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NUMERICAL MODELING OF THE KINEMATICS
OF TURBULENT MIXING IN HE-DRIVEN
BLAST WAVES

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US ARMY ARMAMENT RESEARCH AND DEVELOPMENT COMMAND
BALLISTIC RESEARCH LABORATORY
ABERDEEN PROVING GROUND, MARYLAND

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model does indeed generate turbulent mixing near the contact surface and nowhere else in the flow field. The magnitude of the turbulence depends on the turbulence model parameters, particularly the Rayleigh-Taylor coefficient, C_3 , and the viscosity coefficient, C_4 . Appropriate values for these parameters should be established by comparing the results of parametric calculations with experimental data.

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I. INTRODUCTION

Considered here is the theoretical modeling of turbulent mixing at density discontinuities in nonsteady compressible flows. It is well known that if a density discontinuity (or a strong density gradient) occurs in a pressure gradient of the opposite sign, then the flow field is hydrodynamically unstable in the Rayleigh-Taylor sense (Taylor, 1950).¹ Small perturbations occurring in such a region will amplify with time, and if the perturbations become large enough, they can lead to a local breakdown in the well-ordered flow; i.e., they can lead to turbulence.

One of the more interesting examples of density gradients working against pressure gradients to cause instabilities occurs in blast waves driven by solid high explosives (HE).^{*} After the detonation wave breaks out of the charge, the HE combustion gases expand to a high velocity (~ 6 km/s), pushing an air shock ahead. From one-dimensional inviscid calculations of this problem (Brode, 1957),² we know that a positive pressure gradient is formed throughout the flow field. Such calculations also indicate that there is a large density jump (ρ_{HE}/ρ_{air} can be as large as 70) across the contact surface. However, from high-speed photography of HE experiments, we know that this contact surface (which theoretically should be smooth) actually develops an irregular shape indicating the growth of instabilities. Evidence of mixing at the contact surface can be inferred from test results which show that the HE gases react with the shocked ambient gases and release

^{*} Similar gradients can occur in "shock-tube-type" flows driven by gases at very large initial densities.

1. Sir G. I. Taylor (1950), "Instability of Liquid Surfaces when Accelerated in a Direction Perpendicular to Their Plane," *Proceedings of the Royal Society (London)*, A201, pp. 192-196.
2. H. L. Brode (1957), A Calculation of the Blast Wave from a Spherical Charge of TNT, Rand Corporation, RM-1965.

heat (i.e., afterburn) if the ambient gases contain oxygen (Matle, 1959, and Filler, 1956)^{3,4}. Since this heat release can be of the same order as the energy released by the detonation wave (e.g., for TNT postdetonation energy release is about 2.5 times the detonation energy), it will affect the blast wave flow field and must be taken into account for accurate numerical simulations of such flows.

This report describes the numerical work that RDA has performed to simulate the kinematics* of the turbulent mixing associated with such HE-driven blast waves. A k- ϵ turbulence model was programmed and combined with RDA's minimal-diffusion Flux-Corrected Transport (FCT) module which solves the gas dynamic conservation laws on a sliding grid. Source terms were included in the k- ϵ equations to model the above-described Rayleigh-Taylor mechanism to generate turbulence. The governing equations are described in Section II. Preliminary numerical studies (as described in Section III) indicate that this model does, indeed, generate turbulent kinetic energy at the HE/air interface of HE-driven blast waves. Conclusions and recommendations are offered in Section IV.

* Energetics (i.e., heat release) was neglected for the preliminary work.

3. C. C. Matle (1959), The Contribution of Afterburning to the Air Blast from Explosives, NAVORD Report 6234.
4. W. S. Filler (1956), "Post-Detonation Pressure and Thermal Studies of Solid Explosives in a Closed Chamber," Sixth (Int) Symposium on Combustion, pp. 648-657.

II. FORMULATION

The time evolution of the mean flow is governed by the conservation of mass, momentum and energy which may be written as follows for point ($j=2$), line ($j=1$), or plane ($j=0$) symmetric flow:

$$\frac{\partial}{\partial t} \rho + \frac{1}{r^j} \frac{\partial}{\partial r} (r^j \rho u) = 0 \quad (1)$$

$$\frac{\partial}{\partial t} (\rho u) + \frac{1}{r^j} \frac{\partial}{\partial r} (r^j \rho u^2) = -\frac{\partial}{\partial r} \left(p + \frac{2}{3} \rho k \right) \quad (2)$$

$$\begin{aligned} \frac{\partial}{\partial t} (\rho E) + \frac{1}{r^j} \frac{\partial}{\partial r} (r^j \rho u E) = & -\frac{1}{r^j} \frac{\partial}{\partial r} r^j u \left(p + \frac{2}{3} \rho k \right) \\ & + \frac{1}{r^j} \frac{\partial}{\partial r} r^j \mu_T \left(\frac{1}{\sigma_{t,h}} \frac{\partial h}{\partial r} + \frac{1}{\sigma_{t,k}} \frac{\partial k}{\partial r} \right) + \dot{Q} \end{aligned} \quad (3)$$

where mass-averaged properties of the mixture are

ρ = density
 u = velocity
 E = total energy = $e + \frac{1}{2} u^2 + k$
 e = internal energy
 p = pressure
 $\dot{Q}$ = rate of energy release per unit volume
 h = enthalpy

and the turbulence parameters are

k = turbulence kinetic energy per unit mass
 $\sigma_{T,\beta}$ = turbulent Prandtl number for the variable β
 μ_T = total viscosity = $\mu_f + C_\mu \rho k^2 / \epsilon$
 μ_f = molecular viscosity

For a mixture of N component gases, one must solve $N-1$ species transport equations in addition to the mass conservation law for the mixture (Eq. 1). The species transport equations have the form

$$\frac{\partial}{\partial t} \rho f_a + \frac{1}{r^j} \frac{\partial}{\partial r} (r^j \rho f_a u) = \frac{1}{r^j} \frac{\partial}{\partial r} \left(r^j \frac{\mu_T}{\sigma_{t,f}} \frac{\partial f_a}{\partial r} \right) + \dot{S}_a \quad (4)$$

where f_α = mass-averaged, mass fraction of component α
 $\approx \rho_\alpha / \rho$ (while $\sum_\alpha f_\alpha = 1$)

$\dot{S}_\alpha$ = rate of creation of component α (with $\sum_\alpha \dot{S}_\alpha = 0$)

As shown by Issa (1980),⁵ a one-dimensional k- ϵ turbulence model can be used to simulate turbulent mixing driven by the Rayleigh-Taylor mechanism. The transport equations for the turbulence kinetic energy, k, and the turbulence kinetic energy dissipation rate, ϵ , acquire the following form:

$$\frac{\partial}{\partial t} (\rho k) + \frac{1}{r^j} \frac{\partial}{\partial r} (r^j \rho k u) = \frac{1}{r^j} \frac{\partial}{\partial r} \left(r^j \frac{\mu_t}{\sigma_{t,k}} \frac{\partial k}{\partial r} \right) + G - \rho \epsilon \quad (5)$$

$$\frac{\partial}{\partial t} (\rho \epsilon) + \frac{1}{r^j} \frac{\partial}{\partial r} (r^j \rho \epsilon u) = \frac{1}{r^j} \frac{\partial}{\partial r} \left(r^j \frac{\mu_t}{\sigma_{t,\epsilon}} \frac{\partial \epsilon}{\partial r} \right) + C_1 G / k - C_2 \rho \epsilon^2 / k \quad (6)$$

where

$$G = -\frac{2}{3} \frac{k}{r^j} \frac{\partial}{\partial r} (r^j u) - C_3 \frac{\mu_t}{\rho} \frac{\partial \rho}{\partial r} \frac{\partial p}{\partial r} \quad (7)$$

Here G represents a source/sink for turbulence kinetic energy. The first term in G is proportional to the flow divergence and tends to kill turbulence in expanding flows. The second term is proportional to the product of the mean pressure and density gradients. When these gradients have opposite signs, then G can become positive. As will be shown, the pressure and density gradients do have such opposite signs near the contact surface of an HE-driven blast wave and turbulence indeed grows there. In other regions of the flow (e.g., at the shocks and in the rarefaction wave), the pressure and density gradients have similar signs and turbulence is suppressed.

5. R. I. Issa (1980), Modeling of Turbulent Mixing at Density Discontinuities in Nonsteady Compressible Flows, R & D Associates, RDA-TR-107605-001.

III. NUMERICAL STUDIES

The k-ε turbulence equations described in the previous section were programmed on the computer and incorporated into the one-dimensional hydrocode, RDAFCT. This code uses the FCT module labeled JPBFACT⁶ to solve general conservation laws on a sliding grid:

$$\frac{\partial}{\partial t} \int_{\delta A(t)} \underline{w} dA = - \oint_{\delta A(t)} \underline{w} (\vec{u} - \vec{u}_g) \cdot d\vec{A} + \oint_{\delta A(t)} \underline{\tau} dA \quad (8)$$

where $\underline{w} = (\rho, \vec{u}, pE, pf, \text{etc.})$ and the grid motion satisfies $dA(t) = \vec{u}_g(t) dA(t)$. The module is called successively for each conservation equation (i.e., Eqs. (1) to (6)) to advance the flow field one time step. NRL's newest transport, diffusion and antidiffusion coefficients are employed to give sixth-order phase and fourth-order amplitude properties for the numerical algorithm.

a. Initial conditions--As a test problem, we chose to simulate the evolution of the flow field associated with the detonation of a 1-lb spherical charge of PBX-9404 in air. Predetonation conditions for the charge were

$$R_C = 1.88973 \text{ cm}$$

$$\rho_C = 1.84 \text{ g/cm}^3$$

while the ambient air conditions were taken as

$$p_a = 1.01325 \times 10^6 \text{ dy/cm}^2$$

$$\rho_a = 1.225 \times 10^{-3} \text{ g/cm}^3$$

$$T_a = 288.4^\circ\text{K}$$

It was assumed that the charge was center-detonated. Initial conditions for the numerical calculations were taken at the instant the detonation wave reached the charge radius. It was assumed that the flow field corresponded to that of an ideal, Chapman-Jouquet (CJ) detonation wave; this field was obtained from subroutine CJDET which provides the similarity solution for any given explosive (Kuhl, 1978).⁷

6. J. P. Boris (1976), Flux-Corrected Transport Modules for Solving Generalized Continuity Equations, Naval Research Laboratory, Memorandum Report 3237.

7. A. L. Kuhl, M. R. Seizew (1978), Analysis of Ideal, Strong, Chapman-Jouquet Detonations, TRW Report 78.4735.9-13.

b. Equation-of-state--The detonation products were modeled by the Jones-Wilkins-Lee (JWL) equation-of-state (Dobratz, 1974)⁸ which provides the pressure as a function of density and internal energy in the form

$$p(\rho, e) = A \left(1 - \frac{\omega \rho}{R_1 \rho_0} \right) \exp(-R_1 \rho_0 / \rho) + B \left(1 - \frac{\omega \rho}{R_2 \rho_0} \right) \exp(-R_2 \rho_0 / \rho) + \omega p e \quad (9)$$

The JWL parameters for PBX-9404 are

$$\begin{aligned} A &= 8.545 \text{ Mbars} \\ B &= 0.20493 \text{ Mbars} \\ R_1 &= 4.60 \\ R_2 &= 1.35 \\ \omega &= \gamma - 1 = 0.25 \end{aligned}$$

while the CJ detonation parameters for this explosive are

$$\begin{aligned} p_{CJ} &= \rho_0 w_{CJ}^2 / (\Gamma + 1) = 370 \text{ kbars} \\ \rho_{CJ} &= \rho_0 (\Gamma + 1) / \Gamma = 2.485 \text{ g/cm}^3 \\ w_{CJ} &= 8.8 \text{ km/s} \\ u_{CJ} &= w_{CJ} / (\Gamma + 1) = 2.28 \text{ km/s} \\ q_{CJ} &= E_0 / \rho_0 = 5.543 \times 10^{10} \text{ erg/g} \\ \Gamma_{CJ} &= 2.85 \\ e_{CJ} &= q_{CJ} + 1/2 u_{CJ}^2 = 8.142 \times 10^{10} \text{ erg/g} \end{aligned}$$

Local thermodynamic equilibrium was assumed for the air. The pressure was related to the density and internal energy by an effective gamma:

$$p = (\gamma_e - 1) \rho e \quad (10)$$

where $\gamma_e = \gamma_e(\rho, e)$ was obtained from a table-lookup subroutine which uses Gilmore's data for real air (Gilmore, 1955).⁹ Two gas species were considered: air and detonation products. Computational cells containing air were initialized with $f=0$, while cells containing detonation products were initialized with $f=1$. A transport equation was then included for the species fraction f . In the present nonreactive case, f served

8. B. Dobratz (1974), Properties of Chemical Explosives and Explosive Simulants, Lawrence Livermore Laboratory Report UCRL-51319 Rev. 1.

9. F. R. Gilmore (1955), Equilibrium Composition and Thermodynamic Properties of Air to 24000°K, Rand Report RM-1543.

simply as a flag to discriminate which cells contained air and which cells contained HE. Pressures in mixed cells (where $0.1 < f < 0.9$) were blended according to Dalton's law. For the present study, heat release due to turbulent mixing near the HE/air interface was neglected ($\dot{S}_Q = 0$).

c. Results--As a baseline, we first performed an inviscid calculation of this HE-driven blast wave (i.e., $k = \epsilon = \mu_T = 0$). We found it necessary to use very fine zoning for this problem. The grid spacing was initialized as one tenth of one percent of the shock radius ($\Delta/R_S = .001$) in the outer region of the charge ($0.08 \leq r/R_S \leq 1.0$) yielding 200 cells, and then allowed to increase according to an interest rate formula ($0 < r/R_S < 0.8$) over 50 cells, with a grand total of 250 cells inside the charge. The cell containing the primary or outer shock front was moved with a velocity about equal to the instantaneous shock velocity, w_s , so that this shock remained approximately fixed in the grid. Cell interfaces inside the shock were assigned velocities linearly proportional to the radius:

$$(u_g)_{i+k} = w_s \cdot r_{i+k}/R_S \quad (11)$$

Note that this grid law produces a linear dilation of the grid, and hence preserves the initial mesh space distribution--a very useful attribute for this case. It keeps the cells packed where all the action is--near the contact surface and shock front!

Figures 1-8 show the inviscid flow field spatial distributions as calculated for this HE-driven blast wave at various instants in time, starting from the CJ detonation flow field (cycle 0) out at a point in time where the air shock has reached about two charge radii (cycle 800). Included near the bottom of each figure is the mesh distribution for the last displayed time. Note in particular the density distributions of Figure 1 which show a primary shock (S1), followed by a contact surface (CS), and then a secondary shock (S2). The latter is an inward-facing shock that is being swept outward by the supersonic flow. At later times, this secondary shock starts to move inward and eventually implodes.

Next, a turbulence calculation was performed. Initial conditions were taken as the flow field at the end on the aforementioned inviscid calculation for the following reasons:

- At this point the three discontinuities had separated from each other and were well resolved on the mesh.
- This allowed an accurate calculation of the pressure and density gradients which fed into the turbulence source term, G .

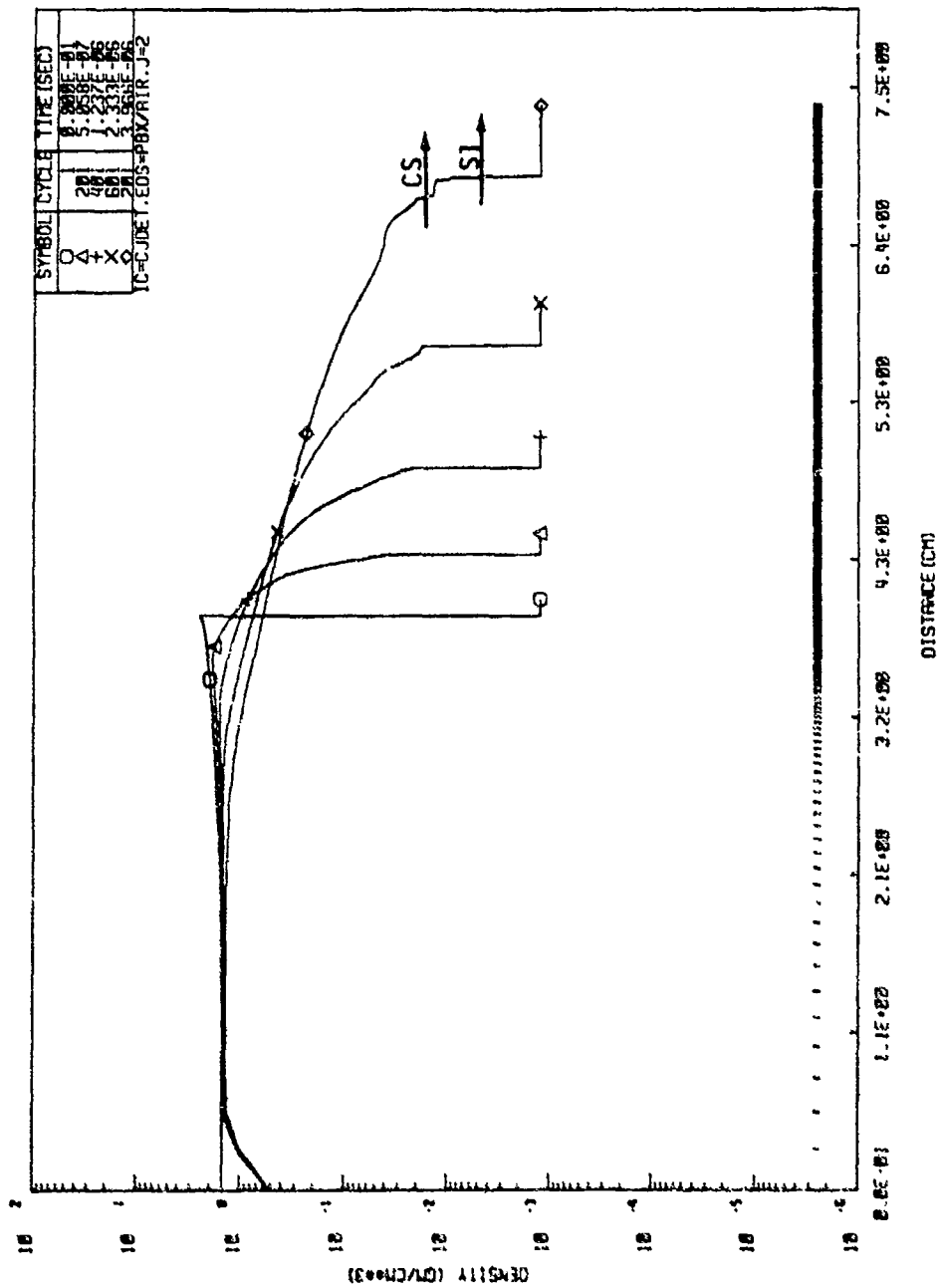


Figure 1. Spatial distribution of the density field at various times (inviscid FCT calculation of a 1-lb spherical PBX-9404 charge detonated in air).

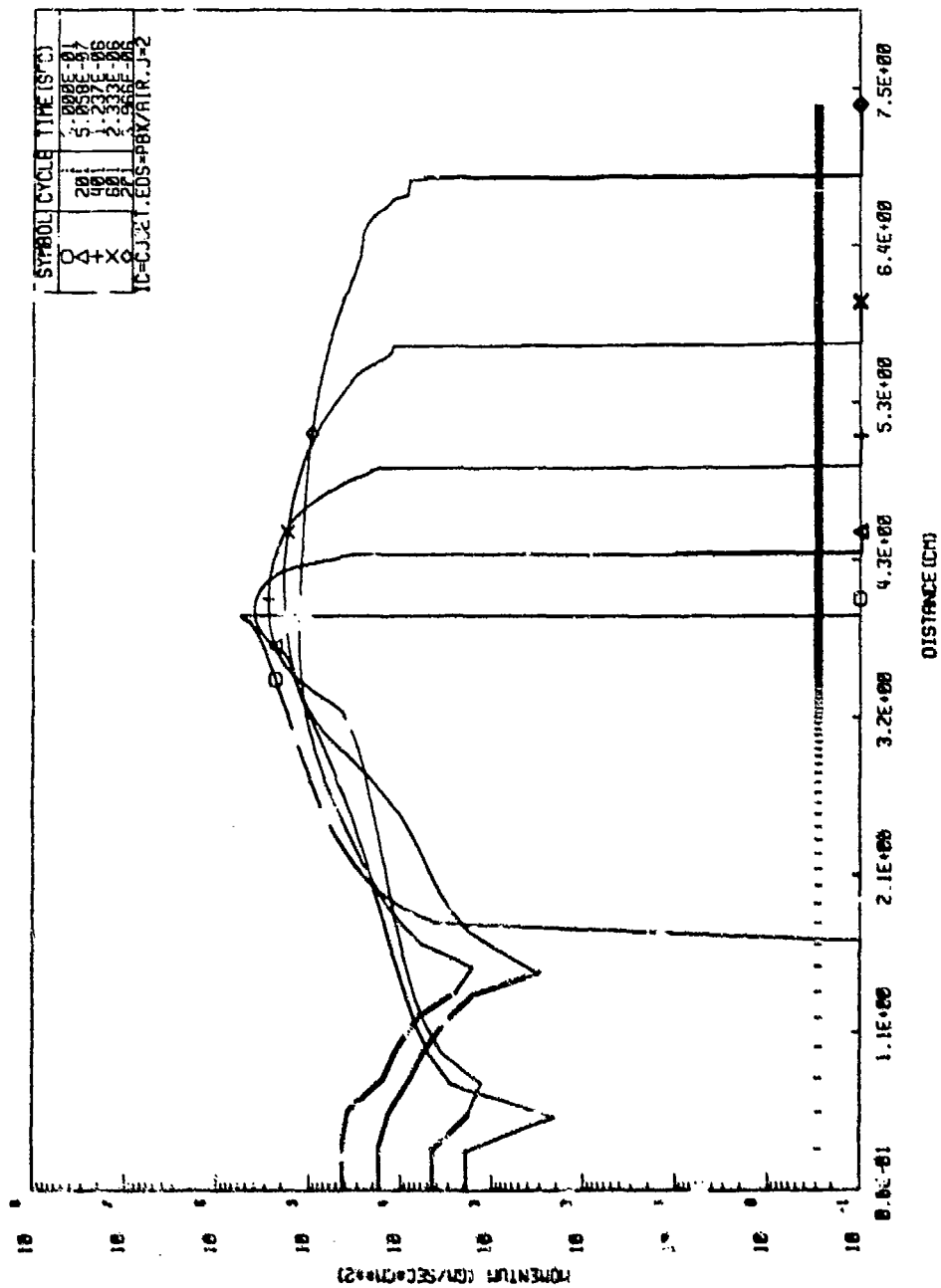


Figure 2. Spatial distribution of the momentum field at various times (inviscid FCT calculation of a 1-lb spherical PBX-9404 charge detonated in air).

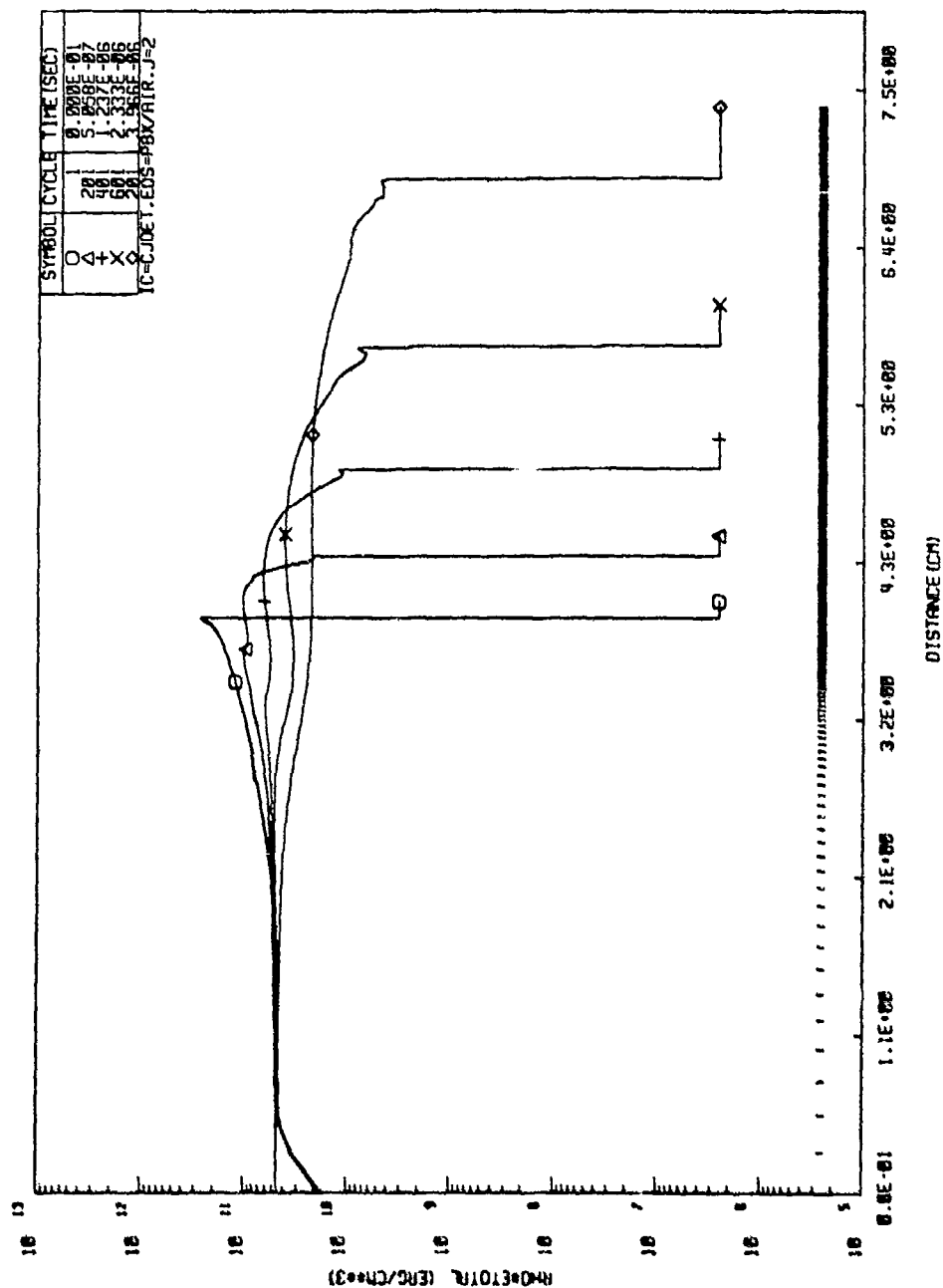


Figure 3. Spatial distribution of the total energy field at various times (inviscid FCT calculation of a 1-lb spherical PBX-9404 charge detonated in air).

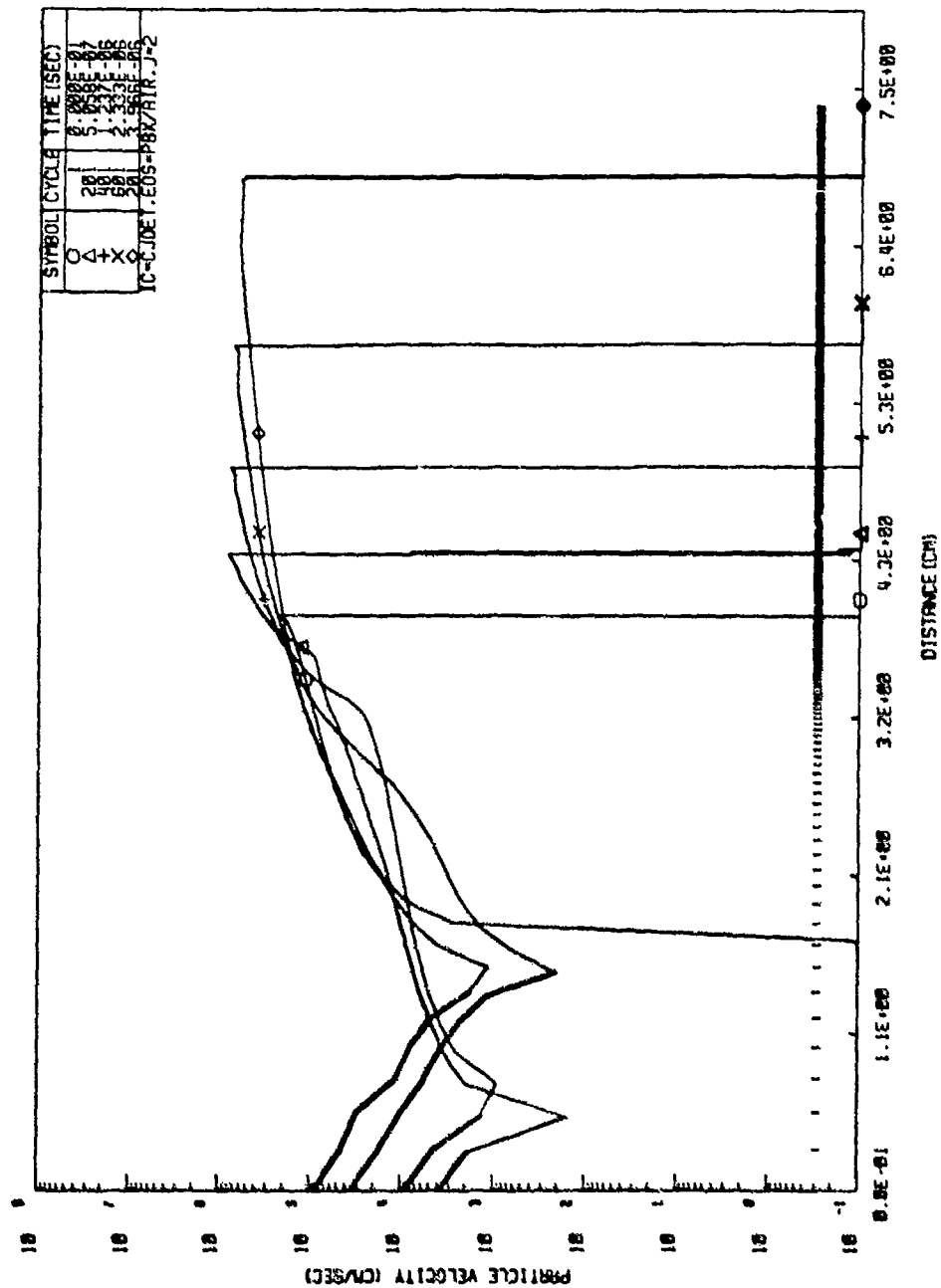


Figure 4. Spatial distribution of the velocity field at various times (inviscid FCT calculation of a 1-lb spherical PBX-9404 charge detonated in air).

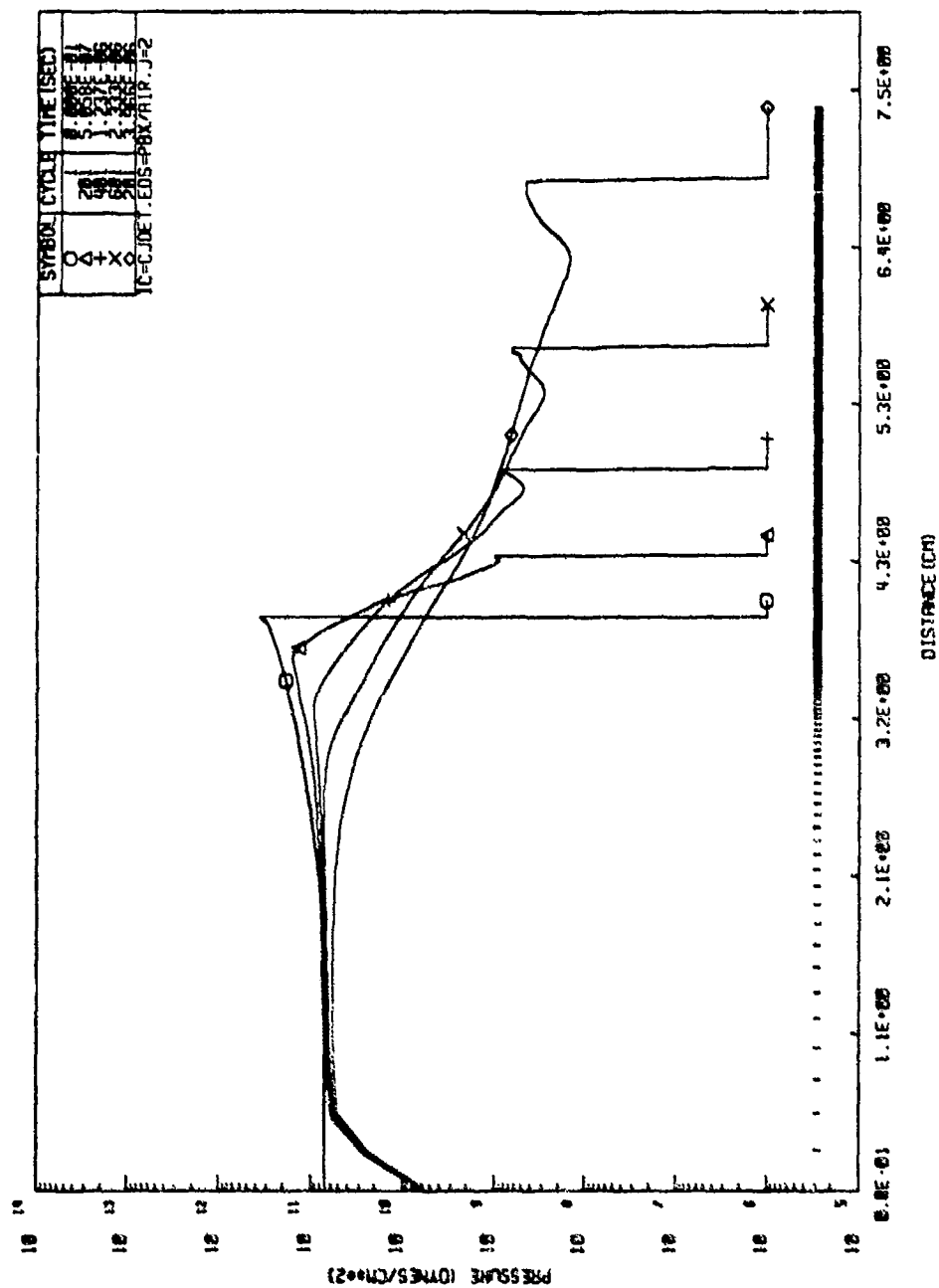


Figure 5. Spatial distribution of the pressure field at various times (inviscid PCT calculation of a 1-lb spherical PBX-9404 charge detonated in air).

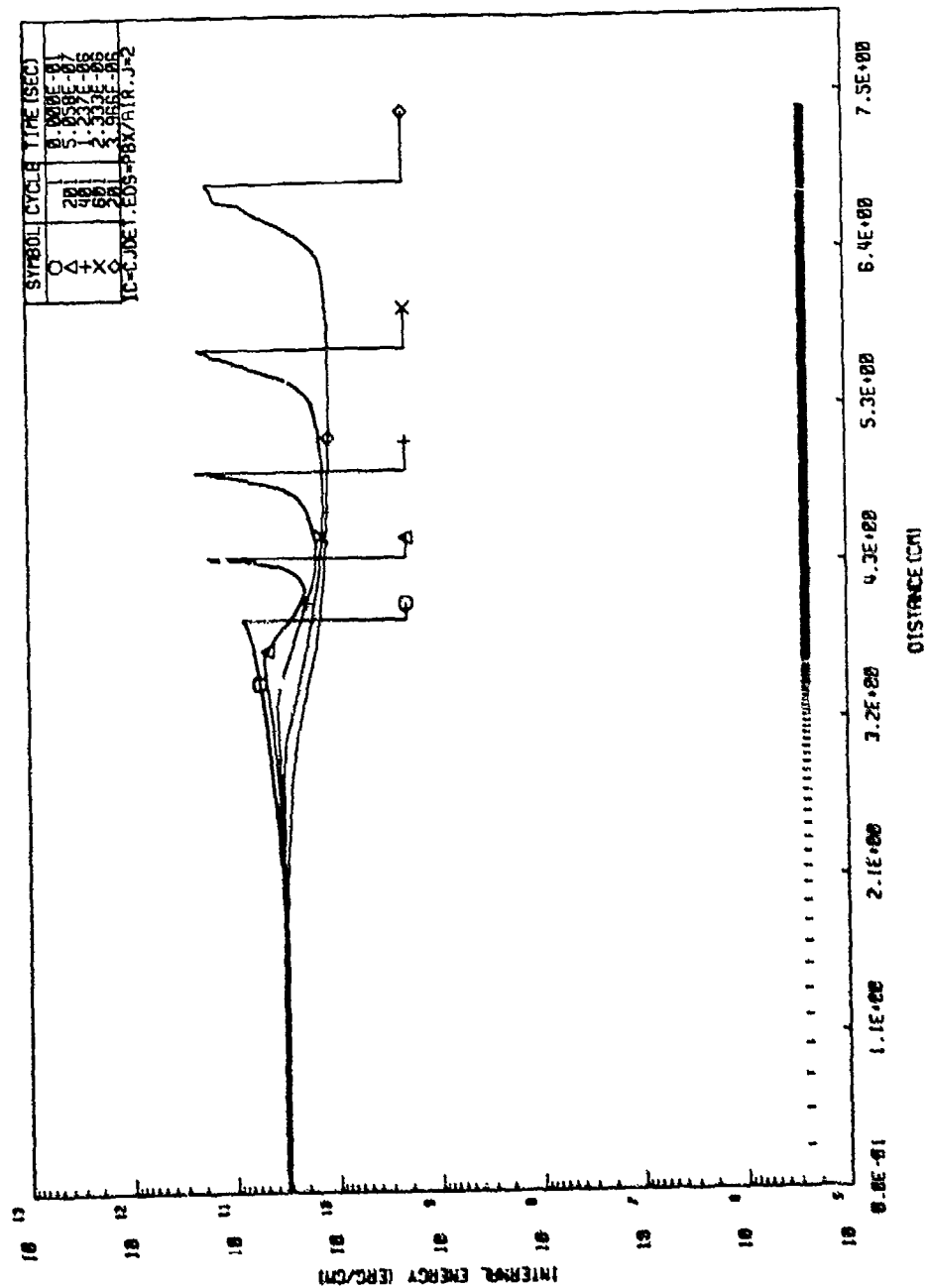


Figure 6. Spatial distribution of the internal energy field at various times (inviscid PCT calculation of a 1-lb spherical PBX-9404 charge detonated in air).

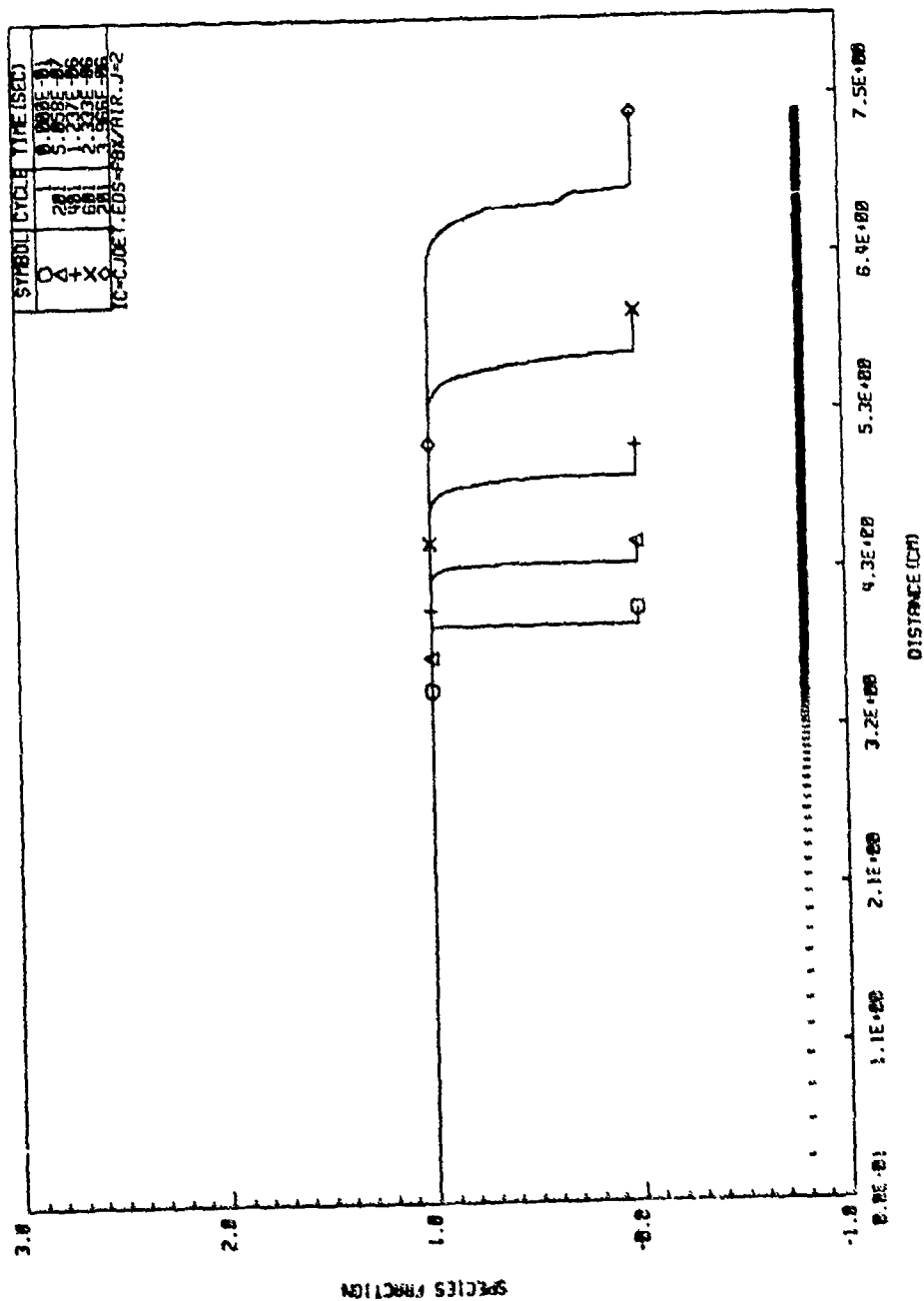


Figure 7. Spatial distribution of the species fraction field at various times (inviscid PCT calculation of a 1-lb spherical PBX-9404 charge detonated in air).

The values of the k- ϵ model parameters were taken as those established from turbulent shear flow

$$\begin{aligned}C_1 &= 1.44 \\C_2 &= 1.92 \\ \sigma_{T,\beta} &= 1.0 \text{ for } \beta = h, k, f \\ \sigma_{T,\epsilon} &= 1.3\end{aligned}$$

while the viscosity coefficient, C_μ , and the Rayleigh-Taylor coefficient, C_3 , were assumed to be:

$$\begin{aligned}C_\mu &= 0.009 \\C_3 &= 1.0\end{aligned}$$

Figures 9 through 19 give the evolution of the flow field at 100 and 200 cycles after the turbulence terms were turned on. These figures show a narrow region of the flow field in the vicinity of the contact surface. Consider in particular Figures 17, 18 and 19 which depict the calculated turbulent kinetic energy, k , dissipation rate, ϵ , and total viscosity, μ_T . Comparing these parameters with the density distribution shows that the turbulent kinetic energy grows rapidly in the vicinity of the contact surface and nowhere else. After 200 cycles, $k \sim 5 \times 10^8$ erg/g while internal and kinetic energies are greater than 10^{10} erg/g. Note that the dissipation rate is also growing; hence, the evolution of the turbulence kinetic energy will depend on the delicate balance between the generation terms and the decay terms. These, in turn, depend on the particular values chosen for C_3 and C_μ . A detailed investigation of these effects is an appropriate subject for future studies.

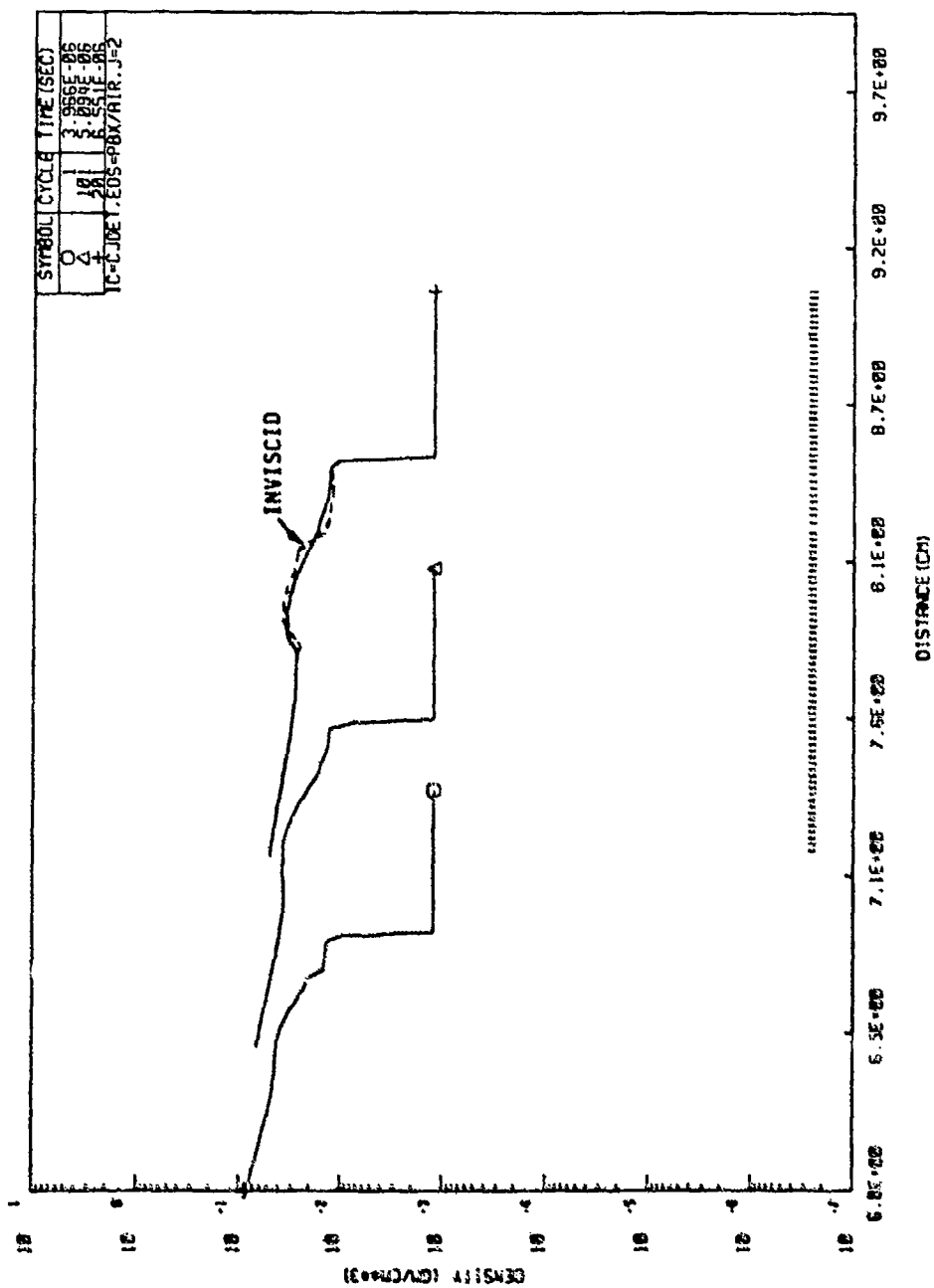
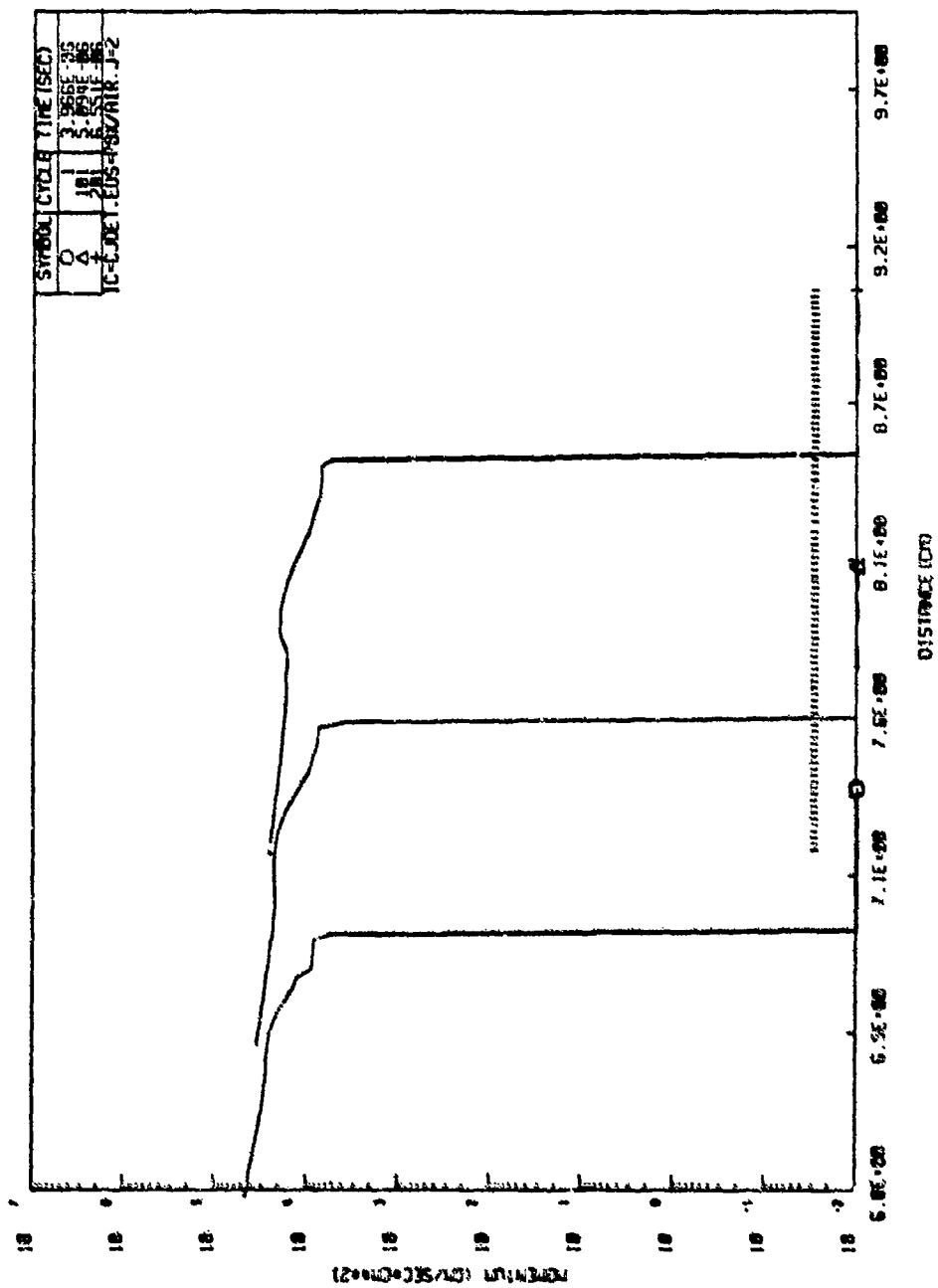


Figure 9. Spatial distribution of the density field at various times (continuation of the PCT calculation of Figures 1-8 with the k-ε turbulence model activated).



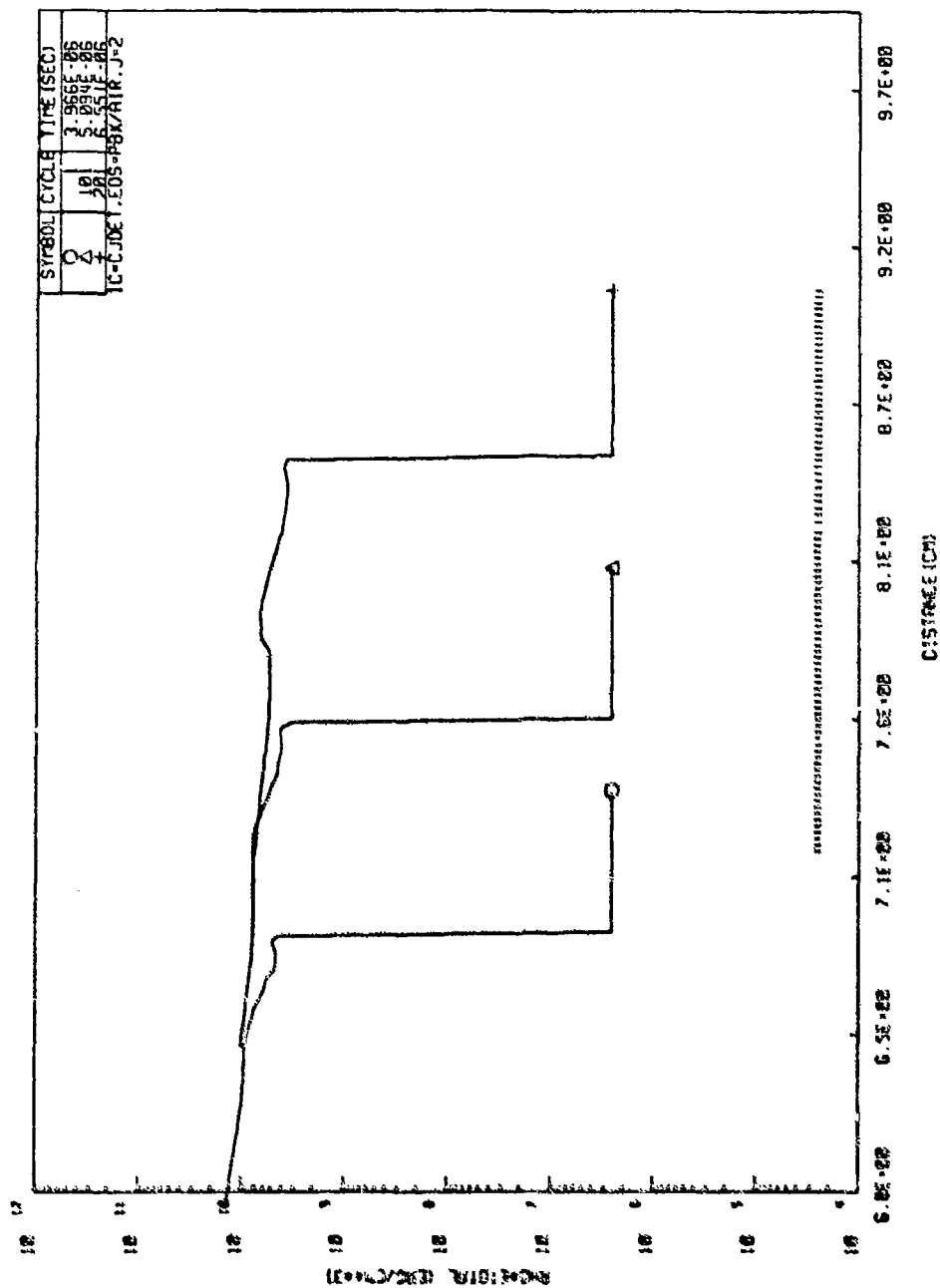


Figure 11. Spatial distribution of the total energy field at various times (continuation of the FCT calculation of Figures 1-8 with the k-ε turbulence model activated).

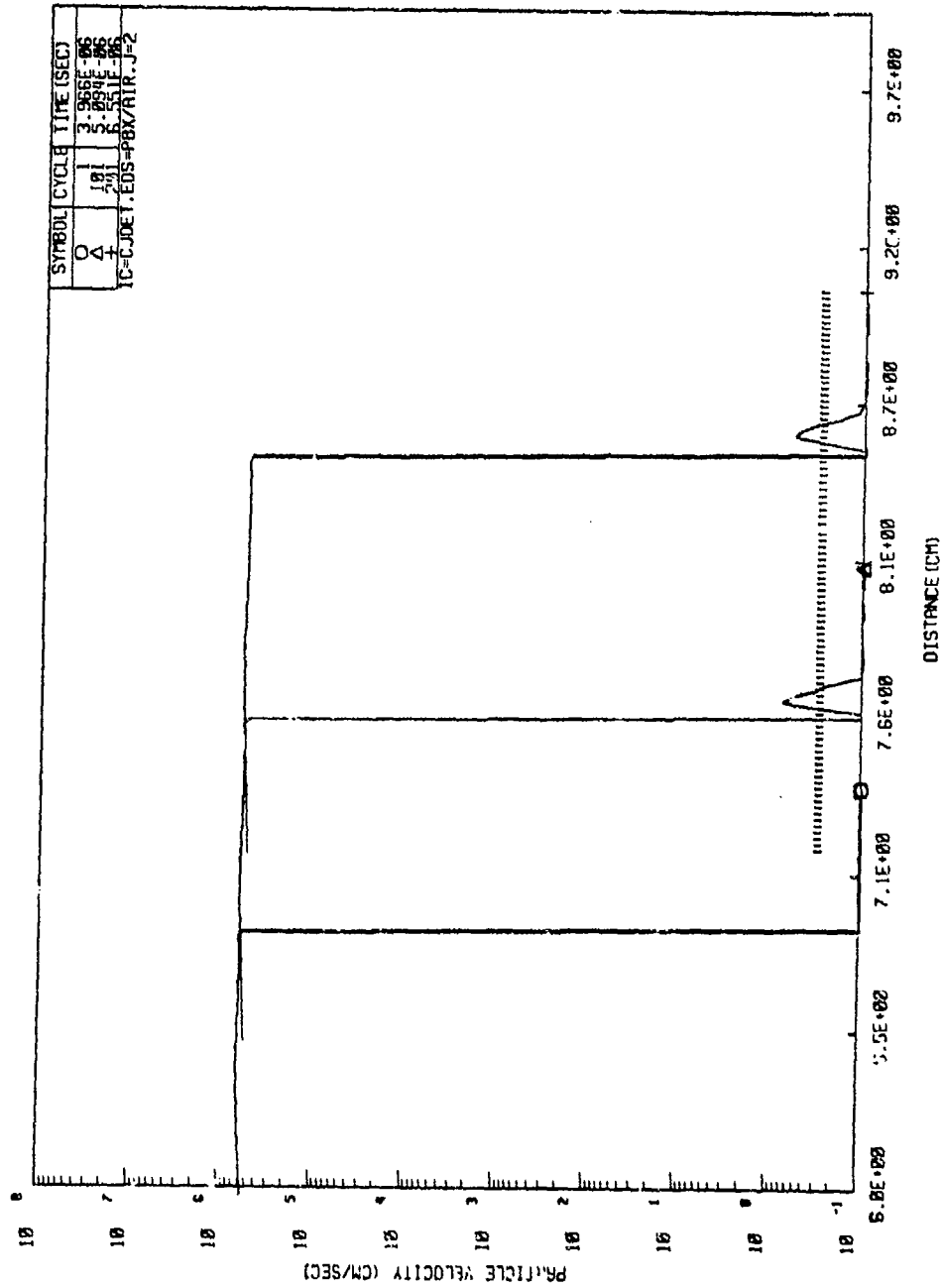


Figure 12. Spatial distribution of the velocity field at various times (continuation of the FCT calculation of Figures 1-8 with the k-ε turbulence model activated).

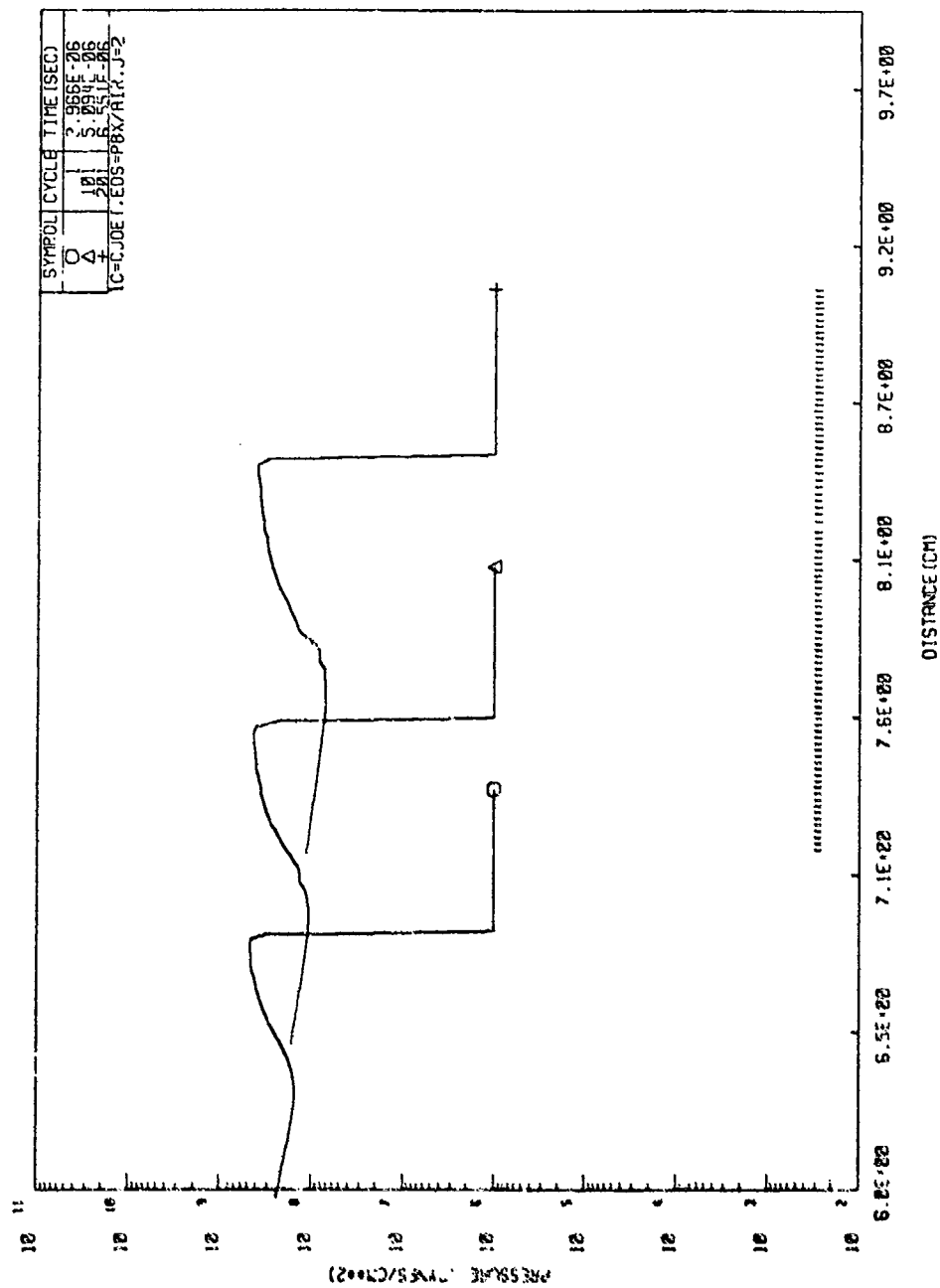


Figure 13. Spatial distribution of the pressure field at various times (continuation of the FCT calculation of Figures 1-8 with the k-ε turbulence model activated).

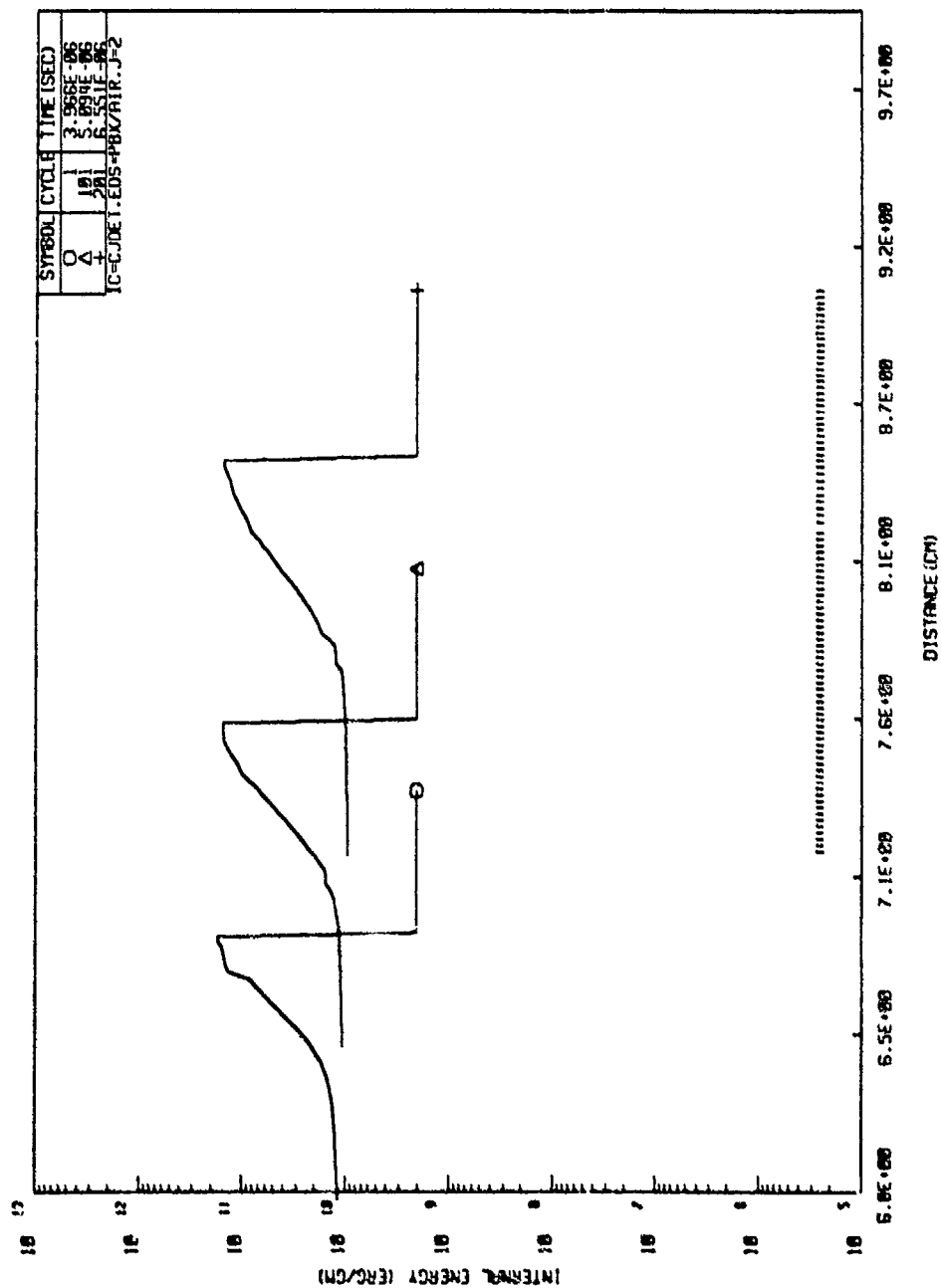


Figure 14. Spatial distribution of the internal energy field at various times (continuation of the PCT calculation of Figures 1-8 with the k-ε turbulence model activated).

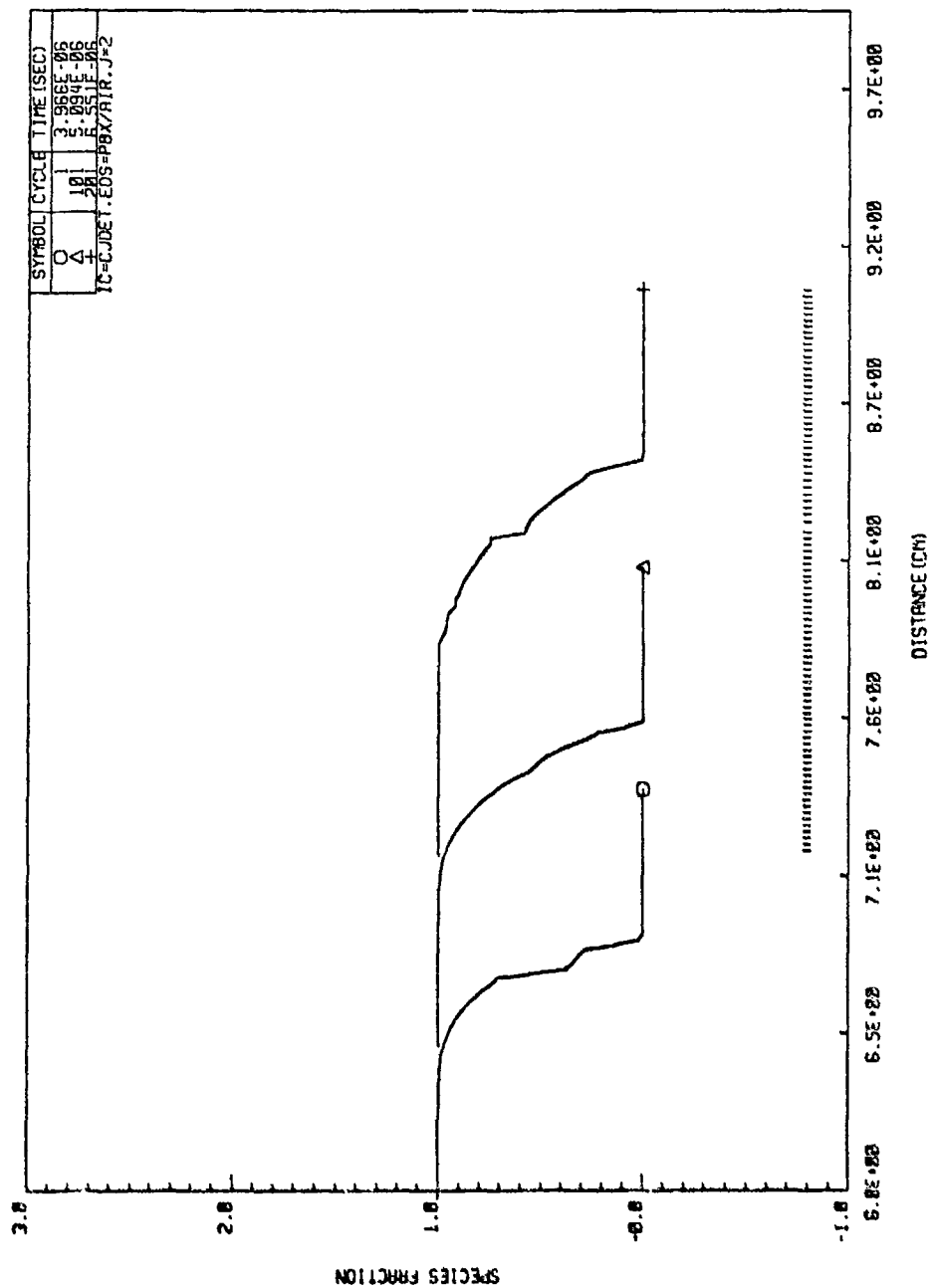


Figure 15. Spatial distribution of the species fraction field at various times (continuation of the FCT calculation of Figures 1-8 with the k- ϵ turbulence model activated).

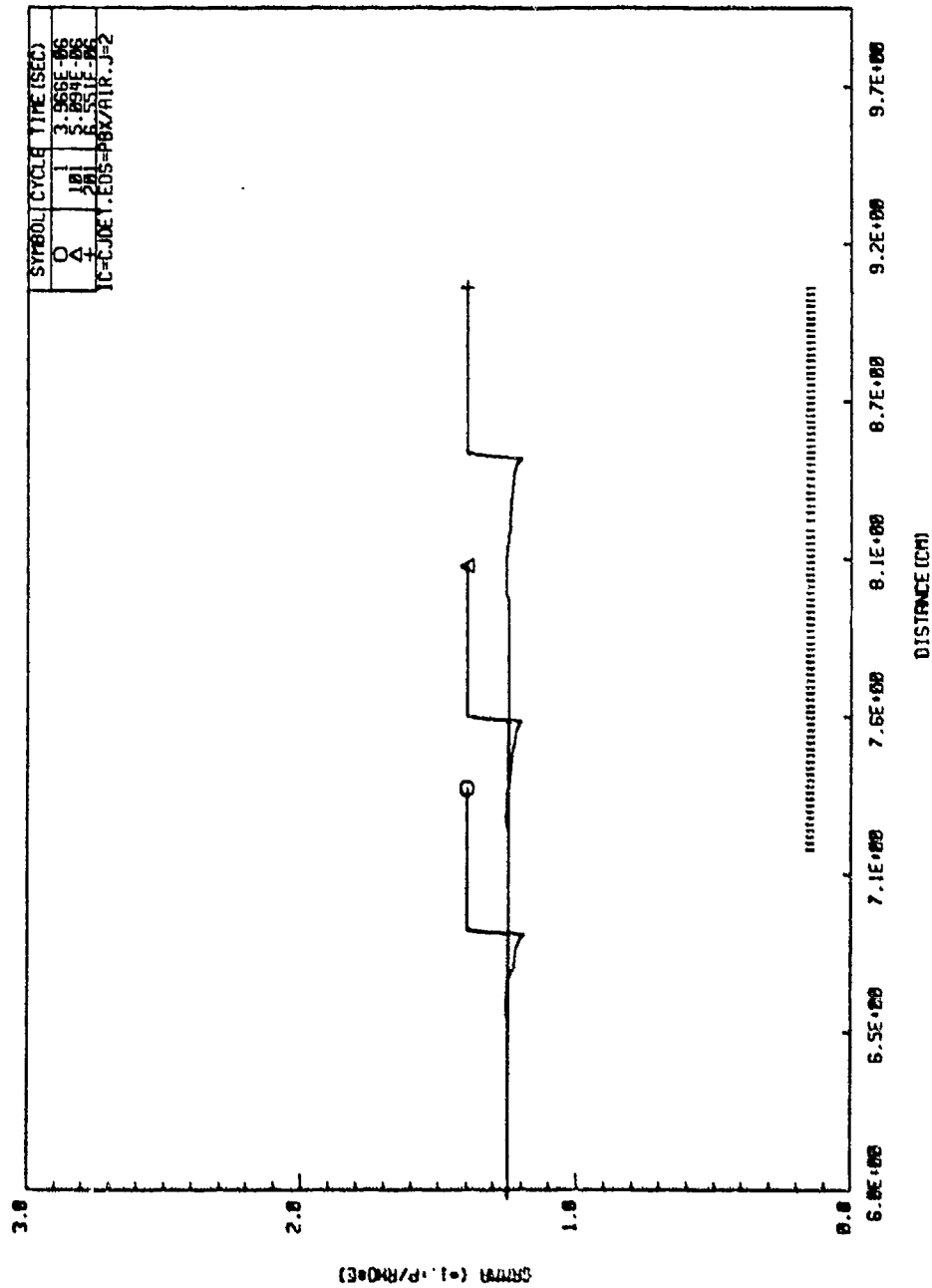


Figure 16. Spatial distribution of the effective gamma field at various times (continuation of the FCT calculation of Figures 1-8 with the k-ε turbulence model activated).

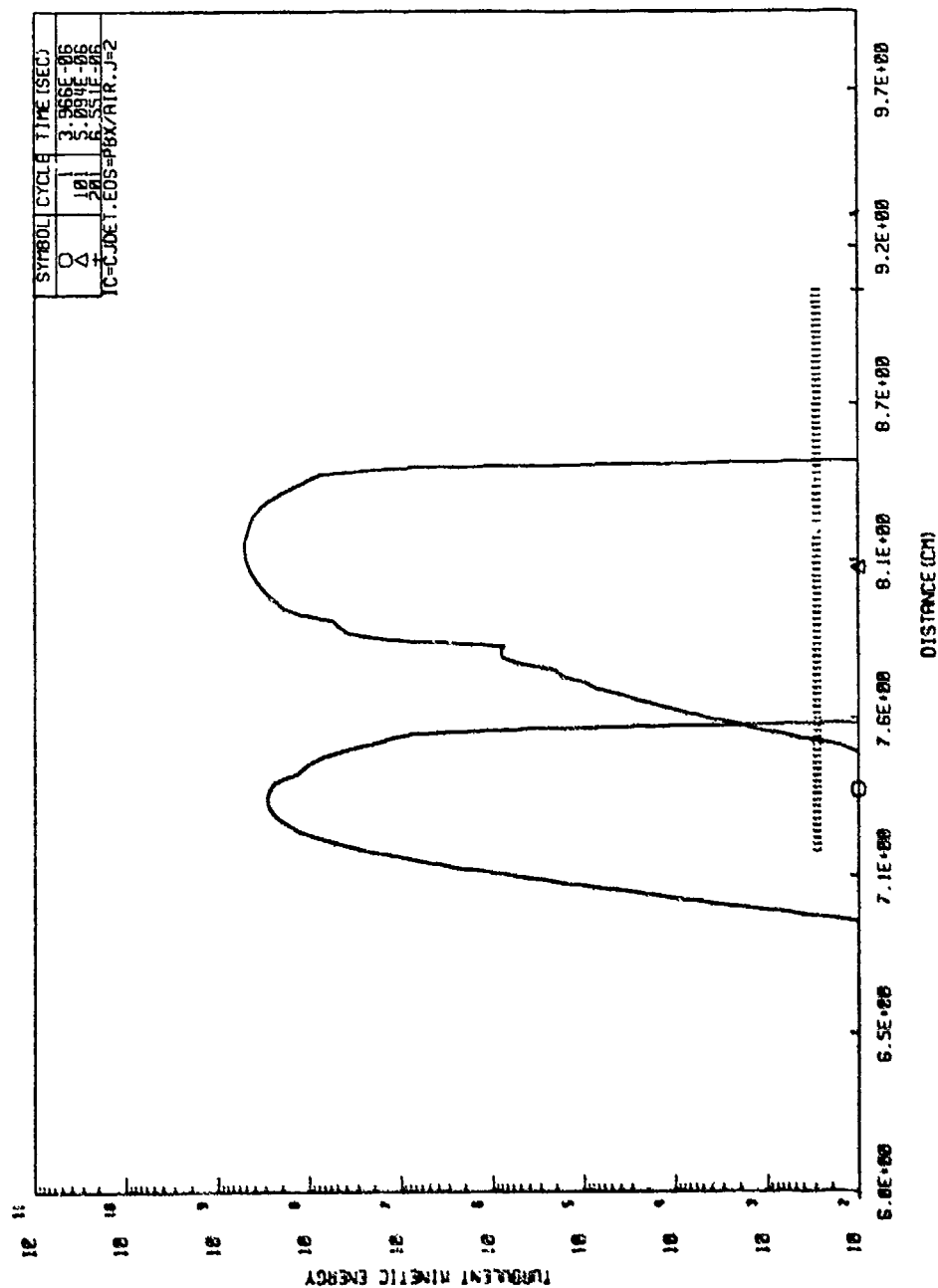


Figure 17. Spatial distribution of the turbulent kinetic energy field at various times (continuation of the FCT calculation of Figures 1-8 with the k-ε turbulence model activated).

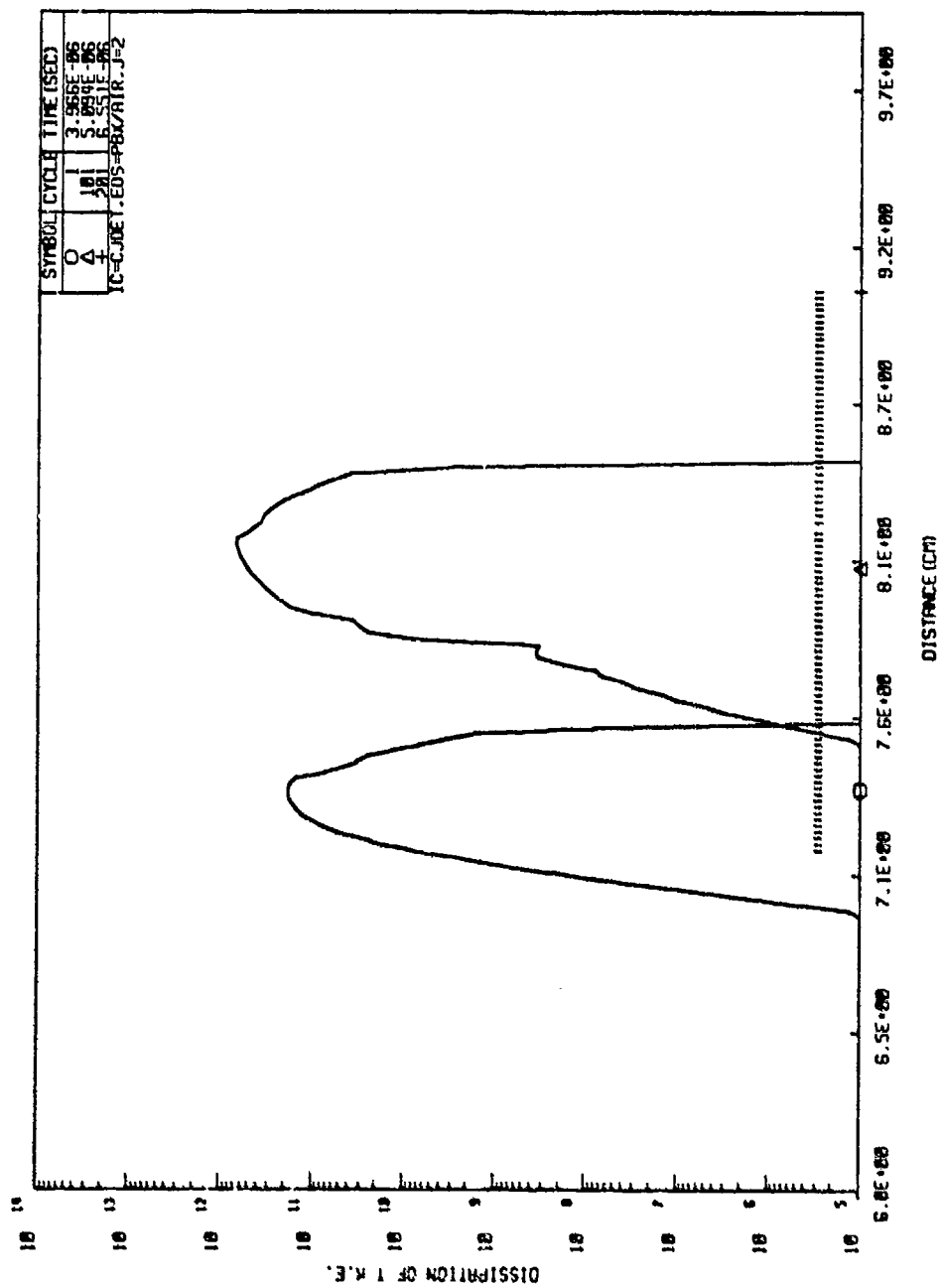


Figure 18. Spatial distribution of the turbulent kinetic energy dissipation rate at various times (continuation of the FCT calculation of Figures 1-8 with the k-ε turbulence model activated).

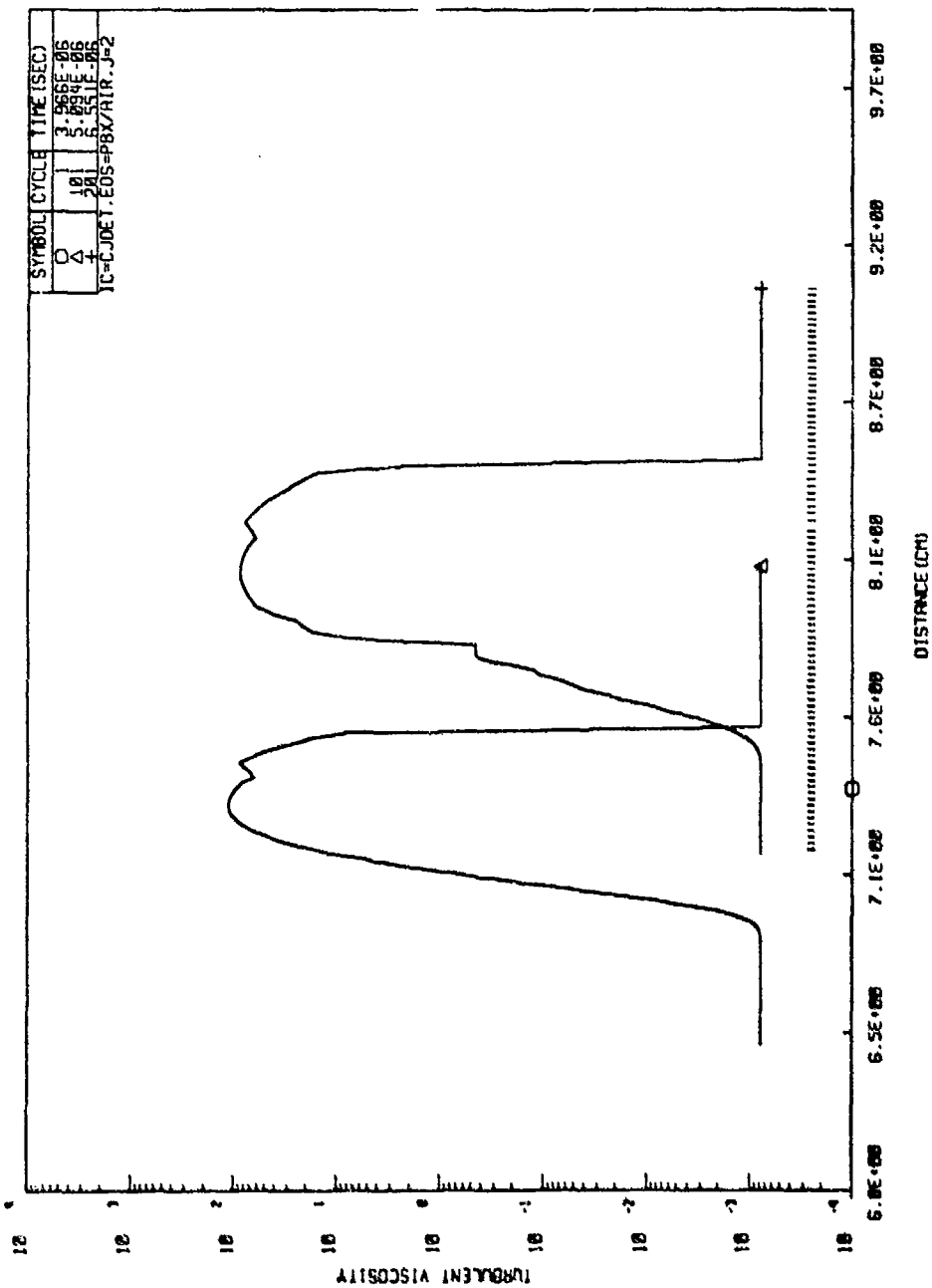


Figure 19. Spatial distribution of the total viscosity (laminar plus turbulent) field at various times (continuation of the FCT calculation of Figures 1-8 with the k-ε turbulence model activated).

IV. CONCLUSIONS AND RECOMMENDATIONS

We have shown here that the present $k-\epsilon$ turbulence model does indeed predict the rapid growth of turbulence in the vicinity of the contact surface for HE-driven blast waves. Parametric studies should be performed with this model to pin down the constants, especially C_3 and C_μ . Such kinematic calculations should be verified with experimental data. In addition, a heat release model should be formulated and incorporated into the hydrocode. Calculations including such energetics (i.e., afterburning) should then be performed for explosives which afterburn more strongly (e.g., TNT and Pentolite) and more weakly (e.g., PBX-9404), and such calculations should then be compared with appropriate experimental data (pressure records, photography and thermal radiation measurements of the fireball) and inviscid calculations to determine the importance of afterburning for various types of explosives.

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