a new limiting system of equations to describe combustion processes at low Mach number in either confined of 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. However, 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

We introduce a new 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; furthermore, our formulation of these equations constitutes a well-posed initial value problem (rigorous proofs are available, [5]). Under additional assumptions guaranteeing infinitely thin flame front structure, this new system of combustion equations in multi-dimensions has a formal asymptotic limit which reduces to the system introduced recently in [7] for combustion in open channels through qualitative considerations. That system was solved numerically through a combination of random vortex element techniques and flame propagation algorithms specifically designed for problems in turbulent combustion [7],[17]. In this paper, our new system, which applies to turbulent combustion in both open and closed vessels, is solved numerically by means of an extension of the above techniques. The new method, 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.

This new limiting system of equations describing zero Mach number combustion to be described in this paper is a valid set of equations describing the physical process under the following three assumptions:

(1.1)

(a) The nondimensional Mach number M, the ratio of typical fluid velocities to typical sound speeds, is small.

(b) The initial pressure P_0 is spatially uniform within terms of order M^2.

(c) The initial temperature T, mass fraction Z, and velocity v are in *chemical-fluid balance* within terms of order M.

The requirement in (1.1)(c) will be explained in detail below, but we would like to emphasize here that this condition is not particularly restrictive. If we use the well-known unique orthogonal decomposition (see [2]) of an arbitrary fluid velocity vector field v into a rotational field w and a potential $\nabla\psi$,

$$v = w + \nabla\psi$$

$$\text{div } w = 0, \qquad w\cdot n\big|_{\partial\Omega} = 0, \qquad \frac{\partial\psi}{\partial n}\bigg|_{\partial\Omega} = 0 \ , \tag{1.2}$$

then given initial values of T,Z, there is a *unique initial value* of the *gradient* of the *potential* $\nabla\psi$, *guaranteeing exact chemical-fluid balance;* however, the *rotational piece* of the *initial velocity* w *can be completely arbitrary,* as long as it is consistent with the assumption in (1.1)(a). We emphasize here that the assmption of the approximate chemical-fluid balance for the initial data is quite essential for the validity of the equations to be described here. In fact, even if the initial Mach number is small and the initial pressure is nearly spatially uniform, when the conditions of chemical-fluid balance are violated, the effects of the acoustic waves can be substantial. In fact, one only has to realize that there exist many combustion systems with

initial data satisfying (1.1)(a),(b) alone which exhibit transition to detonation. Furthermore, a rigorous proof of the validity of the zero Mach number limit equations (described in (1.3) below) under the three assumptions in (1.1) can be given by extending and modifying the analysis in [7]--this will be published elsewhere.

Next we describe these equations in the simplest reacting fluid system. We assume two reacting species--unburnt gas, with mass fraction Z, undergoes one-step irreversible chemical conversion to burnt gas with the same γ-gas law. In this situation, the equations for *zero Mach number combustion* in a *confined region* Ω (to be derived in Section 2 under the assumptions in (1.1)) are the following system of equations for the variables, pressure P, fluid velocity $v = w + \nabla\psi$, temperature T, and mass fraction Z, supplemented by the ideal gas formula $\rho = P/T$, with ρ the density:

(1.3) (a) *Nonlinear O.D.E. for the Mean Pressure* $P(t)$

$$\frac{dP(t)}{dt} = \frac{\gamma q_o \frac{K}{\varepsilon} \int_\Omega \rho Z e^{-A/T}}{\mathrm{Vol}\ \Omega}$$

(b) *Elliptic Equations for the Velocity Potential* ψ

$$\Delta\psi = (\gamma P)^{-1}\left(-\frac{dP}{dt} + \gamma q_o \frac{K}{\varepsilon}\rho Z e^{-A/T} + \varepsilon\gamma\Delta T\right), \qquad \left.\frac{\partial\psi}{\partial n}\right|_{\partial\Omega} = 0$$

(c) *Incompressible Nonhomogeneous Navier-Stokes Equation for the Rotational Piece of Velocity* w

$$\rho\frac{Dw}{Dt} - \varepsilon\,\mathrm{Pr}\,\Delta w + \nabla\tilde{p}^{\infty} = -\rho\frac{D}{Dt}(\nabla\psi), \qquad \mathrm{div}\ w = 0$$

$$w\cdot n\big|_{\partial\Omega} = 0, \qquad w\times n\big|_{\partial\Omega} = -\nabla\psi\times n\big|_{\partial\Omega}$$

(d) Heat Conduction Equation for T

$$\rho \frac{DT}{Dt} = \frac{\gamma-1}{\gamma}\frac{dP}{dt} + \varepsilon \Delta T + q_o \frac{K}{\varepsilon} \rho Z e^{-A/T}$$

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

(e) Reacting Species Equation for Z

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

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

where the above equations are written in suitable nondimensional form with Pr, Le, the Prandtl and Lewis numbers,

(1.4) *the parameter* ε *<u>the flame - thickness factor</u> characterizes the width of the thermal flame struc re to a typical linear dimension for* Ω.

and $\frac{D}{Dt} = \frac{\partial}{\partial t} + v\cdot\nabla$. *The condition of chemical-fluid balance for the initial data mentioned in (1.1) (c) is precisely the condition that the elliptic equation in (1.3) (b) be satisfied at time zero, i.e., there should exist a constant* H_o, *so that*

$$\Delta\psi = (\gamma P)^{-1}(- H_o + \gamma q_o \frac{K}{\varepsilon} \rho Z e^{-A/T} + \varepsilon \Delta T)$$

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

Given arbitrary Z, T, *a choice of* H_o *guaranteeing a unique* $\nabla\psi$ *satisfying the above equations is always possible by classical potential theory.*

In Section 3, following the discussion of Sivashinsky [19], we take the formal limit of the system of equations in (1.3) as the parameter ε described in (1.4) tends to zero---the limit of infinitely thin flame structure. In unconfined chambers, we describe the fashion in which the system in (1.3) reduces to the model described in [7]. In Section 4 we briefly describe the numerical method used in [17] for solving these 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 our new zero Mach number equations. 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. 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. Finally, in the Appendix, we give the zero Mach number combustion equations for a general chemically reacting fluid.

The new formulation presented here uses some of the earlier work of Sivashinsky [19]. However, our derivation and point of view are completely different. In the formulation in [19], the two equations

$$\frac{D\rho}{Dt} + \rho \operatorname{div} v = 0 \tag{1.5}$$

$$\rho T = P(t) \tag{1.6}$$

are used together with the equations in (1.3c, 1.3d and 1.3e) instead of the two equations in (1.3a, 1.3b). For the purposes of numerical modelling, the formulation from [19] has two disadvantages when compared with the one in (1.3): 1) A straightforward discretization of the conservation of mass equation and the temperature equation from (1.3d) introduces spatial discretization errors

in the density and temperature so it is quite difficult to design numerical schemes which enforce the constraint $\rho T = P(t)$ and 2) the evolution of the pressure $P(t)$ is only implicitly defined in [19], so it is difficult to calculate a dynamic update for $P(t)$ as needed for calculations in closed vessels. One theoretical advantage of our formulation (which, to our knowledge, has been discussed nowhere else in the literature) is that the correct initial conditions of chemical fluid balance described above and needed for self-consistency with the zero Mach number asymptotics arise naturally. The zero Mach number equations developed here can be regarded as a model existing between the full compressible Navier-Stokes equations and constant density models [8],[13] where the fluid dynamics essentially decouples from the combustion process. Further details and additional comments regarding zero Mach number combustion in a single space variable can be found in [12].

2. *Derivation of the zero Mach Number Combustion Equations*

Here we present a derivation of the equations of zero Mach number combustion under the simplest ideal assumptions for the chemical reactions. We concentrate on the case of a bounded region $\overline{\Omega}$. We assume that there are only two species present, unburnt gas 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

$$(2.1)\qquad \frac{Dp}{Dt} + \gamma\, p \operatorname{div} v = \Pr \varepsilon\gamma(\gamma-1)M^2\left(\sum_{i,j}\left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i}\right)^2 - \frac{2}{3}(\operatorname{div} v)^2\right) + \gamma \frac{q_o K\rho Z}{\varepsilon} e^{-A/T} + \gamma\varepsilon\Delta T .$$

Momentum Equations

$$(2.2)\qquad \rho\frac{Dv_i}{Dt} + (\gamma M^2)^{-1}\frac{\partial p}{\partial x_i} = \varepsilon \Pr \sum_j \frac{\partial}{\partial x_j}\left(\frac{\partial v_j}{\partial x_i} + \frac{\partial v_i}{\partial x_j} - \frac{2}{3}\delta_{ij} \operatorname{div} v\right)$$

for $i = 1,2,3$.

Temperature Equation

$$(2.3)\quad \rho \frac{DT}{Dt} = \frac{\gamma-1}{\gamma}\frac{Dp}{Dt} + Pr\ \varepsilon(\gamma-1)M^2\left(\sum_{i,j}\left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i}\right)^2 - \frac{2}{3}(\mathrm{div}\ v)^2\right) + \frac{q_o}{\varepsilon}K\rho Z\ e^{-A/T} + \varepsilon\Delta T$$

Species Equation

$$(2.4)\quad \rho \frac{DZ}{Dt} = -\frac{1}{\varepsilon}K\rho Z\ e^{-A/T} + (Le)^{-1}\ \varepsilon\ \mathrm{div}(\rho\nabla Z)$$

together with the ideal gas equation of state,

$$(2.5)\qquad p = \rho T\,.$$

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

(2.6) Nondimensionalization:

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

(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.,

$$c_pT_b = \max_{x\in\bar{\Omega}}\ (c_pT_o(x) + \tilde{q}_oZ_o(x))$$

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

(3) $q_o = \tilde{q}_o/C_pT_b$ is the nondimensional heat release.

(4) The density is given in units of ρ_b with $\rho_b = \frac{P_0}{T_b}$.

(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 $T_u = T_b - c_p^{-1}\,\tilde{q}_o$.

(7) The unit time scale is determined by (5) and (6), *i.e. unit time in (2.1) - (2.5) is measured by diam* $\Omega/|v_b|$.

(8) $Pr = vc_p/\kappa$ is the Prandtl number

$Le = \kappa/\rho_b c_p d$ is the Lewis number

where v is the viscosity, d is the species diffusion coefficient, and κ is the coefficient of heat conduction.

(9) The parameter ε *the flame-thickness factor is defined by*

$$\varepsilon = \ell_T/\text{diam}\ \Omega$$

where ℓ_T is the length scale associated with the internal thermal structure of flames

$$\ell_T = \kappa(\rho_b|v_b|c_p)^{-1} .$$

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

$$K = K_o\rho_b^{-1}\ c_p^{-1}|v_b|^{-2}\ \kappa$$

with K_o the frequency factor and A is the nondimensional activation energy in units of T_bR_o, with R_o the universal gas constant.

(11) The quantity M is the Mach number

$$M = |v_b|/(\gamma\ P_o/\rho_b)^{\frac{1}{2}}.$$

For simplicity in exposition, we have assumed that all diffusion coefficients and the frequency factor are constants. Also, ε is typically a small parameter, but we will not exploit this fact in this section.

Inviscid Reacting Gases

First we treat the case when the reacting gas is inviscid, i.e., Pr = 0. Then the system of equations in (2.1)-(2.5) is supplemented by the *boundary conditions*

$$(2.7)\qquad \begin{aligned} &\text{(a)}\quad v\cdot n = 0 && \text{on}\quad \partial\Omega \\ &\text{(b)}\quad \frac{\partial T}{\partial n} = \frac{\partial Z}{\partial n} = 0 && \text{on}\quad \partial\Omega . \end{aligned}$$

The adiabatic boundary conditions in (2.7)(b) have been assumed to avoid additional complications with thermal boundary layers, etc. With the hypothesis of small Mach number, we assume the asymptotic expansions in terms of Mach number given by

$$(2.8)\qquad \begin{aligned} p &= P_o(x,t) + MP_1 + \gamma M^2 P_2 + O(M^3) \\ v &= v_o(x,t) + Mv_1(x,t) + O(M^2) \\ T &= T_o(x,t) + MT_1(x,t) + O(M^2) \\ Z &= Z_o(x,t) + MZ_1(x,t) + O(M^2) . \end{aligned}$$

Before beginning the derivation, we recall two well-known facts (see [4],[20]):

Fact #1. For a bounded domain Ω, the boundary value problem

$$(2.9)\qquad \begin{aligned} \Delta\psi &= F && \text{in}\quad \Omega \\ \left.\frac{\partial\psi}{\partial n}\right|_{\partial\Omega} &= g \end{aligned}$$

has a solution with $\nabla\psi$ uniquely determined if and only if $\int_\Omega F = \int_{\partial\Omega} g$ and

<u>Fact #2.</u> Every vector field v has the unique orthogonal decompositon

(2.10) $v = w + \nabla\phi$ where

$$\operatorname{div} w = 0, \qquad w\cdot n\big|_{\partial\Omega} = 0$$

and

$$\Delta\phi = \operatorname{div} v, \qquad \frac{\partial\phi}{\partial n}\bigg|_{\partial\Omega} = v\cdot n\big|_{\partial\Omega}.$$

We set $Qv = w$ and observe that $Q(\nabla\phi) = 0$. We substitute (2.8) into (2.1)-(2.4) and equate powers of M.

First, we concentrate on the momentum equation in (2.2). The terms of order M^{-2}, M^{-1}, respectively, imply

$$\nabla P_o(x,t) = 0$$

(2.11)

$$\nabla P_1(x,t) = 0 .$$

For the terms of order zero in the momentum equation, we first apply Q and use the fact from (2.10) that $Q(\nabla p) = 0$, then

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

with $\frac{D}{Dt} = \frac{\partial}{\partial t} + (v_o\cdot\nabla)$. From the equations in (2.11) and (2.12), we conclude that

(2.13)

(a) $P_o \equiv P_o(t)$

and

(b) there is a scalar pressure p^∞, with $\frac{P_0}{T_0}\frac{Dv_0}{Dt} = -\nabla p^\infty$.

The equations of order zero for the temperature and mass fraction from (2.3), (2.4) are straightforward and given by

$$(2.14)\quad \begin{aligned} &\text{(a)} \quad \frac{P_0}{T_0}\frac{DT_0}{Dt} = \frac{\gamma-1}{\gamma}\frac{dP_0}{dt} + \frac{q_0}{\varepsilon} K\rho_o Z_o\, e^{-A/T_0} + \varepsilon\,\Delta T_o \\ &\text{(b)} \quad \frac{P_0}{T_0}\frac{DZ_0}{Dt} = -\frac{K}{\varepsilon}\frac{P_0}{T_0} Z_o\, e^{-A/T_0} + (Le)^{-1}\,\varepsilon\, \mathrm{div}\left(\frac{P_0}{T_0}\nabla Z_o\right). \end{aligned}$$

The only subtle part of the derivation occurs in our discussion of the pressure equation--in fact, our use of the pressure equation from (2.1) rather than the conservation of mass is a significant difference in our formulation when compared with the one in **[19]** . Conservation of mass is a consequence of the two separate equations to be derived below. Using (2.13)(a) in (2.1), we compute that the order zero terms in the pressure equation are given by

$$(2.15)\qquad \frac{dP_0}{dt} = -\gamma P_o\, \mathrm{div}\, v_o + \gamma \frac{q_o}{\varepsilon} K\rho_o Z_o\, e^{-A/T_0} + \gamma\varepsilon\,\Delta T_o .$$

The self-consistency of the perturbation expansion in (2.8) requires that the order zero equation in (2.15) is satisfied. The left-hand side of (2.15) is a scalar function of time alone, while the right-hand side of (2.15) involves functions of both space and time. Therefore, there must exist a scalar function $\mathcal{H}(t)$ of time alone, so that simultaneously

$$(2.16)\quad \begin{aligned} &\text{(a)} \quad \frac{dP_0}{dt} = \mathcal{H}(t) \\ &\text{(b)} \quad \mathcal{H}(t) = -\gamma P_o\, \mathrm{div}\, v_o + \gamma \frac{q_o}{\varepsilon} K\rho_o Z_o\, e^{-A/T_0} + \gamma\varepsilon\,\Delta T_o . \end{aligned}$$

How should $\mathcal{H}(t)$ be chosen? We use the orthogonal decomposition from <u>Fact #2</u> to decompose v_o as

(2.17) $$v_o = w_o + \nabla\psi_o ,$$

so that from the boundary condition in (2.7)(a) we rewrite (2.16)(b) as an equation for ψ_o, namely,

(2.18) $$(\Delta\psi_o) = (\gamma P_o)^{-1}(- \mathcal{H}(t) + \frac{\gamma}{\varepsilon} q_o K\rho_o Z_o \, e^{-A/T_0} + \gamma\varepsilon \, \Delta T_o)$$

$$\left.\frac{\partial\psi_0}{\partial n}\right|_{\partial\Omega} = 0 .$$

Now, from Fact #1 in (2.9), the elliptic equation in (2.18) has a solution with $\nabla\psi_o$ uniquely determined if and only if the integral of the right-hand side of (2.18) over Ω vanishes. This requirement uniquely determines $\mathcal{H}(t)$ by the equation

$$- \mathcal{H}(t) \int_\Omega dx + \frac{1}{\varepsilon} \int_\Omega \gamma \, q_o \, K\rho_o Z_o \, e^{- A/T_0} + \varepsilon \int_\Omega \gamma\Delta T_o = 0 ,$$

i.e.,

(2.19) $$\mathcal{H}(t) = \frac{\frac{1}{\varepsilon} \int_\Omega \gamma \, q_o \, K\rho_o Z_o \, e^{- A/T_0}}{\mathrm{Vol}(\Omega)} .$$

Here we have used the boundary condition in (2.7)(b) to integrate to zero the contribution from heat conduction. This choice of $\mathcal{H}(t)$ allows us to satisfy (2.16)(b) with a unique choice of $\nabla\psi_o$ and simultaneously to obtain an evolution equation for the mean pressure $P_o(t)$. With $\mathcal{H}(t)$ from (2.19), the equations from (2.13)(b), (2.14), and (2.16) yield the

<u>Equations for Zero Mach Number Inviscid Combustion</u>

(2.20) (a) <u>Nonlinear O.D.E. for Mean Pressure</u>

$$\frac{dP_0}{dt} = \frac{\frac{1}{\varepsilon} \int_\Omega \gamma q_o K\rho_o Z_o \, e^{-A/T_0}}{\mathrm{Vol}(\Omega)} .$$

(b) Elliptic Equation

$$\Delta\psi_o = (\gamma P_o)^{-1}\left(-\frac{dP_0}{dt} + \gamma q_o \frac{K}{\varepsilon}\rho Z_o e^{-A/T_0} + \gamma\varepsilon\Delta T_o\right)$$

$$\left.\frac{\partial\psi_0}{\partial n}\right|_{\partial\Omega} = 0 .$$

(c) Nonhomogeneous Incompressible Fluid Equation

$$\rho(P_o,T_o)\frac{D}{Dt}w_o = -\rho(P_o,T_o)\frac{D}{Dt}\nabla\psi_o - \nabla p^{\infty}$$

$$\operatorname{div} w_o = 0 , \qquad w_o\cdot n|_{\partial\Omega} = 0 .$$

(d) Reaction-Diffusion Equations

(1) $$\rho(P_o,T_o)\frac{DT_0}{Dt} = \frac{\gamma-1}{\gamma}\frac{dP_0}{dt} + \frac{q_0}{\varepsilon}K\rho Z_o e^{-A/T_0} + \varepsilon\Delta T_o$$

(2) $$\rho(P_o,T_o)\frac{DZ_0}{Dt} = -\frac{K}{\varepsilon}\rho Z_o e^{-A/T_0} + (Le)^{-1}\varepsilon\operatorname{div}(\rho\nabla Z_o)$$

$$\frac{\partial T_0}{\partial n} = \frac{\partial Z_0}{\partial n} = 0 \qquad \text{on } \partial\Omega$$

where the formulae

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

and

$$v_o = w_o + \nabla\psi_o, \qquad \operatorname{div} w_o = 0, \qquad w_o\cdot n|_{\partial\Omega} = 0$$

complete the description of this system. Since each of the steps associated with (2.20)(a)-(d) is a well-posed equation, it is intuitively clear that the system in (2.20) defines a well-posed system of equations--in fact, a rigorous

proof of this fact will appear in **[5]**. The requirement of *approximate chemical-fluid balance* for the initial data is an immediate consequence of (2.11) which requires initially

$$p(x,0) = 1 + O(M^2) ,$$

and the fact that the elliptic equation in (2.20)(b) must be satisfied at time $t = 0$. For arbitrary initial data $Z_o(x)$, $T_o(x)$, the equation in (2.20)(b) imposes a constraint upon the initial velocity only as regards the fluid dynamic potential $\nabla\psi_o$, and w_o can be completely arbitrary initially at $t = 0$.

Equations for Zero Mach Number Viscous Combustion

When $Pr \neq 0$, the system of equations in (2.1)-(2.5) should satisfy the *boundary conditions*

$$(2.21) \quad \begin{aligned} &\text{(a)} \quad v\big|_{\partial\Omega} = 0 \qquad \text{(no slip)} \\ &\text{(b)} \quad \frac{\partial T}{\partial n} = \frac{\partial Z}{\partial n} = 0 . \end{aligned}$$

The no-slip boundary conditions together with the nonzero viscosity coefficient in the momentum equation changes the boundary conditions and nature of the limiting equation in (2.20)(c). However, since the viscous stress contributions to the pressure and temperature equations are $O(M^2)$, the equations for (2.20)(a), (b), and (d) are unchanged in the viscous case. By repeating the derivation given above in the inviscid case, we compute that the Equations for Zero Mach Number Viscous Combustion are given by

Nonlinear O.D.E. (2.20)(a)

(2.22)(a) Elliptic Equation (2.20)(b)

Reaction-Diffusion Equations (2.20)(d)

and the *Nonhomogeneous Incompressible Navier-Stokes Equation*

$$(2.22)(b) \quad \rho(P_o,T_o)\,\frac{D}{Dt}\,w_o - \varepsilon\,\mathrm{Pr}\,\Delta w_o + \nabla\tilde{p}^{\infty} = -\,\rho(P_o,T_o)\,\frac{D}{Dt}\,\nabla\psi_o$$

(actually, we have defined a reduced pressure $\tilde{p}^{\infty} = p^{\infty} - \frac{4}{3}\varepsilon\,\mathrm{Pr}\,\Delta\psi_o$ to simplify the equations in (2.22)(b) even further) with the boundary conditions

$$(2.22)(c) \quad \mathrm{div}\, w_o = 0, \qquad w_o \cdot n\big|_{\partial\Omega} = 0, \qquad w_o \times n\big|_{\partial\Omega} = -\,\nabla\psi_o \times n\big|_{\partial\Omega}.$$

The linearized equations obtained from (2.22)(b)-(c) are nonhomogeneous Stokes equations and yield a well-posed problem (see **[20]**)--in fact, a rigorous proof of the nonlinear well posedness for the system in (2.22) will appear in **[5]**. We remark here that in this case the requirement of approximate chemical fluid balance also imposes the condition

$$w_o \times n\big|_{\partial\Omega} = -\,\nabla\psi_o \times n\big|_{\partial\Omega}$$

initially at time $t = 0$.

Zero Mach Number Combustion in Unbounded Domains

The derivation which we have presented applies just as well to combustion in unbounded domains. We use the same nondimensional form of the equations in (2.1)-(2.5) with the change that diam Ω is replaced by some typical large mean length scale which in Section 3 is assumed to be much bigger than the length scale ℓ_T. The crucial difference in the derivation rests on the following fact:

For unbounded domains such as channels or all of space, the elliptic equation

$$\Delta\psi = F$$

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

has a unique solution for *any* F which is square integrable.

In repeating the derivation given above, this fact has the important consequence that $\mathcal{H}(t)$ from (2.16) can be chosen so that

(2.23)(a) $$\mathcal{H}(t) \equiv 0 .$$

Thus, the *pressure remains constant* independent of time, while (2.16)(b) becomes the elliptic equation

(2.23)(b)
$$\Delta\psi_o = (\gamma P_o)^{-1}(\gamma\, q_o \frac{K}{\varepsilon}\rho Z_o\, e^{-A/T_0} + (\gamma\varepsilon\,\Delta T_o)$$
$$\left.\frac{\partial\psi_0}{\partial n}\right|_{\partial\Omega} = 0 .$$

The remaining equations for zero Mach number combustion from either (2.20) or (2.22) are unchanged.

We remark that ***the equations in either (2.20) or (2.22) conserve mass***, i.e., with

$$\rho = \frac{P_0(t)}{T_0(x,t)}, \qquad v_o = \nabla\psi_o + w_o, \qquad \frac{D\rho}{Dt} + \rho \operatorname{div} v_o = 0 .$$

The reader can check this by direct calculation with (2.22) or he can use our observation that the compressible system in (2.1)-(2.5) conserves mass and the equations in (2.20) or (2.22) are the limit of equations that conserve mass, therefore these systems conserve mass too.

3. Zero Mach Number Combustion with Infinitely Thin Flame Structure

Here we discuss the further simplification of the general multi-dimensional zero Mach number combustion equations derived in the last section, under 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 **[19]**.)

These assumptions are satisfied for many typical combustion processes when the diam Ω is the order of one meter. (We drop all subscript zeros for the equations in (2.22), (2.31) in this section.)

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

$$Z(x,0) = \begin{cases} 1, & \phi_o(x) < 0 \\ 0, & \phi_o(x) > 0 \end{cases}$$

(3.1)

$$T(x,0) = \begin{cases} T_u \equiv 1-q_o, & \phi_o(x) < 0 \\ T_b \equiv 1, & \phi_o(x) > 0. \end{cases}$$

This initial data including the fluid velocity has a jump discontinuity across the surface $S_o = \{x \in \Omega | \phi_o(x) = 0\}$ and is a stochiometric mixture composed of unburnt gas for those points $x \in \Omega$ with $\phi_o(x) < 0$ and burnt gas for

those points $x \in \Omega$ with $\phi_o(x) > 0$. After we have finished the discussion in this section, 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_o, provided that the non-dimensional adiabatic equation expressing conservation enthalpy across S_o,

$$T_b(x) = T_u(x) + q_o Z(x) \qquad \text{for } x \in S_o \tag{3.2}$$

is valid at all points of S_o.

As described in [19] and following the well-known ideas of Landau [11], under the above assumption and with the special initial data for (2.22) given in (3.1), it follows that as $\varepsilon \to 0$, formally

$$\frac{1}{\varepsilon} K Z e^{-A/T_0} \to m(x,t)\delta_{S(t)}, \qquad x \in S(t) \tag{3.3}$$

where $S(t)$ is a surface described by $S(t) = \{x|\phi(x,t) = 0\}$ with $\phi(x,0) = \phi_o(x)$ and $\delta_{S(t)}$ is the surface Dirac measure concentrated on $S(t)$ (see [6]). Here the function $-m(x,t)$ is the mass flux across $S(t)$ and is determined by

$$\rho_b(v_b \cdot n - V) = \rho_u(v_u \cdot n - V) = -m(x,t) \qquad \text{for } x \in S(t), \quad V = \phi_t/|\nabla\phi| \tag{3.4}$$

where n is the outward spatial normal to $S(t)$. The equation in (3.4) expresses the conservation of mass across the surface $S(t)$ which is valid for solutions of (2.22) in the limit as $\varepsilon \to 0$. As $\varepsilon \to 0$, from (3.3), the reaction-diffusion equations in (2.22)(a) reduce to

$$\text{(a)} \qquad \frac{dP}{dt} = \frac{\gamma\, q_o \int_{S(t)} m(x,t)\,dA}{\mathrm{Vol}(\Omega)}$$

$$\text{(3.5)} \qquad \text{(b)} \quad \rho \frac{DT}{Dt} = \frac{\gamma-1}{\gamma}\frac{dP}{dt}\,, \quad \text{for} \quad \phi(x,t) > 0 \quad \text{and} \quad \phi(x,t) < 0$$

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

where (b) and (c) are supplemented by the jump conditions across $S(t)$ appropriate for data of the form in (3.1) given by

$$\text{(3.6)} \qquad \begin{aligned} &T_b(x,t) - T_u(x,t) = q_o \qquad \text{for} \quad x \in S(t) \\ &Z_b(x,t) = 0, \quad Z_u(x,t) = 1 \qquad \text{for} \quad x \in S(t)\,, \end{aligned}$$

while the elliptic equation from (2.22)(a) becomes

$$\text{(3.7)} \qquad \begin{aligned} &\Delta\psi = (\gamma P)^{-1}\left(-\frac{dP}{dt} + \gamma\, q_o\, m\, \delta_{S(t)}\right) \\ &\left.\frac{\partial\psi}{\partial n}\right|_{\partial\Omega} = 0\,. \end{aligned}$$

The nonhomogeneous Navier-Stokes equations from (2.22)(b) become

$$\text{(3.8)} \qquad \begin{aligned} &\rho \frac{Dv}{Dt} - (\varepsilon\, \mathrm{Pr})\Delta w - \nabla\tilde{p}^{\infty} = 0 \quad \text{for} \quad \phi(x,t) > 0 \quad \text{and} \quad \phi(x,t) < 0 \\ &v|_{\partial\Omega} = 0 \end{aligned}$$

with $v = w + \nabla\psi$, $\mathrm{div}\, w = 0$, $w\cdot n|_{\partial\Omega} = 0$. The equations in (3.8) are supplemented by the jump conditions from (3.4) across $S(t)$ and the density is given in the two regions by

$$\text{(3.9)} \qquad \rho = \begin{cases} P(t)/T_u(x,t)\,, & \phi(x,t) < 0 \\ P(t)/T_b(x,t)\,, & \phi(x,t) > 0\,. \end{cases}$$

(Alternatively, we could use the conservation form of the momentum equation in (3.8) across $\phi = 0$.)

We have retained the viscosity term $(\varepsilon\ Pr)\Delta w$ in (3.8) for emphasis because the no slip boundary conditions $v|_{\partial\Omega} = 0$ create boundary layers since $\varepsilon\ Pr \neq 0$ 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 front is idealized as infinitely thin and represented by the surface $S(t)$. With the initial data in (3.1), it is very easy to solve the equations in (3.5)(c) to obtain

$$(3.10) \qquad Z(x,t) = \begin{cases} 1\,, & \phi < 0 \\ 0\,, & \phi > 0\,. \end{cases}$$

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 [1], [10], 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.,

$$(3.11) \qquad m(x,t) = m(T_u,P) = m(\rho_u,P)\,.$$

Landau postulated that $m(\rho_u,P)$ should be determined by the local laminar flame velocity (see [11]) and others ([1], [10]) 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

$$(3.12) \qquad m(\rho_u,P) = Q\,\rho_u^{1-a}\,P^a$$

where $a, Q > 0$ are constant and $1 > a \geq \frac{1}{2}$ (see [10], $a = \frac{1}{2}$ corresponds to the laminar case). Now, the equation in (3.11) 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,

$$\text{(3.13)} \qquad \begin{aligned} &\phi_t + \frac{m(\rho_u(t),P(t))}{\rho_u} |\nabla\phi| + v_u \cdot \nabla\phi = 0 \\ &\phi(x,0) = \phi_o(x) \ . \end{aligned}$$

Thus, from (3.13) the points $\vec{r}(t)$ on $S(t)$ are described by the equation

$$\text{(3.14)} \qquad \frac{d\vec{r}}{dt} = \frac{m(\rho_u(t),P(t))}{\rho_u} \vec{n}(\vec{r}) + v_u(\vec{r})$$

where $\vec{n}(\vec{r})$ is the outward normal to $S(t)$. With the assumption in (3.11), the equation in (3.5)(a) becomes

$$\text{(3.15)} \qquad \frac{dP}{dt} = \frac{q_o \ \gamma \ m(\rho_u(t),P(t))A(t)}{\mathrm{Vol}(\Omega)}$$

with $A(t)$ the area of $S(t)$. Next 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,

$$\text{(3.16)} \qquad \frac{D}{Dt} \log(\rho_u^\gamma/P) = 0$$

and therefore, for the special initial data in (3.9),

$$\rho_u(t) = P^{1/\gamma}(t)\rho_u(0) = P^{1/\gamma}(t)\rho_u^o \,. \tag{3.17}$$

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 $\varphi > 0$ by solving the linear boundary problem for the first order equation

$$\begin{aligned} &\frac{D}{Dt} T_b(x,t) = 0 \\ &T_b(x,t)|_{S(t)} = q_0 + \frac{P(t)}{\rho_u(t)} \\ &T_b(x,0) = 1 \end{aligned} \tag{3.18}$$

It should be apparent to the reader that the more general initial data discussed above (3.2) are handled by straightforward modification.

4. 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 (3.1) and with the main additional *assumption* at the beginning of Section 3 and postulate (3.11), we have derived the equations for zero Mach number combustion with infinitely thin flame structure described in (3.7), (3.8), (3.14) and (3.15) as a limiting case of the equation from (2.22). 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 (4.1)

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

(b) Eikonal Equation for the Flame Front $S(t)$ (4.2)

$$\frac{d\vec{r}}{dt} = v_u(\vec{r}) + \frac{m(\rho_u(t), P(t))}{\rho_u} \vec{n}(\vec{r})$$

(c) Elliptic Equation (4.3)

$$\Delta\varphi = (\gamma P)^{-1}\left(-\frac{dP}{dt} + \frac{q_0 \gamma m(\rho_u(t), P(t))\delta_s}{\mathrm{Vol}(\Omega)}\right)$$

$$\frac{\partial\varphi}{\partial n} = 0$$

(d) Nonhomogeneous Incompressible Navier–Stokes Equation (4.4)

$$\rho \frac{Dw}{Dt} - \varepsilon \,\mathrm{Pr}\, \Delta w - \nabla p^{\infty} = -\rho \frac{D\nabla\varphi}{Dt}$$

$$\mathrm{div}\, w = 0$$

$$w \cdot n \,|_{\partial\Omega} = 0 \qquad w \times n \,|_{\partial\Omega} = -\nabla\varphi \times n \,|_{\partial\Omega}$$

with the orthogonal decomposition $v = \nabla\varphi + w$. Here, we again note that q_0 is the non-dimensional heat release, $A(t)$ is the area of the flame front at time t, Vol (Ω) is the volume of the vessel under consideration, $\vec{r}(t)$ is a point on the flame front at time t, $v_u(\vec{r})$ is the velocity at the point r as taken as a limit from the unburnt side, $\vec{n}(\vec{r})$ is the normal to the front at $\vec{r}$, and δ_F 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 in [7], the fact above (2.23) is valid and the constant pressure approximation $\frac{dP}{dt} \equiv 0$ applies for the system in (2.22b) and therefore in our equations. In this situation, the equations (4.1-4.4) reduce to those introduced by Ghoniem, Chorin and Oppenheim in [7] and studied extensively in [17]. We now describe the numerical algorithm for approximating the system of equations (4.1-4.4).

Given that w is divergence-free and that $\nabla\varphi$ is irrotational ($\nabla\times\nabla\varphi=0$), we define ξ to be the vorticity ($\xi = \nabla\times w$) and take the curl of (4.4) to produce the vorticity transport equation

$$\frac{D\xi}{Dt} = \frac{1}{R}\nabla^2\xi \tag{4.5}$$

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

The form for the mass flux given in (3.12) is

$$m(\rho_u, P) = Q\rho_u^{1-a}P^a \tag{4.6}$$

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

$$\rho_u(t) = (P(t))^{1/\gamma} \rho_u(0) \tag{4.7}$$

where δ_F is the surface Dirac measure. We shall now describe the technique for approximating the combustion model (4.1-4.3,4.5-4.7).

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 [3], 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 [17], 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 [17].

The vorticity ξ in (4.1) 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 (4.2), 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 [15]). This problem is avoided through introducing a grid on the domain and assigning each cell a number (a "volume fraction", see [14],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 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 [2]). 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 $\nabla\varphi$ 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 Equation (4.3); a fast Poisson solver is used to solve the Neumann problem for φ. Straightforward finite differences on the fast solver grid provide $\nabla\varphi$ and hence u. Again, the tangential boundary "no-slip" condition is satisfied by the creation of vortex sheets. The vortex elements are then advected under the field $\nabla\varphi$, and the flame is advected by the velocity field $u = w + \nabla\varphi$ 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 (Equation 4.1) in computing $\nabla\varphi$. To advance from one time step to the next, the position of the flame is used to calculate $\frac{dP}{dt}$ using (4.1). 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 non-linear ordinary differential equation (4.1). Finally, Equation (4.7) is used to update the density of the unburnt gas used in the mass flux calculation in (4.6).

RESULTS

In previous work [17,18], 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 [17] 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 [16].

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 $Q = .2$ was chosen, with $\alpha = .5$ (Equation 4.6). 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 to $q_0 = 1.333$ (see [18] for details on these choices of values for q_0 and Q). In Figure 1, the results of this experiment are shown. The black region corresponds to burnt fluid, and 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. 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 $\nabla\varphi$, 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 .24 (compared with $k = .2$ at $t = 0$).

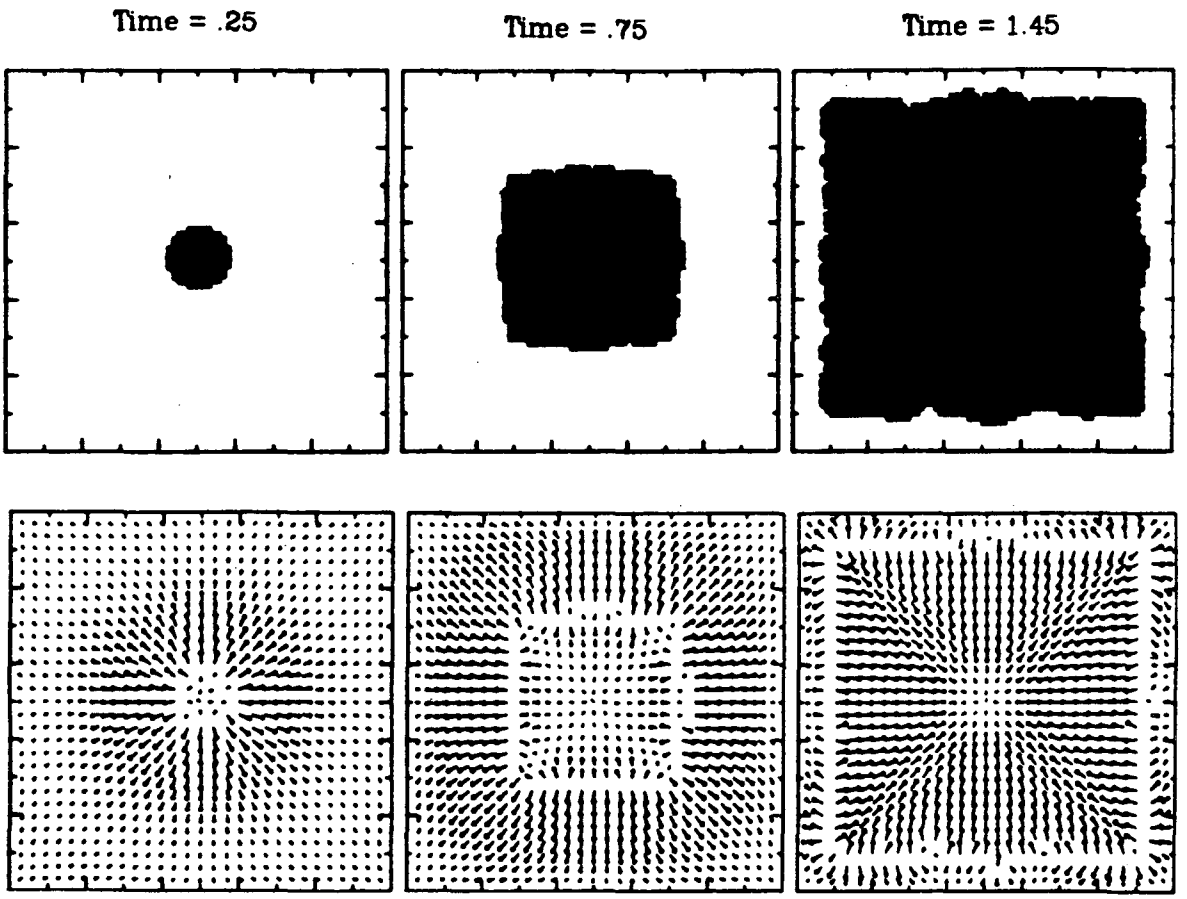

Figure 1: Inviscid, Motionless Fluid Ignited in Center, $q_0 = 1.333$

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 $Q = .14$, four different experiments were performed. The 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.

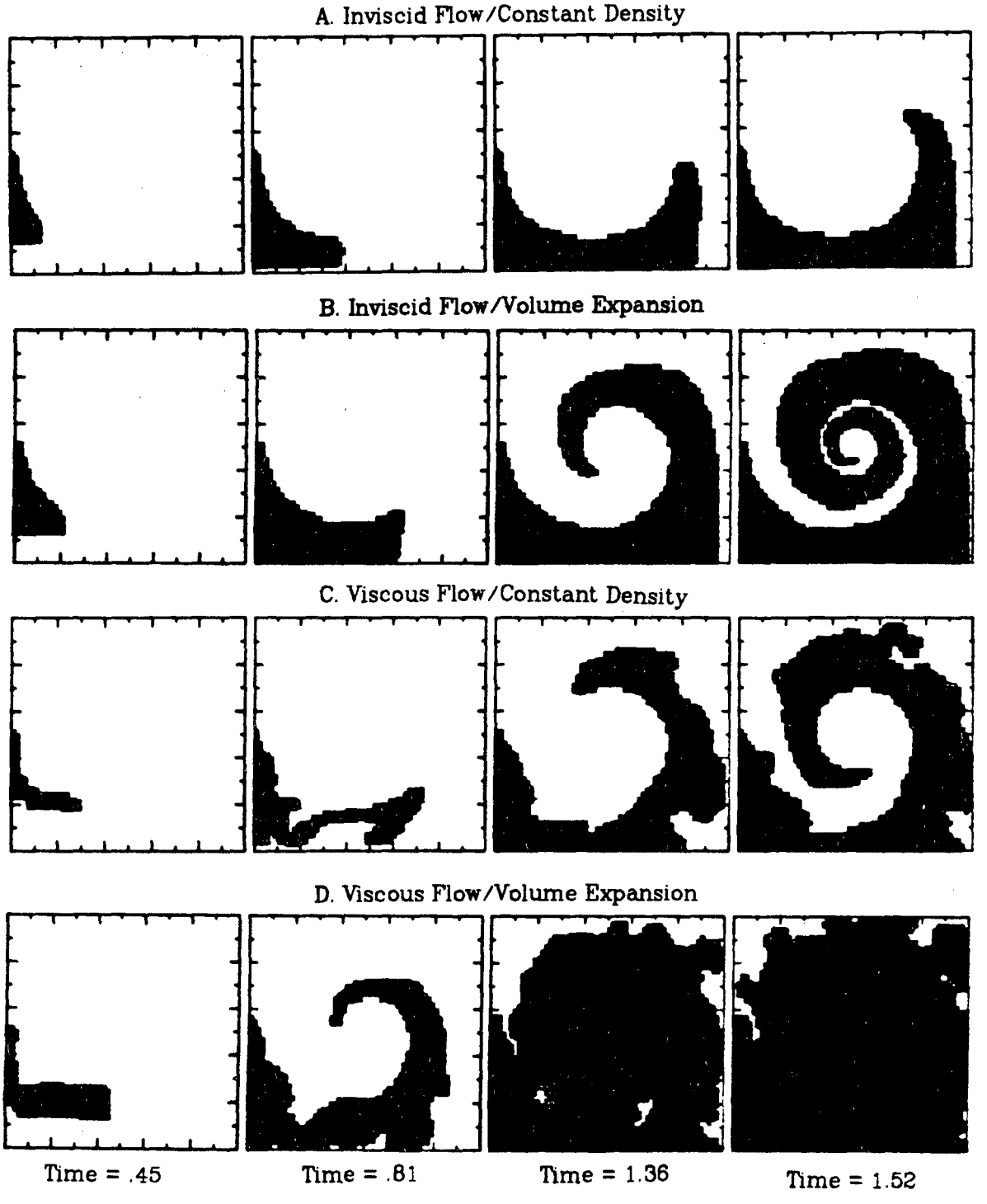

Figure 2: Swirling Fluid

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 [17] 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.

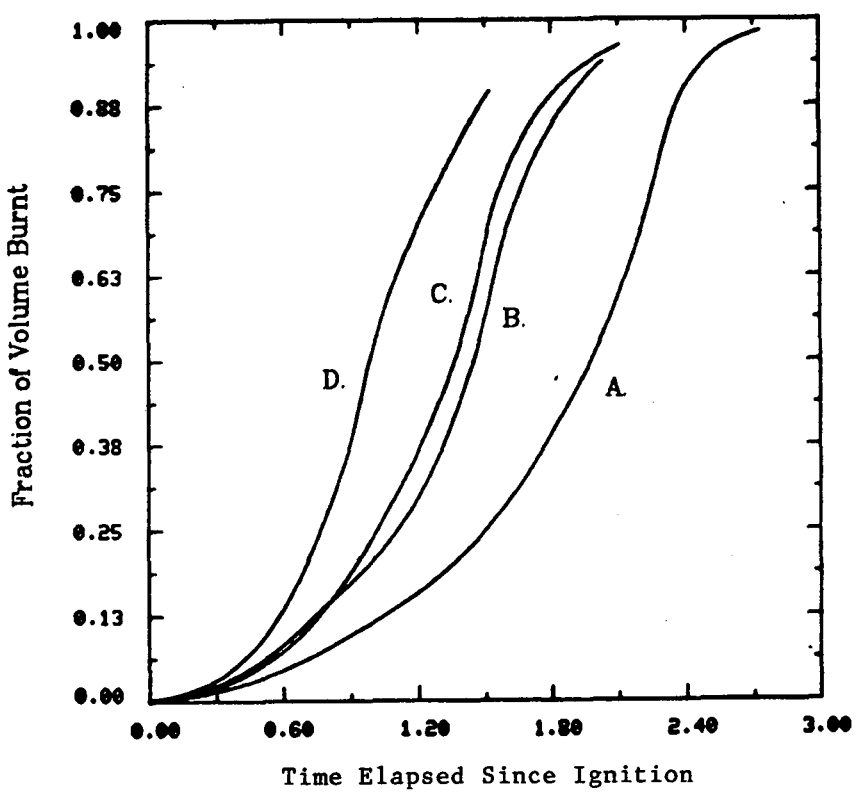

Figure 3

APPENDIX

Equations of Zero Mach Number Combustion in a General Reacting Fluid

The basic equations for a general reacting fluid with m-species in terms of the variables p, T, v, Z_i, $i = 1,\ldots,m$, where Z_i is the mass fraction of the i-th species, are given in nondimensional form (see [21]) by

Pressure Equation

$$\text{(A.1)} \quad \frac{1}{\rho c_f^2}\frac{Dp}{Dt} + \operatorname{div} v = \frac{M^2}{T\rho c_p}\sigma : \nabla v + \frac{1}{Tc_p}\sum_{i=1}^{m}(\mathrm{Pr\ Re\ Le}^i)^{-1}\nabla Z_i \cdot \nabla h_i$$

$$+ \frac{1}{(\mathrm{Pr\ Re}\ \rho T c_p)}\Delta T + \sum_{i=1}^{m}\left(\frac{\partial\mu_i}{\partial p}\right)_{T,Z}(\mathrm{Pr\ Re\ Le}^i)^{-1}\operatorname{div}(\rho\nabla Z_i)$$

$$+ \sum_{i=1}^{m}\left[\left(\frac{\partial\mu_i}{\partial p}\right)_{T,Z} - \frac{h_i}{\rho T c_p}\right]\Phi_i \ .$$

Momentum Equations

$$\text{(A.2)} \qquad \rho\frac{Dv}{Dt} + (M)^{-2}\nabla p = (\mathrm{Re})^{-1}\operatorname{div}\sigma \ .$$

Temperature Equation

$$\text{(A.3)} \quad \rho c_p\frac{DT}{Dt} + c_f^2\rho\operatorname{div} v = \frac{M^2}{\mathrm{Re}}\left(1 + \frac{c_f^2}{Tc_p}\right)\sigma : \nabla v + \frac{1}{\mathrm{RePr}}\left(1 + \frac{c_f^2}{Tc_p}\right)\Delta T$$

$$+ \sum_{i=1}^{m}(\mathrm{Le}^i\ \mathrm{PrRe})^{-1}\left(1 + \frac{c_f^2}{c_pT}\right)\rho\nabla Z_i \cdot \nabla h_i$$

$$+ \sum_{i=1}^{m}(\mathrm{Le}^i\ \mathrm{RePr})^{-1}\ c_f^2\ \rho\left(\frac{\partial\mu_i}{\partial p}\right)_{T,Z}\operatorname{div}(\rho\nabla Z)$$

$$+ \sum_{i=1}^{m}\left[c_f^2\ \rho\left(\frac{\partial\mu_i}{\partial p}\right)_{T,Z} - \left(1 + \frac{c_f^2}{c_pT}\right)\right]\Phi_i \ .$$

Reacting Species Equations

(A.4) $$\rho \frac{DZ_i}{Dt} = (\mathrm{Pr\ Re\ Le}^i)^{-1} \operatorname{div}(\rho \nabla Z_i) + \Phi_i \ , \qquad i = 1,\ldots,m \ .$$

In (A.1)-(A.4), we have assumed that the i-th species is an ideal gas so that with $\gamma_i(T) = c_p^i(T)/C_v^i(T)$ and W_i the molecular weight of the i-th species,

(1) $h_i(T)$ is the enthalpy of the i-th species

$$h_i(T) = \left(\frac{R}{W_i} \int_{T_f}^{T} \frac{\gamma_i(s)}{\gamma_i(s)-1}\, ds\right) + h_{i,f} \ , \qquad i = 1,\ldots,m$$

(2) $$p = \rho T \sum_{i=1}^{m} \frac{R\, Z_i}{W_i}$$

(3) c_f is the frozen sound speed,

(A.5) $$c_f^2 = \left(\frac{\partial p}{\partial \rho}\right)_{S,Z}$$

(4) With $h = \sum_{i=1}^{m} h_i\, Z_i$, the enthalpy, c_p is given by

$$c_p = \left(\frac{\partial h}{\partial T}\right)_{p,Z}$$

(5) $\mu_i(p,T,Z)$ is the chemical potential of the i-th species, $i=1,\ldots,m$

(6) $\Phi_i(p,T,Z)$ is the chemical source term for the i-th species

(7) $\sigma = (\sigma_{ij})$, $\sigma_{ij} = \frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i} - \frac{2}{3} \operatorname{div} v\, \delta_{ij}$

while the important nondimensional parameter M is the Mach number

(A.6) $$M^2 = \frac{|v_b|^2}{\tilde{P}_o/\tilde{\rho}_o} .$$

With the assumption that the Mach number is small, we make the Ansatz

$$P = P_o + M\, P_1 + O(M^2)$$

$$v = v_o + O(M)$$

$$T = T_o + O(M)$$

$$Z = Z_o + O(M)$$

and repeat the analysis of Section 2 to derive the following:

<u>Equations for Zero Mach Number Combustion in a Reacting Fluid in a Confined Chamber</u>

Nonlinear O.D.E. for Mean Pressure

(A.7) $$\frac{dp}{dt} = \mathcal{H}(t) .$$

Elliptic Equation

(A.8) $$\Delta\psi = g - \frac{\mathcal{H}(t)}{\rho c_f^2} , \qquad \left.\frac{\partial\psi}{\partial n}\right|_{\partial\Omega} = 0 .$$

Incompressible Nonhomogeneous Navier-Stokes Equation

$$\rho \frac{Dw}{Dt} + \nabla\tilde{p}^{\infty} + (Re)^{-1}\Delta w = -\rho \frac{D}{Dt}\nabla\psi$$

(A.9) $$\operatorname{div} w = 0 , \qquad w\cdot n|_{\partial\Omega} = 0$$

$$w \times n|_{\partial\Omega} = -\nabla\psi \times n|_{\partial\Omega} , \qquad v = w + \nabla\psi .$$

Temperature Equation

$$\text{(A.10)} \quad \rho c_p \frac{DT}{Dt} = \mathcal{H}(t) + (\mathrm{Re}\ \mathrm{Pr})^{-1}\mathrm{div}(\nabla T) + \sum_{i=1}^{m} (\mathrm{Le}^i\ \mathrm{Pr}\mathrm{Re})^{-1}\rho\ \nabla Z_i \cdot \nabla h_i - \sum_{i=1}^{m} h_i \Phi_i \ .$$

Reacting Species Equations

$$\text{(A.11)} \quad \rho \frac{DZ_i}{Dt} = (\mathrm{Le}^i\ \mathrm{Pr}\mathrm{Re})^{-1}\ \mathrm{div}(\rho\ \nabla Z_i) + \Phi_i \ , \qquad i = 1,\ldots,m \ ,$$

with $\left.\frac{\partial T}{\partial n}\right|_{\partial\Omega} = \left.\frac{\partial Z}{\partial n}\right|_{\partial\Omega} = 0$. Here the source term g and the scalar $\mathcal{H}(t)$ are given by

$$\text{(A.12)} \qquad \mathcal{H}(t) = \frac{\int_\Omega g}{\int_\Omega (\rho\ c_f^2)^{-1}}$$

and

$$\text{(A.13)} \quad g = (\mathrm{Pr}\ \mathrm{Re})^{-1} \frac{1}{\rho T c_p} + \frac{1}{T c_p} \sum_{i=1}^{m} (\mathrm{Le}^i\ \mathrm{Pr}\mathrm{Re})^{-1}\ \nabla Z_i \cdot \nabla h_i$$

$$+ \sum_{i=1}^{m} \left(\frac{\partial \mu_i}{\partial p}\right)_{T,Z} (\mathrm{Le}^i\ \mathrm{Pr}\mathrm{Re})^{-1}\mathrm{div}(\rho \nabla Z_i) + \sum_{i=1}^{m} \left[\left(\frac{\partial \mu_i}{\partial p}\right)_{T,Z} - \frac{h_i}{\rho T c_p}\right]\Phi_i \ .$$

Acknowledgment: The authors thank Alexandre Chorin, J.B. Keller, and G.I. Sivashinsky for interesting discussions related to this work.

REFERENCES

[1] Carrier, G.F., Fendell, F.E., and Feldman, P.S., *Dynamics of Reactive Systems*, Academic Press, New York (1980), 333-352.

[2] Chorin, A.J., "Flame Advection and Propagation Algorithms", Journal of Computational Physics, Vol.35, 1980, pp.1-11

[3] Chorin, A.J., "Numerical Studies of Slightly Viscous Flow", Journal of Fluid Mechanics, Vol.57, 1973, pp.785-796.

[4] Chorin, A.J. and Marsden, J., *A Mathematical Introduction to Fluid Mechanics*, Springer-Verlag, New York, 1979.

[5] Embid, P., "The equations of zero Mach number combustion, PhD. these, U.C. Berkeley, 1984 (to appear).

[6] Gelfand, I.M., and Shilov, G.E., *Generalized Functions*, Vol. I, Academic Press, New York, 1964.

[7] Ghoniem, A.F., Chorin, A.J., and Oppenheim, A.K., "Numerical Modelling of Turbulent Flow in a Combustion Tunnel", Philos. Trans. Roy. Soc, London Sr. A (1981), 1103-1119.

[8] van Harten, A., and Matkowsky, B.J., "A New Model in Flame Theory", SIAM J. Appl. Math. 42 (1982), 850-868.

[9] Klainerman, S., and Majda, A., "Compressible and Incompressible Fluids", Comm. Pure Appl. Math, Vol. 35, 1982, p.629-651.

[10] Kurylo, J., Dwyer, H.A., and Oppenheim, A.K., "Numerical Analysis of Flow Fields Generated by Accelerated Flames", AIAA J. 18 (1980), 302-308.

[11] Landau, L.D., "On the Theory of Slow Combustion", J. Exp. Theor. Phys. 14 (1944), 240-249.

[12] Majda, A., "Equations of Low Mach Number Combustion", Center for Pure and Applied Mathematics, University of California, Berkeley, 1982, Report No. 112, November 1982.

[13] Matkowsky, B.J., and Sivashinsky, G.I., "An Asymptotic Derivation of Two Models in Flame Theory Associated with the Constant Density Approximation", SIAM J. Appl Math. 37 (1979), 686-699.

[14] Noh, W.T. and Woodward, P., SLIC (Simple Line Interface Calculation). Proc. 5th Int. Conf. Numer. Math. Fluid Mechanics, Springer-Verlag, Berlin, 1976, pp.330-339.

[15] Sethian, J.A. "An Analysis of Flame Propagation", PhD. Dissertation, University of California, Berkeley, June 1982.

[16] Sethian, J.A. "Numerical Simluation of Flame Propagation in a Closed Vessel", Proc. Fifth Int. GAMM Conf. Numer. Meth. Fluid Mechanics, Rome, Italy, Oct.5-7, 1983.

[17] Sethian, J.A. "Turbulent Combustion in Open and Closed Vessels", Lawrence Berkeley Laboratory, LBL-15744, 1983, to appear in the Journal of Computational Physics, May 1984.

[18] Sethian,J.A. "The Wrinkling of a Flame Due to Viscosity", Fire Dynamics and Heat Transfer, Proc. 21st Nat. Heat Transfer Conf., J.Quintiere, Ed.,p.29-32, 1983.

[19] Sivashinsky G.I., "Hydrodynamic Theory of Flame Propagation in an Enclosed Volume", Acta Astronautica 6 (1979), 631-634.

[20] Temam, R., *The Navier-Stokes Equations*, North Holland Press, Amsterdam, 1977.

[21] Williams, F.A., *Combustion Theory*, Addison-Wesley, Reading, MA, 1964.

This report was done with support from the Department of Energy. Any conclusions or opinions expressed in this report represent solely those of the author(s) and not necessarily those of The Regents of the University of California, the Lawrence Berkeley Laboratory or the Department of Energy.

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