AIAA 95-1720

A Multi-Fluid Algorithm for Compressible, Reacting Flow

John B. Bell
Phillip Colella
Jeffrey A. Greenough
Daniel L. Marcus

Lawrence Livermore National Laboratory
Livermore, CA 94551

12th AIAA Computational Fluid Dynamics Conference
June 19-22, 1995 / San Diego, CA

A MULTI-FLUID ALGORITHM FOR COMPRESSIBLE, REACTING FLOW*

John B. Bell, Phillip Colella, Jeffrey A. Greenough, and Daniel L. Marcus †
Center for Computational Sciences and Engineering
Lawrence Livermore National Laboratory
Livermore, CA 94551

Abstract

We present an alghorithm for the solution of compressible, reacting flow problems in which burned and unburned fluids are thermodynamically distinct and separated by a thin flame. We use a higher-order, adaptive Godunov method for the fluid dynamics and the motion of the flame front normal to itself, and a thermodynamically consistent representation of burned and unburned components to represent the effect of burning. Results of one-dimensional and two-dimensional calculations are presented.

Introduction

This paper is concerned with the solution of compressible, reacting flow problems in which burned and unburned fluid are treated as thermodynamically distinct materials separated by a thin reaction zone. The dynamics of the flame is specified by a flame speed model which determines flame speed from the thermodyanmic state of the unburned fluid. The burned and unburned fluids are represented using a volume-of-fluid representation for the thermodynamic quantities. In particular, for each zone in the computational mesh we let ρ^α, e^α, and f^α represent density, internal energy, and volume fraction occupied by fluid α, where $\alpha = B, U$ denotes burned and unburned, respectively.

The fluid dynamical aspect of the flow is modeled using a high-resolution upwind finite difference method based on the formulation of Colella et al. [1]. In this approach the fluid is advanced under the assumption of local pressure equilibrium and a single velocity in each cell. The motion of the flame in this presentation takes the form of an eikonal equation for the volume fraction which is also solved using a higher-order upwind scheme. Consistent with the assumption of local pressure equilibrium, we restrict the algorithm to relatively low-Mach number flow regimes. Even so, the pressure equilibrium assumption is sometimes violated. In these situations, as in [1], we use a relaxation scheme to restore pressure equilibrium in multifluid cells.

Governing equations

A system of PDE's consistent with the above assumptions is the following:

$$\frac{D}{Dt}(\rho^\alpha f^\alpha) + \rho^\alpha f^\alpha \nabla \cdot U = \dot{M}^\alpha \qquad (1)$$

*This work was performed under the auspices of the U.S. Department of Energy by the Lawrence Livermore National Laboratory under contract W-7405-Eng-48. Support under contract W-7405-Eng-48 was provided by the Applied Mathematical Sciences Program and the HPCC Grand Challenge Program of the Office of Scientific Computing at DOE and by the Defense Nuclear Agency under IACRO 94-831. Prof. Colella was supported at UC Berkeley by DARPA and the National Science Foundation under grant DMS-8919074; and by a National Science Foundation Presidential Young Investigator award under grant ACS-8958522; and by the Department of Energy High Performance Computing and Communications Program under grant DE-FGO3-92ER25140.

†Member, AIAA

$$\frac{DU}{Dt} + \frac{1}{\hat{\rho}}\nabla p = 0 \quad (2)$$

$$\frac{De^\alpha}{Dt} + p\frac{D}{Dt}(\frac{1}{\rho^\alpha}) = 0 \quad (3)$$

$$p^\alpha = p^\alpha(\rho^\alpha, e^\alpha) \quad (4)$$

$$p^\alpha(x,t) = p(x,t) \quad (5)$$

$$\sum_\alpha f^\alpha = 1 \quad (6)$$

where

$$\hat{\rho} = \sum_\alpha \rho^\alpha f^\alpha$$

In these equations $\dot{M}^\alpha$ represents the transport of mass across the front, Equations (1) - (3) are conservation laws for mass, momentum, and energy. Equation (4) is an equation of state for each component. Equation (5) represents our local pressure equilibrium assumption.

The solution procedure is a fractional step scheme. It consists of a multi-fluid integration step, alternated with a step to advance the flame front. In flame advancement step the flame is moved normal to itself by solving an eikonal equation with speed determined by the local flame speed (see below). An update to the burned and unburned fluid states is then specified from the volume of fluid that is "burned" during the flame advance.

More precisely, at the flame front the eikonal solution determines δf^B, the volume of fluid that is converted from unburned to burned in each cell. By relating δf^B to the change in mass of burned material $\dot{M}^\alpha$ in a thermodynamically consistent way, we obtain

$$\delta f^B := \Delta t \dot{M}^B(\frac{1}{\bar{\rho}^B} - \frac{f^B Q}{\Gamma^B}) \quad (7)$$

where

$$Q = \hat{\Gamma}(\frac{1}{\bar{\rho}^B} - \frac{1}{\rho^U})$$

This equation is used to determine $\dot{M}^\alpha$. To maintain thermodynamic consistency, the thermodynamic state of the burned material on the right hand side of (7) is defined using jump relations combined with the constant pressure assumption. Thus, for the update we use

$$\bar{\rho}^B = \frac{\frac{\Gamma^B}{\Gamma^B - 1}p}{h^B}$$

and

$$\bar{e}^B = e^U + p(1/\rho^U - 1/\bar{\rho}^B) + q_0$$

where q_0 is the chemical energy in the unburned fluid and h^B is the enthalpy in the burned fluid given by

$$h^B = h^U \equiv e^U + p/\rho^U + q_0$$

By using these definition and noting that from conservation of mass $\dot{M}^B = -\dot{M}^U$, the thermodnamic updates for mass and energy of burned and unburned material are given by

$$\rho^B f^B := \rho^B f^B + \Delta t \dot{M}^B \quad (8)$$

$$\rho^U f^U := \rho^U f^U + \Delta t \dot{M}^U \quad (9)$$

$$\rho^B f^B e^B := \rho^B f^B e^B + \Delta t \dot{M}^B(\bar{e}^B + \frac{U \cdot U}{2} + \frac{f^B p Q}{\Gamma^B}) \quad (10)$$

$$\rho^U f^U e^U := \rho^U f^U e^U + \Delta t \dot{M}^U(e^U + \frac{U \cdot U}{2} + \frac{f^U p Q}{\Gamma^U}) \quad (11)$$

Note that the transfer of energy across the flame front is treated implicitly through the definition of $\bar{\rho}^B$ and $\bar{e}^B$.

Results

Eikonal equation

In order to demonstrate the part of the algorithm that consists of a solution to the eikonal equation

$$\frac{\partial \phi}{\partial t} + s|\nabla \phi| = 0$$

we solve this equation for a simple test problem. The initial conditions are $\phi = 1$ inside a square centered at the origin and $\phi = 0$ everywhere else. The speed $s = 1$, and the

resolution is 100^2 zones. Figure 1 shows the calculation at $t = 0$, $t = 0.9$, and $t = 1.8$. The front "burns out" as expected, smoothing the corners of the square.

One-dimensional deflagration

We next apply the full algorithm to a one-dimensional deflagration problem [2, 6]. The calculation is carried out on $x \in [0, 1.6]$ with 800 zones. The left boundary is a reflecting wall and the right boundary is open. The time step is determined by the CFL condition.

Unburned: $(x < 0.75$ and $x > 0.81), p = 1.0, \rho = 1.0, u = 0.0$.

Burned: $(0.75 < x < 0.81); p = 1.4072, \rho = 0.2082, u = 0.0$.

The flame speed relative to the fluid is given by

$$s = k(\frac{p_0}{\rho_0})^q$$

Here, p_0 and ρ_0 are taken from the unburned state, k = 0.095, and q = 2.0.

The results are shown in an x-t diagram in Figure 2. Only $x \in [0, 0.8]$ is shown. We see the shocks moving to the left and right, followed by the deflagration. The left-moving shock reflects off the wall, decelerating the left-moving flame and overtaking and slightly acelerating the right-moving flame.

Two dimensional deflagration with adaptive refinement

Here we examine flame propagation in a closed duct. When initiated by a spark at one end of the duct, this configuration is expected to evovle an inverted cusp, the characteristic "tulip" shape [7, 8].

We implement the flame capturing algorithm described above in conjunction with a multi-fluid adaptive mesh refinement code [5] that selectively refines regions of the grid that require high resolution. This procedure uses a hierachically nested sequence of logically rectangular grids upon which the solution is recursively calculated untuil the desired degree of acuracy is achieved. This proceudre has been highly effective in shock physics calculations, where steep gradients move through the flow domain, and has been shown to be one to two orders of magnitude more efficient than equivalent calculations on a uniform grid [4, 3]

We begin with a base grid of 160 x 16 zones, and alow a single level of refinement by a factor of two. A "spark" of burned material is placed at the end of a closed tube according to the following conditions:

Unburned: $p = 1.0, \rho = 1.0, u = 0.0$.

Burned: $p = 0.9449, \rho = 0.1407, u = 0.0$.

Figures 3-9 show the evolution of the flow; we plot pressure, volume fraction, energy density, and density of burned material, and density of unburned material. As the flame propagates down down the tube, the characteristic tulip shape is clearly evident. The pressure field exhibits a complex system of interacting waves and a high-pressure region ahead of the flame front.

References

[1] P.Colella, H.M. Glaz, R. Ferguson, "Multifluid algorithms for Eulerian finite-difference methods," submitted to *J. Comp. Phys.*

[2] J. Hilditch and P. Colella, "A front tracking method for compressible flames in one dimension" to appear *SIAM J. Sci. Comp.*

[3] J. B. Bell, M. Berger, J. Saltzman, and M. Welcome, "Three dimensional adaptive mesh refinement for hyperbolic conservation laws," *SIAM J. Sci. Stat. Comput.* ,**15**(1), 127-138, 1994.

[4] M.J. Berger and P. Colella, "Local adaptive mesh refinement for shock hydrodynamics." *J. Comp. Phys.*, **82**, 64-84, 1989.

[5] J.S. Greenough, V. Beckner, R.B. Pember, W.Y. Crutchfield, J.B. Bell, P. Colella, "An adaptive, multifluid, interface-capturing method for compressible flow in complex geometries,"

26th AIAA Fluid Dynamics Conference, San Diego, CA, June 19-22, 1995.

[6] Z. Teng, A.J. Chorin, and T. Liu, "A Riemann problem for reacting gases," *SIAM J. Appl. Math.* 1982.

[7] D. Dunn-Rankin, P.K. Barr, R.F. Sawyer, "Numerical and experimental study of "tulip"flame formation in a closed vessel," Twenty-First International Symposium on Combustion, 1986, 1291-1301.

[8] M. Gonzales, R. Borghi, A. Saouab, "Interaction of a flame front with its self-generated flow in an enclosure: the "tulip-flame" phenomenon," Combust. Flame, 88, 201-220, 1992.

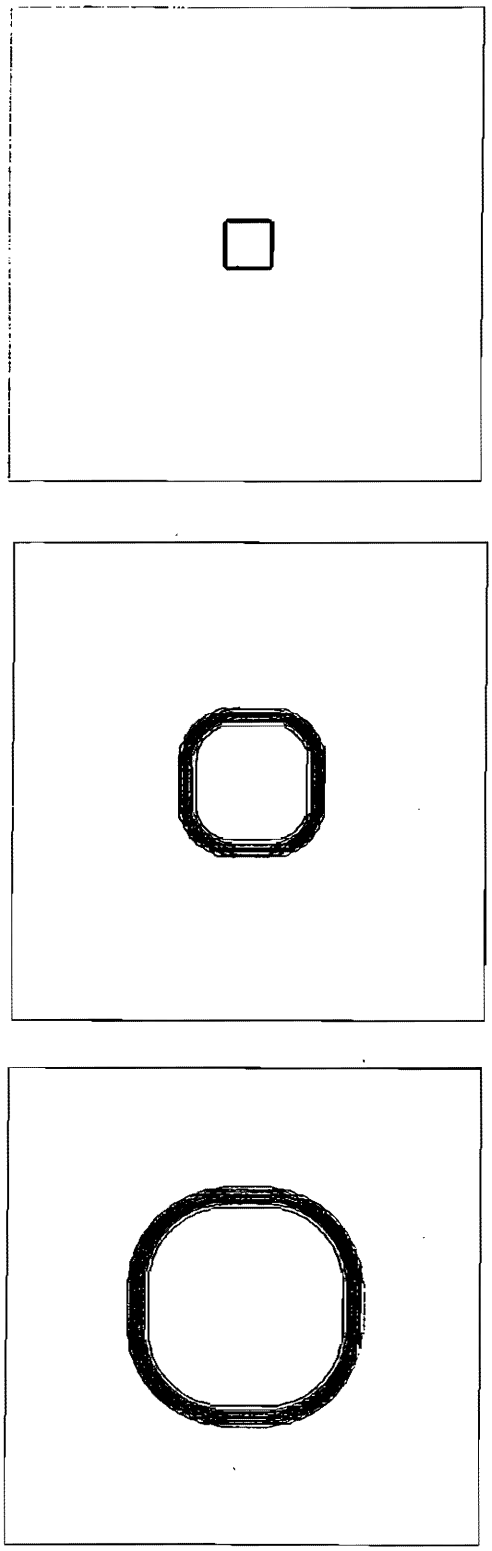


Figure 1. Numerical solution of eikonal equation

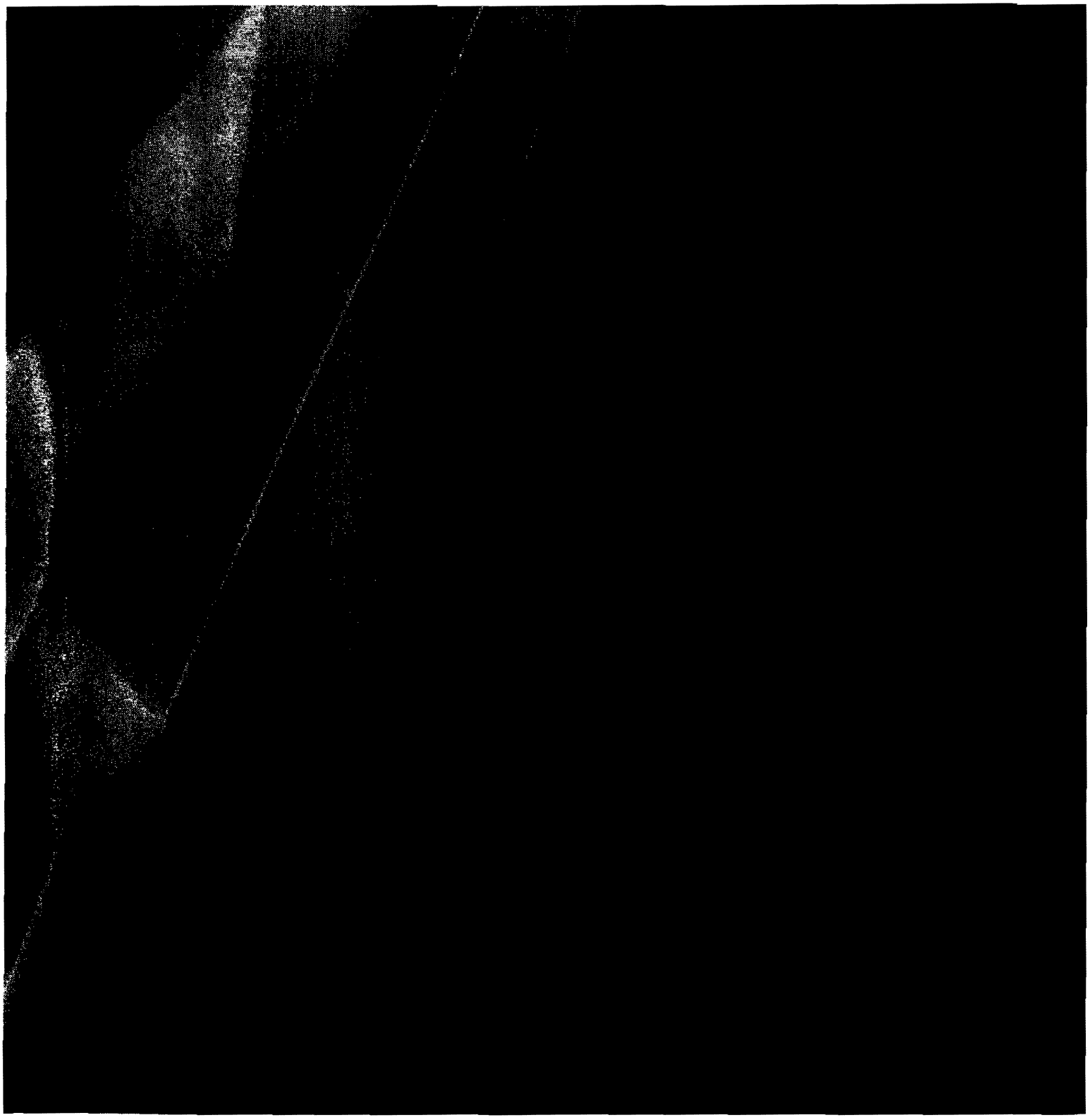


Figure 2. Pressure vs. time for one-dimensional deflagration.

Time = 0.004

Pressure

Volume fraction (burned)

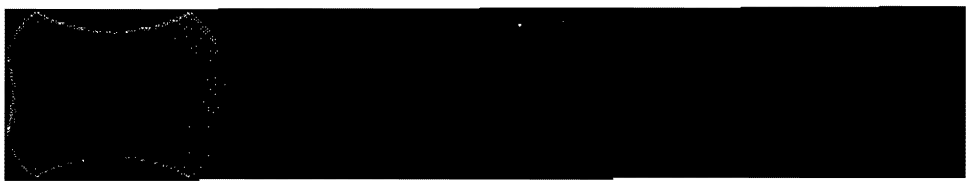
Energy density (burned)

Density (burned)

Density (unburned)

Figure 3. Flame propagation down a closed duct; t = 0.004.

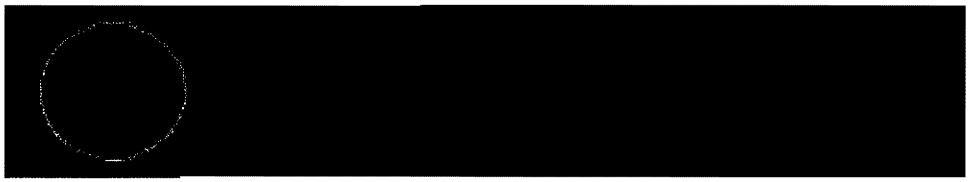
Time = 0.130



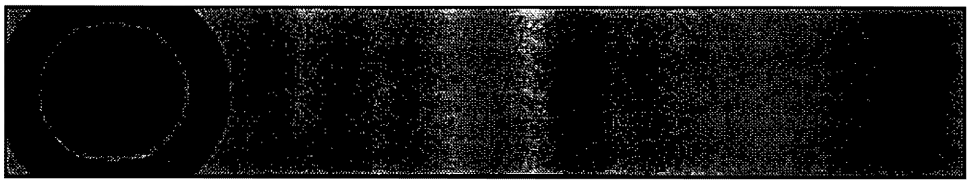
Pressure

Volume fraction (burned)

Energy density (burned)



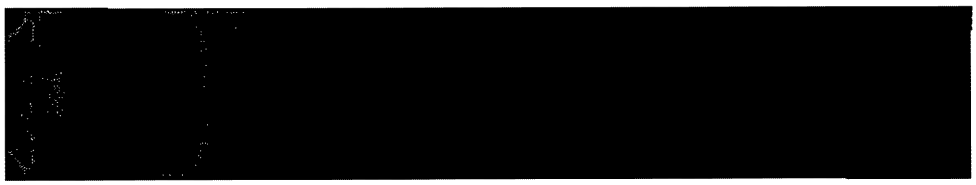
Density (burned)



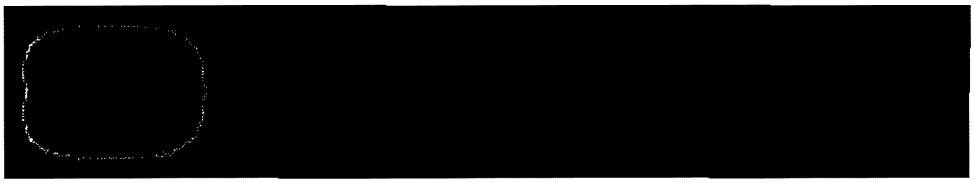
Density (unburned)

Figure 4. Flame propagation down a closed duct; t = 0.130.

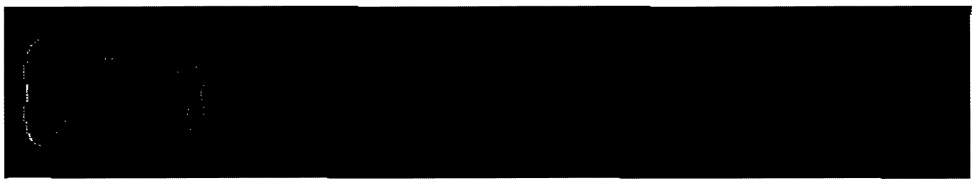
Time = 0.185



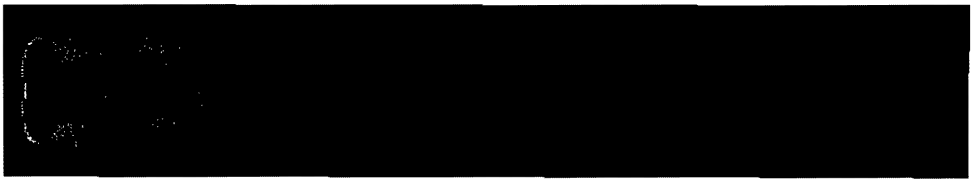
Pressure



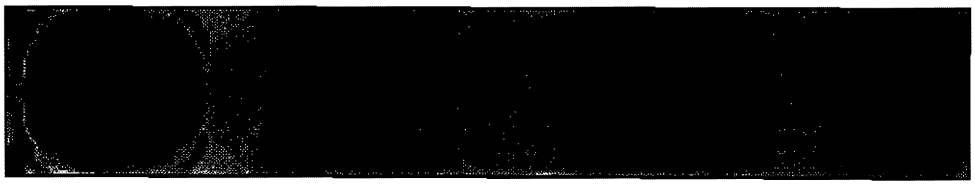
Volume fraction (burned)



Energy density (burned)



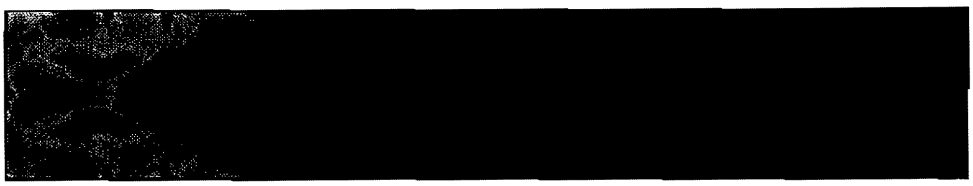
Density (burned)



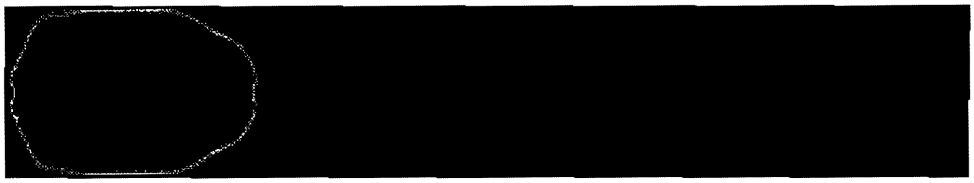
Density (unburned)

Figure 5. Flame propagation down a closed duct; t = 0.185.

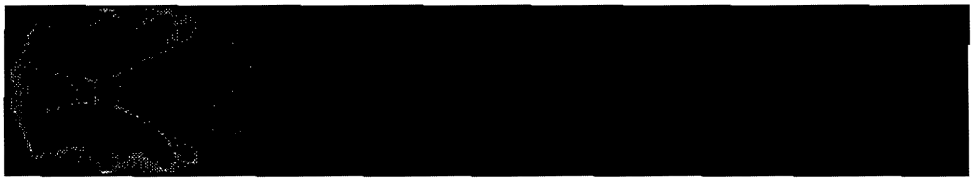
Time = 0.265



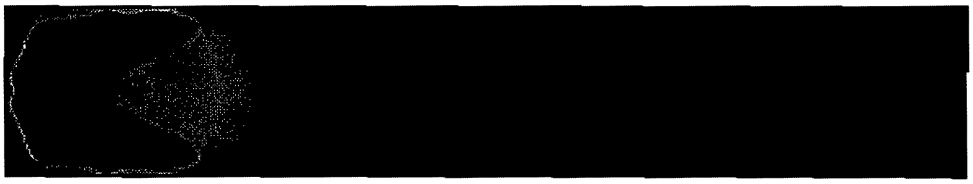
Pressure



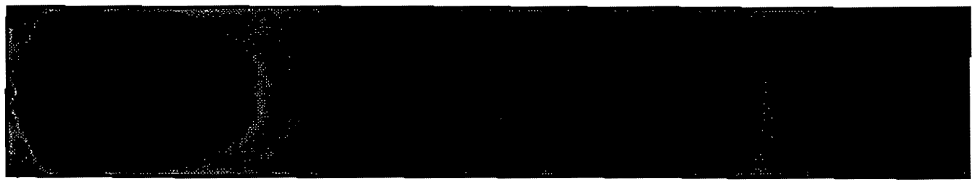
Volume fraction (burned)



Energy density (burned)



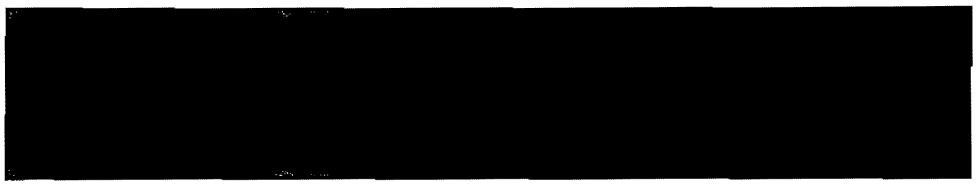
Density (burned)



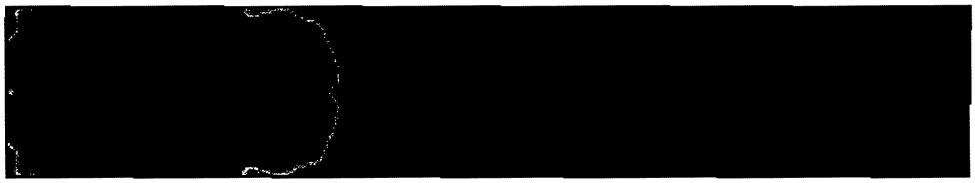
Density (unburned)

Figure 6. Flame propagation down a closed duct; t = 0.265.

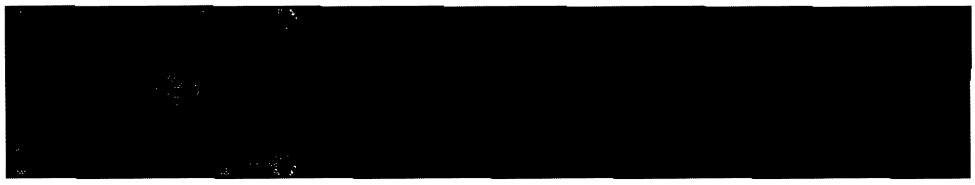
Time = 0.363



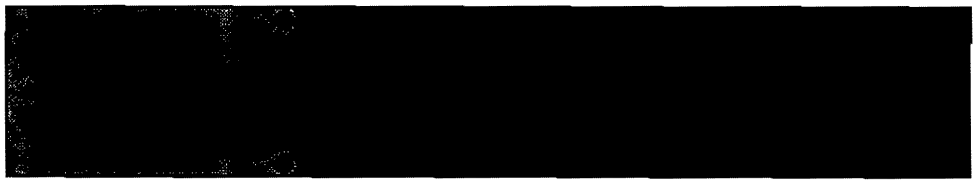
Pressure



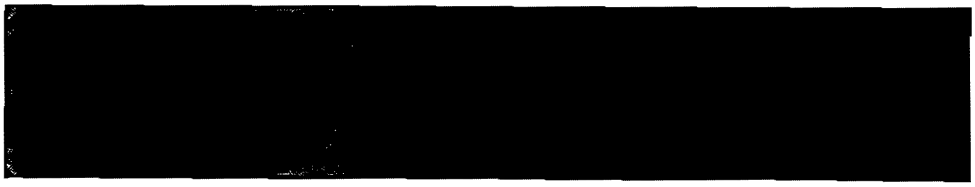
Volume fraction (burned)



Energy density (burned)



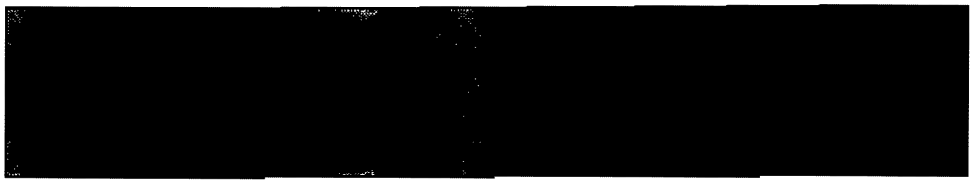
Density (burned)



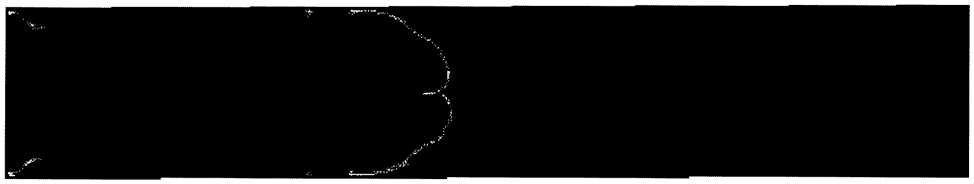
Density (unburned)

Figure 7. Flame propagation down a closed duct; t = 0.363.

Time = 0.450

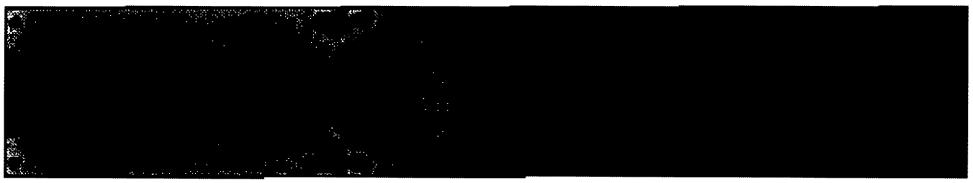


Pressure

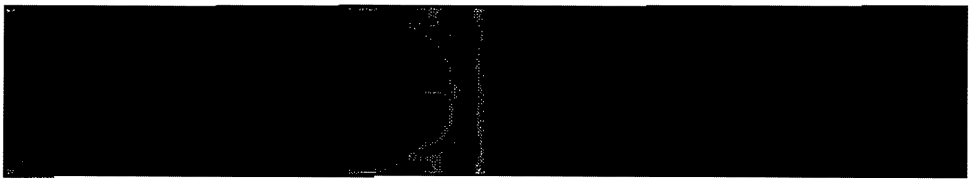


Volume fraction (burned)

Energy density (burned)



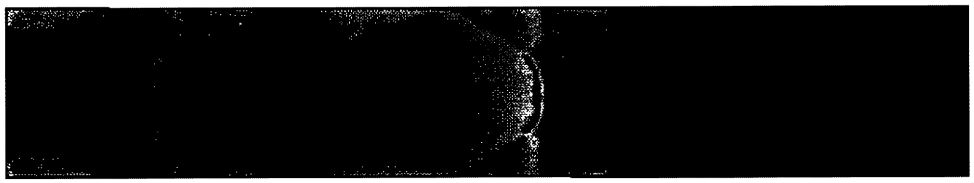
Density (burned)



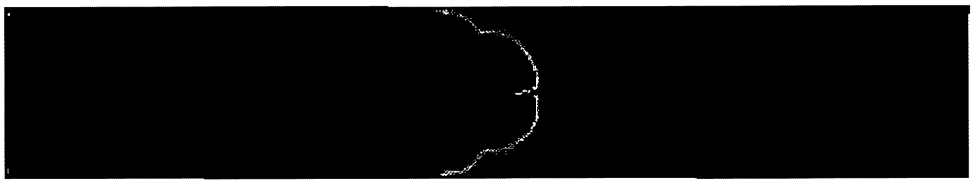
Density (unburned)

Figure 8. Flame propagation down a closed duct; t = 0.450.

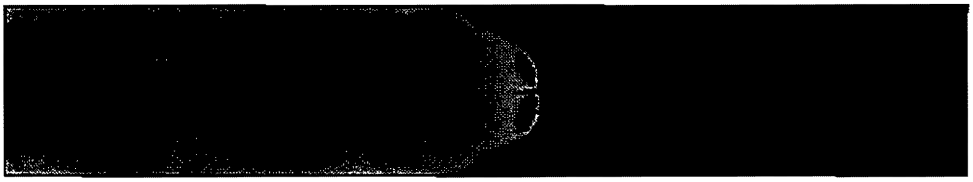
Time = 0.530



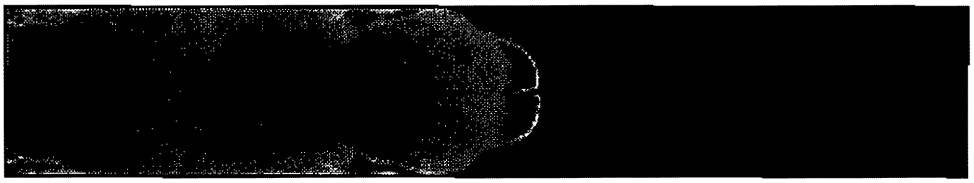
Pressure



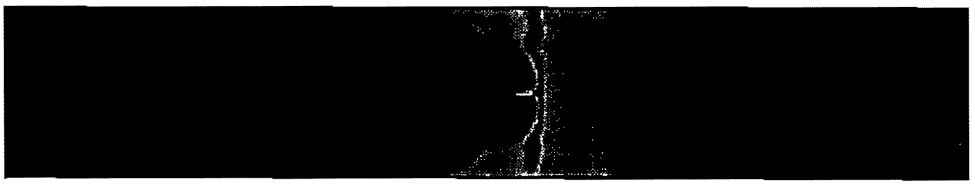
Volume fraction (burned)



Energy density (burned)



Density (burned)



Density (unburned)

Figure 9. Flame propagation down a closed duct; t = 0.530.