Lawrence Berkeley National Laboratory
Recent Work

Title
NUMERICAL SIMULATION OF FLAME PROPAGATION IN A CLOSED VESSEL

Permalink
https://escholarship.org/uc/item/77g7j8mj

Author
Sethian, J.A.

Publication Date
1983-10-01

eScholarship.org Powered by the California Digital Library
University of California

LBL-16828 c.2

Lawrence Berkeley Laboratory
UNIVERSITY OF CALIFORNIA

Physics, Computer Science & Mathematics Division

RECEIVED
LAWRENCE
BERKELEY LABORATORY
DEC 13 1983
LIBRARY AND
DOCUMENTS SECTION

Presented at the Fifth GAMM Conference on Numerical Methods in Fluid Mechanics, Rome, Italy, October 5-7, 1983

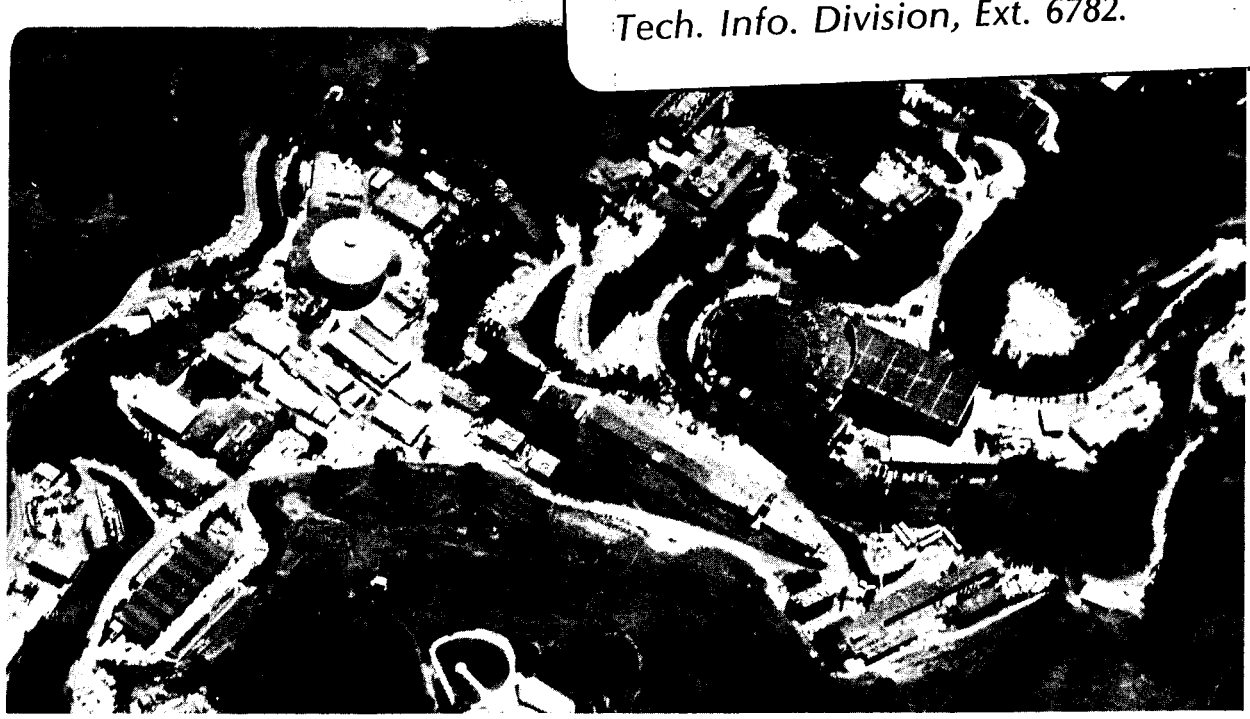
NUMERICAL SIMULATION OF FLAME PROPAGATION IN A CLOSED VESSEL

J.A. Sethian

October 1983

TWO-WEEK LOAN COPY

This is a Library Circulating Copy which may be borrowed for two weeks. For a personal retention copy, call Tech. Info. Division, Ext. 6782.



LBL-16828 c.2

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

DISCLAIMER

This document was prepared as an account of work sponsored by the United States Government. While this document is believed to contain correct information, neither the United States Government nor any agency thereof, nor the Regents of the University of California, nor any of their employees, makes any warranty, express or implied, or assumes any legal responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by its trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof, or the Regents of the University of California. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof or the Regents of the University of California.

LBL-16828

NUMERICAL SIMULATION OF FLAME PROPAGATION IN A CLOSED VESSEL[1]

James A. Sethian

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

October 1983

---

[1]Presented at the Fifth GAMM Conference on Numerical Methods in Fluid Mechanics, Rome, Italy, October 5-7, 1983.

This work was supported in part 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.

NUMERICAL SIMULATION OF FLAME PROPAGATION IN A CLOSED VESSEL

J.A. Sethian

Department of Mathematics
and
Lawrence Berkeley Laboratory

University of California
Berkeley, California, 94720

SUMMARY

We present a numerical simulation of a flame propagating in a swirling, premixed, combustible fuel inside a closed vessel. The model we approximate is appropriate for viscous, turbulent combustion, and includes the effects of exothermic volume expansion along the flame front. The method, which is particularly suited for flow at high Reynolds number, uses random vortex element techniques coupled to a flame propagation algorithm based on Huyghen's principle. We analyze the various effects of pressure, boundary conditions, exothermicity and viscosity on the speed and shape on the burning flame.

INTRODUCTION

A particularly challenging problem in the study of turbulent combustion is the interaction between hydrodynamic turbulence and the propagation of a flame. At high Reynolds number, turbulent eddies and recirculation zones form, due to viscous effects, which affect the motion of a flame. Conversely, exothermic effects along the flame front influence the fluid motion. In many situations, this interaction is of great importance. For example, in the design of internal combustion engines, one might attempt to direct the flow in such a way that the largest amount of fuel is burned as quickly as possible, thus minimizing the amount of unburnt fuel expelled at the end of a stroke.

Questions of flame stability and the interaction between hydrodynamics and flame propagation have received considerable attention over the past few decades. Much of the analysis has concentrated on perturbation analysis of various models of combustion; for example, in [1], the effect of viscosity on the hydrodynamic stability of a plane flame front was examined. An excellent, though now outdated review of such techniques may be found in [2]; a more recent review may be found in [3].

Taking a different approach, in our work we are concentrating on numerical methods to analyze such problems. At the foundation of our investigations is the Random Vortex Method [4], a numerical technique that is specifically designed for high Reynolds number flow, and portrays in an accurate and natural manner the formation of turbulent eddies and coherent structures in the flow. This technique has been successfully applied to a variety of situations, for example, flow past a cylinder [5] and blood flow past heart valves [6], and was first applied to turbulent combustion over a backwards facing step in [7].

In [8], we used these techniques to model turbulent combustion in open and closed vessels, and in [9] analyzed the effect of viscosity on the rate of combustion. We showed that viscosity wrinkles the flame front, increasing the surface area of the flame and thus accelerating the combustion process. In these investigations, exothermic effects, that is, volume expansion along the flame front, were ignored, hence the fluid motion affected the flame, but there was no feedback mechanism by which combustion could influence fluid motion. Recently, a model for combustion in closed vessels was formulated in [10] which includes exothermic effects in confined chambers and allows the flame to influence the hydrodynamics. In this paper, we use the techniques

described in [8] to approximate the solution of these equations. We investigate the role of pressure, boundary conditions, exothermicity and viscosity on the speed and shape of the burning flame.

THE MODEL: EQUATIONS OF MOTION

We consider two-dimensional, viscous flow inside the vessel. On solid walls, we require that the normal and tangential velocities be zero. In this model, combustion is characterized by a single step, irreversible chemical reaction; the fluid is a pre-mixed fuel in which each fluid particle exists in one of two states, burnt and unburnt. When the temperature of a particle becomes sufficiently high, it undergoes an instantaneous change in volume due to heating and becomes burnt. Thus we regard the interface between the burnt and unburnt regions as an infinitely thin flame front, acting as a source of specific volume and propagating in a direction normal to itself into the unburnt fluid. We assume that the Mach number M (the ratio of typical fluid velocities to typical sound speeds) is small, thus acoustic wave interactions are ignored.

The equations of motion for the above model applied to turbulent combustion in unconfined chambers may be found in [8]. In an unconfined vessel, the pressure remains constant, since expansion along the flame front merely pushes the fluid through the exit. Recently, Majda [10] has formulated a set of equations for low Mach number combustion in closed vessels that includes a time-dependent spatially uniform mean pressure term. Under the physically reasonable assumptions that the Mach number M is small, the initial pressure is spatially uniform within terms of order M^2, and the initial conditions for velocity, pressure and mass fraction are consistent within order M, formal asymptotic limits of the equations for fully compressible combustion can be taken to obtain a mathematically rigorous model of combustion that removes the detailed effects of acoustic waves, while retaining exothermic effects and spatial density variations. One can think of this model as existing "in between" constant density models, in which the fluid mechanics essentially decouples from the flame propagation, and the fully compressible combustion equations. In the case of combustion in unconfined chambers, the pressure remains constant and the equations reduce to those presented in [8]. We now describe the equations, for details, see [10].

Let $\vec{u} = (u,v)$ be the velocity of the fluid in the domain D. We let $\vec{u} = \vec{w} + \nabla\varphi$ where $\vec{w}$ is divergence-free (that is, $\nabla\cdot\vec{w} = 0$) and $\nabla\varphi$ is irrotational ($\nabla\times\nabla\varphi = 0$). Defining ξ to be the vorticity ($\xi = \nabla\times\vec{w}$), we take the curl of the momentum equation to produce the vorticity transport equation

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

where R is the Reynolds number and $\frac{D}{Dt}$ is the total derivative $\partial_t + (\vec{u}\cdot\nabla)$. Here, we have ignored the term $(\nabla\times\frac{\nabla P}{\rho})$ which corresponds to vorticity production across the flame front. The boundary conditions are that $\vec{u} = 0$ on ∂D.

With the assumption of an infinitely thin reaction zone, we view the flame front as a curve γ separating the burnt fluid from the unburnt fluid, where $\gamma(s,t)$ parameterizes by s, $0\le s\le S$, the position of the front at time t. Thus, for each s and t, $\gamma(s,t)$ yields the coordinates (X_F, Y_F) of a fluid particle that is "on fire". The burning of the front in a direction normal to itself, plus the advection of the front by the fluid, can be described by the system of partial differential equations

$$\frac{\partial X_F}{\partial t} = k(Y_F)_s\left(\frac{1}{((X_F)_s^2 + (Y_F)_s^2)^{1/2}}\right) + u(X_F, Y_F) \tag{2}$$

$$\frac{\partial Y_F}{\partial t} = -k(X_F)_s\left(\frac{1}{((X_F)_s^2 + (Y_F)_s^2)^{1/2}}\right) + v(X_F, Y_F) \tag{3}$$

The burning speed k may be determined by examining the mass flux m across the flame front to obtain

$$k = \frac{m(\rho_u(t), P(t))}{\rho_u(t)} \tag{4}$$

where $\rho_u(t)$ and $P(t)$ are the density of the unburnt gas and mean pressure, at time t, respectively. A typical form for the mass flux (see [11]) is

$$m(\rho_u, P) = Q\rho_u^{1-\alpha} P^{\alpha} \tag{5}$$

where Q is the local laminar flame velocity and α is a constant. Under the assumption of a γ-gas law, the unburnt fluid density may be obtained from the pressure through the relation

$$\rho_u(t) = (P(t))^{1/\gamma} \rho_u(0) \tag{6}$$

where $\rho_u(0)$ is the density of the unburnt fuel initially. The mean pressure in the vessel changes as a result of the expansion of fluid particles along the flame front as they change from unburnt to burnt. The rate of change $\frac{\partial P}{\partial t}$, which clearly depends on the length of the flame front and the volume of the vessel, is of the form

$$\frac{dP}{dt} = \frac{q_0 \gamma m(\rho_u(t), P(t))}{Vol(D)} \int_0^S \gamma(s,t)\, ds \tag{7}$$

where q_0 is a constant corresponding to exothermic expansion, and $Vol(D)$ is the volume of the vessel.

Finally, we need to determine $\nabla\varphi$, the exothermic velocity field resulting from volume expansion along the flame front. The divergence of this velocity field corresponds to the amount of expansion (or compression) at any point. Since $\nabla\varphi \cdot \vec{n} = 0$ on ∂D (no flow through the walls), by the divergence theorem we must have that $\int_D \nabla^2\varphi = 0$. Using this fact, together with (7), yields the elliptic equation

$$\nabla^2\varphi = \frac{1}{\gamma P}\left(-\frac{dP}{dt} + q_0 \gamma m(\rho_u, P)\, \delta_F\right) \tag{8}$$

$$\nabla\varphi \cdot \vec{n} = 0$$

where δ_F is the surface Dirac measure concentrated on the flame front. Equations (1-8) form our model for combustion in closed vessels.

THE NUMERICAL APPROXIMATION

Numerical modeling of high Reynolds number flow is typically accomplished through the application of finite difference schemes to the above equations. 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 [4], 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 allows us to follow the development of large-scale coherent, turbulent structures within the flow. In [8], vortex methods were applied to problems in turbulent combustion in open vessels. Our application of these techniques to the equations for combustion in closed vessels is very similar, and is described below.

The vorticity ξ in (1) is approximated by a set of vortex "blobs", whose positions and strengths at any time yield the associated velocity field $\vec{v}$. The distribution of vorticity is updated in two stages. First, the vortex elements are moved under the flow field $\vec{v}$, 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 $\vec{v}$ 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 (Equations 2 and 3) , 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 [12]). We avoid this problem by imposing a grid on the domain and assigning each cell a number (a "volume fraction", see [13]) corresponding to the amount of burnt fluid in that cell at any given time. We allow each cell on the boundary of the burnt gas to ignite 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 [14]). The motion of the flame is broken up into two stages: first, we model burning by allowing the flame to propagate in a direction normal to itself at the prescribed speed and second, we advect the burned fluid by the yet to be determined velocity field $\vec{u}$. By updating these volume fractions according to the advection and burning processes, we may track the motion of the flame.

To determine the velocity field $\vec{u}$, we must solve for the exothermic velocity field $\nabla\varphi$ produced by volume expansion along the flame front. We calculate $\frac{dP}{dt}$ from (7) using the position of the flame as determined by the Huyghen's principle construction described earlier. This allows us to determine the right hand side of (8); 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 $\vec{u}$. 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 $\vec{u} = \vec{v} + \nabla\varphi$ to produce the new positions for the vortex blobs and flame. Finally, the non-linear ordinary differential equation (7) is solved to update the pressure, and (6) is used to update the density of the unburnt gas used in the mass flux calculation (5).

RESULTS

We performed a series of experiments to measure the effect of exothermicity on the propagation of a flame. We began by igniting a motionless, inviscid fluid at the center of a closed square. We chose a non-dimensional local laminar flame velocity $Q = .2$, with $\alpha = .5$ (Equation 5). We took $P(0) = 1.$ and $\rho_u(0) = 1.$, and assumed that a fluid particle increased its volume by a factor of five upon burning, this corresponded to $q_0 = 1.333$ (see [9] for details). 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 30x30 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 $t = 0$).

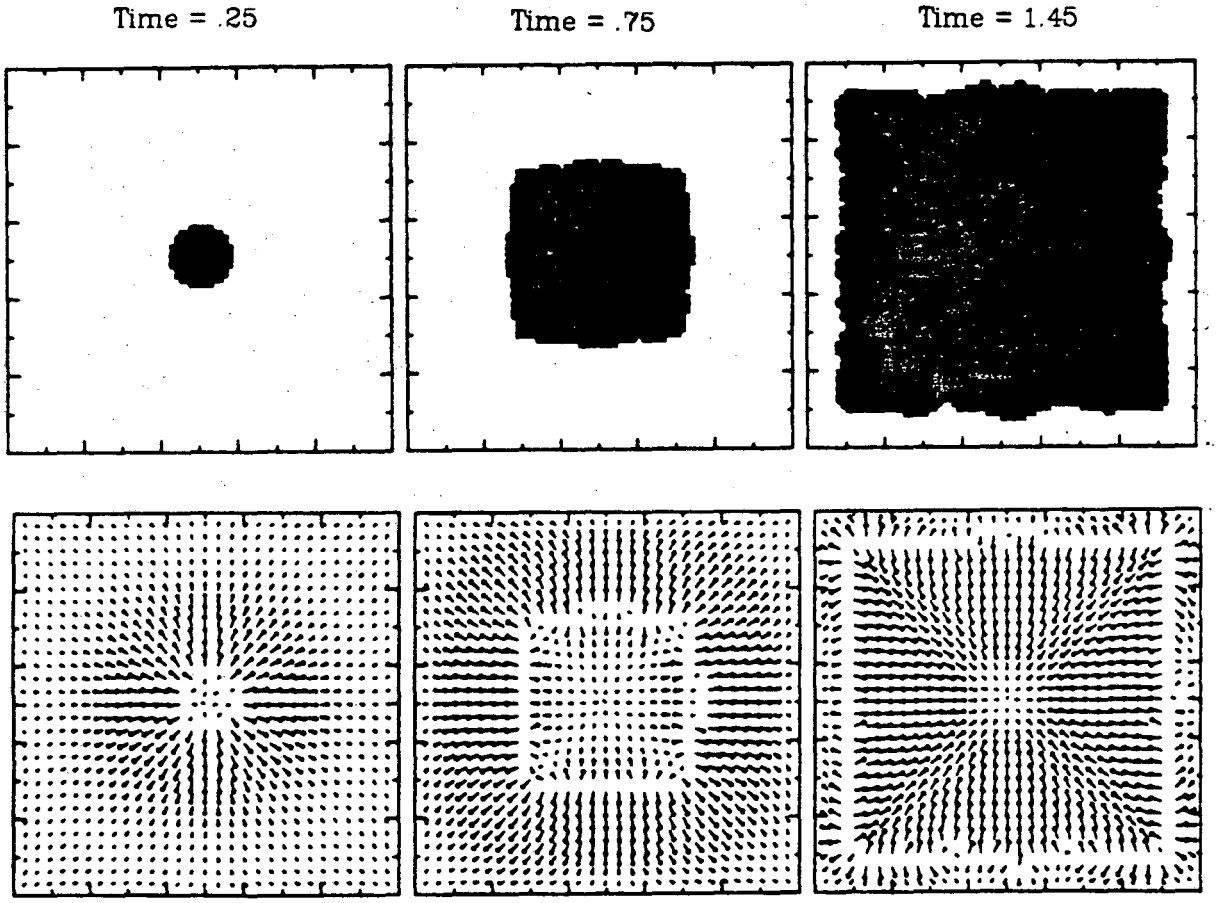


Figure 1: Inviscid, Motionless Fluid Ignited in Center, $q_0 = 1.333$

In the second set of experiments (Figure 2), we investigated the relative effects of viscosity and exothermicity on the rate at which combustion takes place in the vessel. 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 $Q = .14$, we performed four different experiments. 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, $R=1000.$, $q_0=1.333$. In the two viscous runs, the flow was started two seconds before ignition so that recirculation zones would have time to develop.

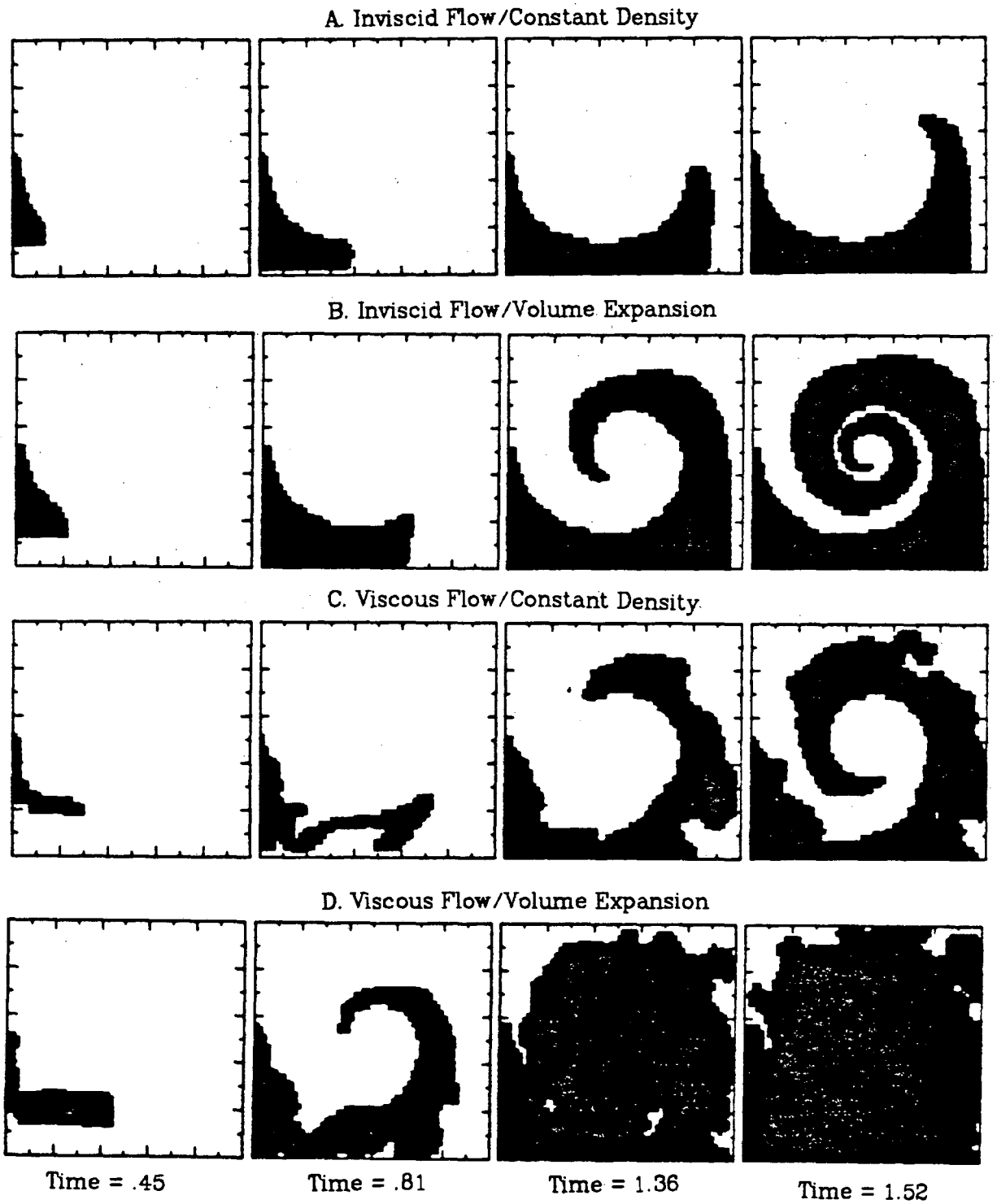


Figure 2: Swirling Fluid

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. In Figure 3, we illustrate these comments by plotting the percentage of the volume burnt as a function of time elapsed since ignition.

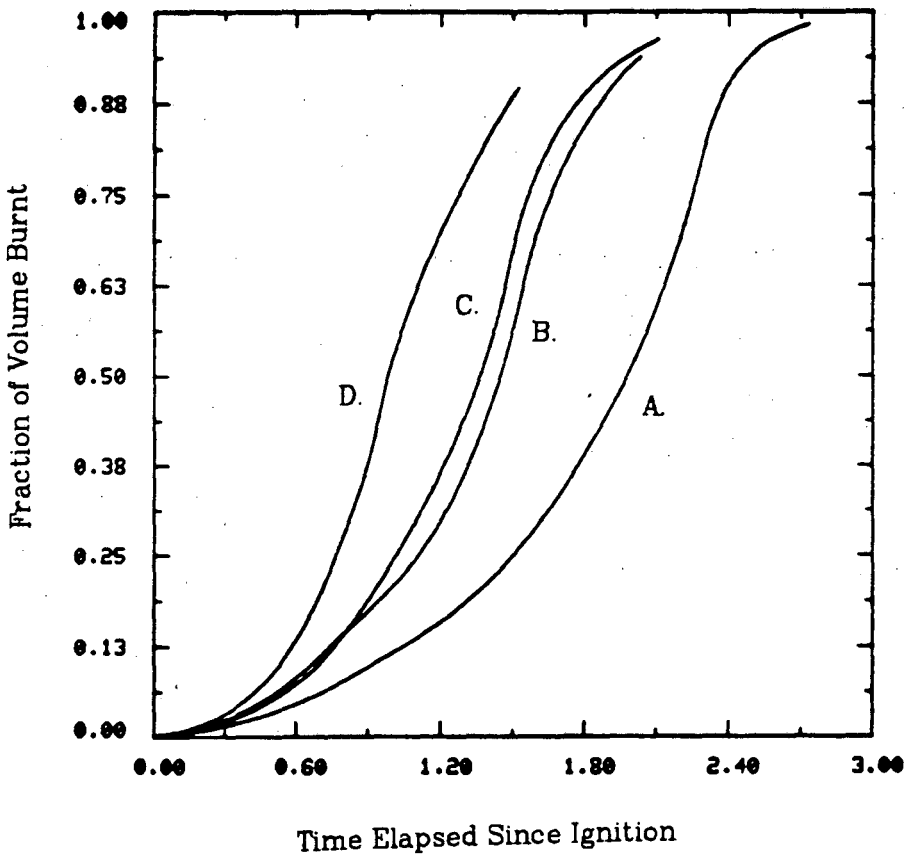


Figure 3

REFERENCES

1. Frankel, M.L., and Sivashinsky, G.I., "The Effect of Viscosity on Hydrodynamic Stability of a Plane Flame Front", Combustion and Science Technology, Vol. 29, pp.207-224.
2. Markstein, G.H., Nonsteady Flame Propagation, Pergammon Press, MacMillan and Company, New York, 1964.
3. Sivashinsky, G.I., "Instabilities, Pattern Formation, and Turbulence in Flames", to appear.
4. Chorin, A.J., "Numerical Studies of Slightly Viscous Flow", Journal of Fluid Mechanics, Vol. 57, 1973, pp. 785-796
5. Cheer, A.Y. "A Study of Incompressible 2-D Vortex Flow Past A Circular Cylinder" Lawrence Berkeley Laboratory, LBL-9950, 1979, to appear in Siam Journal of Scientific and Statistical Computing, 1983.
6. McCracken, M.F. and Peskin, C.S., "A Vortex Method For Blood Flow Through Heart Valves", Journal of Computational Physics, Vol.35, 1980, p.183-205.
7. Ghoniem, A.F., Chorin, A.J., Oppenheim, A.K. "Numerical Modeling of Turbulent Flow in A Combustion Tunnel", Philosophical Transactions of the Royal Society of London, Vol. 304, 1982, pp. 303-325.
8. Sethian, J.A. "Turbulent Combustion in Open and Closed Vessels", Lawrence Berkeley Laboratory, LBL-15744, 1983, to appear in the Journal of Computational Physics.
9. 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.
10. Majda, A., "Equations of Low Mach Number Combustion", Center for Pure and Applied Mathematics, University of Cal., Berkeley, 1982, to appear, SIAM Jour.of Appl. Math.
11. Kurylo, J., Dwyer,H.A., and Oppenheim, A.K., "Numerical Analysis of Flow Fields Generated by Accelerated Flames", AIAA J., Vol.18, 1980, pp.302-308.
12. Sethian, J.A. "An Analysis of Flame Propagation", Lawrence Berkeley Laboratory, LBL-14125, 1982
13 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.
14. Chorin, A.J., "Flame Advection and Propagation Algorithms", Journal of Computational Physics, Vol.35, 1980, pp.1-11

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.

Reference to a company or product name does not imply approval or recommendation of the product by the University of California or the U.S. Department of Energy to the exclusion of others that may be suitable.

TECHNICAL INFORMATION DEPARTMENT
LAWRENCE BERKELEY LABORATORY
UNIVERSITY OF CALIFORNIA
BERKELEY, CALIFORNIA 94720