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ON THE PIC METHOD FOR MODELING THE SHAPED-CHARGED PROBLEMS

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The PIC (particle-in-cell) method has been used for computing compressible, multimaterial problems for more than twenty years. The present work extends the same numerical approximation with operator splitting to hydro-elastic-plastic flow problems in two-dimensional Eulerian coordinates. Applying the operator splitting method, the basic set of cylindrical equations is split in radial (r) and axial (z) directions. The calculations, performed in each direction separately, are alternated for each time advancement to maintain the accuracy of one-dimensional procedure. A shaped-charge problem is treated using the present code and the results are compared with the experimental data as well as those from other codes.

Introduction

It has been of considerable interest to resolve multi-material compressible flow problems with material interface, a Lagrangian approach would be a quite natural choice, e.g., HEMP [1], TOODY [2], MAGEE [3,4]. However, for a large material distortion, the Lagrangian calculations can no longer be continued, and subsequently an Eulerian or a combined Lagrangian-Eulerian type scheme has been applied.

Although many schemes have been invented in the various Eulerian code developments, materials are treated in two ways, namely the Particle-in-Cell Method [5], where materials are represented by discrete mass points called Particles, and the continuous Eulerian method as in SOIL[6], HELP [7] and CSQ [8]. In the continuous method, the computing economy is gained, however, the Lagrangian-type capability of PIC method is lost and subsequently replaced by various interface treatments.

In developing the present code, the PIC capability is sought to be maintained while improving the accuracy and the computing economy. Recently, Clark [9] proved the accuracy of the standard PIC method to be 1st order in hydrodynamic computation of multi-material problems and proposed a second order scheme. Here a similar second order scheme is used to compute multi-material elastic-plastic flow including phase transition and spall. A hemispherical, copper-lined, shaped charge with 75/25 OCTOL as high explosive (HE) is calculated using the present code. The results are compared with the experimental data as well as those from other codes.

THE CONSERVATION EQUATIONS FOR A STRESS SUPPORTING MEDIUM

The conservation equations in two-dimensional cylindrical or plane Eulerian coordinate can be written as below

Mass

$$\frac{D\rho}{Dt} + \rho \left(\frac{\partial u}{\partial r} + \alpha \frac{u}{r} + \frac{\partial v}{\partial z}\right) = 0 \quad (1)$$

Momentum

$$\rho \frac{Du}{Dt} = \frac{\partial}{\partial r} \sigma^{rr} + \frac{\partial}{\partial z} \sigma^{rz}$$

$$+ \frac{\alpha}{r} (\sigma^{rr} - \sigma^{\theta\theta})$$

$$\rho \frac{Dv}{Dt} = \frac{\partial}{\partial y} \sigma^{zz} + \frac{\partial}{\partial r} \sigma^{rz} + \frac{\alpha}{r} \sigma^{rz} \quad (2)$$

Energy

$$\rho \frac{DI}{Dt} = \sigma^{rr} \frac{\partial u}{\partial r} + \alpha\sigma^{\theta\theta} \frac{u}{r}$$

$$+ \sigma^{zz} \frac{\partial v}{\partial z}$$

$$+ \sigma^{rz} \left(\frac{\partial u}{\partial z} + \frac{\partial v}{\partial r}\right) \quad (3)$$

where $\alpha = 0$ for plane geometry,

$\alpha = 1$ for cylindrical geometry,

$$\frac{D}{Dt} = \frac{\partial}{\partial t} + u\frac{\partial}{\partial r} + v\frac{\partial}{\partial z}$$

$$\sigma^{ij} = s^{ij} - P\delta_{ij}$$

$$P = - 1/3\ \sigma^{ii}$$
$$= 1/3\ (\sigma^{rr} + \sigma^{zz} + \sigma^{\theta\theta})$$

u, v = velocities
ρ = density
t = time

s^{ij} = stress deviator, and
I = specific internal energy

EQUATIONS OF STATE

When a stress supporting medium flows under a wide range of stresses, it exhibits a variety of different physical characteristics. Depending on its retention of elastic character, the flow may be elastic or plastic. When melting, it would be- [illegible] each regime of flow, we need proper models or equations of state, and criteria defining the transition from one regime to another. Here a straight forward approach is taken, yet there does not seem to exist any better model.

(a) Stresses in Elastic Regime

When a material flows elastically, Hooke's law in current form can be written as below

$$\frac{DS^{rr}}{Dt} = 2G \left(\frac{\partial u}{\partial r} + \frac{1}{3\rho} \frac{D\rho}{Dt}\right) + \delta^{rr} \quad (4)$$

$$\frac{DS^{zz}}{Dt} = 2G \left(\frac{\partial v}{\partial r} + \frac{1}{3\rho} \frac{D\rho}{Dt}\right) + \delta^{zz} \quad (5)$$

$$\frac{DS^{rz}}{Dt} = G \left(\frac{\partial u}{\partial z} + \frac{\partial v}{\partial r}\right) + \delta^{rz} \quad (6)$$

$$\frac{DS^{\theta\theta}}{Dt} = 2G \left(\alpha\frac{u}{r} + \frac{1}{3\rho} \frac{D\rho}{Dt}\right)$$

$$= \frac{D}{Dt} (-S^{rr} - S^{zz}) \quad (7)$$

$$\text{or} \quad S^{rr} + S^{zz} + S^{\theta\theta} = 0$$

Where G = modulus of elasticity in shear

= f (ρ, I, material),

and δ^{ij} = correction for rigid body rotation

In tensor form

$$\frac{D}{Dt} S^{ij} = 2G\ \dot{e}^{ij} + \delta^{ij} \quad (8)$$

where $\dot{e}^{ij}$ = strain rate deviator

$$= \begin{bmatrix} \frac{\partial u}{\partial r} + \frac{1}{3\rho}\frac{D\rho}{Dt} & \frac{1}{2}\left(\frac{\partial u}{\partial z} + \frac{\partial v}{\partial r}\right) \\ \frac{1}{2}\left(\frac{\partial u}{\partial z} + \frac{\partial v}{\partial r}\right) & \frac{\partial v}{\partial z} + \frac{1}{3\rho}\frac{D\rho}{Dt} \\ 0 & 0 \end{bmatrix}$$

$$\begin{matrix} 0 \\ 0 \\ \alpha \frac{u}{r} + \frac{1}{3\rho}\frac{D\rho}{Dt} \end{matrix} \Bigg] \quad (9)$$

(b) Stresses in Plastic Regime

For plastic flows, Prandtl and Reuss considered both plastic and elastic strain simultaneously and arrived at the following flow equation

$$\dot{S}^{ij} = 2G\dot{e}^{ij} - \frac{G\dot{W}}{\frac{1}{3}(Y^\circ)^2} S^{ij} \quad (10)$$

where $\dot{W} = \sum_{ij} S^{ij}\,\dot{e}^{ij}$ is the plastic work/unit volume

and Y° = yield stress in simple tension.

Expanding (10)

$$\frac{DS^{rr}}{Dt} = 2G\left[\frac{\partial u}{\partial r} + \frac{1}{3\rho}\frac{D\rho}{Dt}\right]$$

$$- \frac{G\dot{W}}{1/3(Y^\circ)^2} S^{rr} + \delta^{rr} \quad (11)$$

$$\frac{DS^{zz}}{Dt} = 2G\left[\frac{\partial v}{\partial z} + \frac{1}{3\rho}\frac{D\rho}{Dt}\right]$$

$$- \frac{G\dot{W}}{1/3(Y^\circ)^2} S^{zz} + \delta^{zz} \quad (12)$$

$$\frac{DS^{rz}}{Dt} = G\left[\frac{\partial u}{\partial z} + \frac{\partial v}{\partial r}\right]$$

$$- \frac{G\dot{W}}{1/3(Y^\circ)^2} S^{rz} + \delta^{rz} \quad (13)$$

$$S^{\theta\theta} = -\left(S^{rr} + S^{zz}\right) \quad (14)$$

$$\dot{W} = \left(\frac{\partial u}{\partial r} + \frac{1}{3\rho}\frac{D\rho}{Dt}\right) S^{rr}$$

$$+ \left(\frac{\partial u}{\partial z} + \frac{\partial v}{\partial r}\right) S^{rz} + \left(\frac{\partial v}{\partial z} + \frac{1}{3\rho}\frac{D\rho}{Dt}\right)$$

$$S^{zz} + \left(\alpha\frac{u}{r} - \frac{1}{3\rho}\frac{D\rho}{Dt}\right) S^{\theta\theta}$$

$$= \frac{\partial u}{\partial r} S^{rr} + \left(\frac{\partial u}{\partial z} + \frac{\partial v}{\partial r}\right) S^{rz}$$

$$+ \frac{\partial v}{\partial z} S^{zz} + \alpha \frac{u}{r} S^{\theta\theta} \quad (15)$$

Physically $\dot{W}$ is the work done per unit volume in changing the shape of the madium. And Eqs. (11-14) holds at the yield limit and for $\dot{W} \geq 0$. When $\dot{W} < 0$, the material is unloading elastically from a plastic state and Eq. (4-7) is to be used. Therefore, for a plastic regime of flow, Eqs. (11-15) have to be solved.

(c) Hydrostatic Pressure

Various forms of equation of state for pressure are available and we will simply write this as below.

$$P = f\,(\rho,\ I,\ \text{Material}) \quad (16)$$

(d) Yield Criterion

To check whether a material is in elastic or plastic state, von Mises criterion is employed here. Denoting three principle directions by subscripts 1, 2, and 3.

$$S_1 = 1/2(S^{rr} + S^{zz}) + 1/2$$

$$\left[(S^{rr} - S^{zz})^2 + (2\,S^{rz})^2\right]^{1/2}$$

$$S_2 = 1/2(S^{rr} + S^{zz})$$

$$- 1/2\left[(S^{rr} - S^{zz})^2\right.$$

$$\left. + (2\,S^{rz})^2\right]^{1/2}$$

$$S_3 = S^{\theta\theta} \quad (17)$$

The second invariant of S^{ij} tensor is then defined by

$$\Phi = S_1^2 + S_2^2 + S_3^2$$

$$= (S^{rr})^2 + (S^{zz})^2 + (S^{\theta\theta})^2 \qquad (18)$$

Then von Mises yield criterion says that a material is in

elastic state when $\Phi \leq 2/3\ (Y°)^2$

or

plastic state when $\Phi > 2/3\ (Y°)^2$

Now let's suppose that a small time step, Δt, is chosen such that the Prandtl-Reuss relation is valid. During the time increment Δt, a material can be in an elastic period Δt_1, then in a plastic period Δt_2, i.e., $\Delta t = \Delta t_1 + \Delta t_2$.

Then for a rigorous computation of S^{ij}, Δt_1, has to be obtained such that

$$\Phi_{\Delta t_1} = 2/3\ (Y°)^2 \qquad (19)$$

is satisfied. An iterative procedure might be considered. However, considering the accuracy of the yield criterion itself and plastic flow model, a simpler method seems profitable. An experience with a Lagrangian computation shows that the following scheme proposed by Wilkins [1] is adequate in computing stress deviators on yield surface, $(S^{ij})^*$.

$$(S^{ij})^* = (S^{ij})\ f$$

where

$$f = 2/3\ (Y°)^2/\Phi \qquad (20)$$

Therefore, if the flow becomes plastic during Δt period. S^{ij} is first calculated based on elastic assumptions, then the new stress deviators on yield surface $(S^{ij})^*$ are approximated by (20)

(e) Stress Correction for Rigid Body Rotation

The magnitude of stresses does not change during a rigid body rotation, and the new stresses after rotation as well as after deformation have to be expressed in terms of the original coordinate system. The correction for rigid body rotation, as well as, after deformation have to be expressed in terms of the original coordinate system. The correction for rigid body rotation is relatively straight forward. However, there doesn't seem to exist a unique way of correcting stresses for deformation. One possibility is to include this effect into the governing differential equation (i. e., Bertholf [2]). Even though technically interesting, the inclusion of deformation correction does not appear to be very significant for practical purposes.

Suppose S^{ij} is rotated by ω during a time increment, Δt, then the new stress deviator in original coordinate system, S_o^{ij}, can be written as

$$S_o^{rr} = S^{rr} \cos^2 \omega + S^{zz} \sin^2 \omega + 2S^{rz} \sin \omega \cos \omega$$

$$S_o^{zz} = S^{rr} \sin^2 \omega + S^{zz} \cos^2 \omega - 2S^{rz} \sin \omega \cos \omega$$

$$S_o^{rz} = S^{rz} (\cos^2 \omega - \sin^2 \omega) - (S^{rr} - S^{zz}) \sin \omega \cos \omega \qquad (21)$$

where $\sin \omega = \frac{\Delta t}{2} \left(\frac{\partial u}{\partial z} - \frac{\partial v}{\partial r}\right)$.

Instead of including δ^{ij} to differential equations as in Eqs. (4-7) and (11-14), S^{ij} correction can be done to the resulting stresses at the end of each computational time step. Thus, it is convenient to define

$$\delta_o^{ij} = \Delta t \, \delta^{ij} = S_o^{ij} - S^{ij}$$

$$\text{or } S_o^{ij} = S^{ij} + \delta_o^{ij} \qquad (22)$$

Then

$$\delta_o^{rr} = 1/2 \left(S^{rr} - S^{zz}\right)(\cos 2\omega - 1) + S^{rz} \sin 2\omega$$

$$\delta_o^{zz} = - \delta_o^{rr} \qquad (23)$$

and

$$\delta_o^{rz} = S^{rz} \left(\cos 2\omega - 1\right) - 1/2 \left(S^{rr} - S^{zz}\right) \sin 2\omega \qquad (24)$$

For a small ω, we may further simplify (23) by

$$\sin 2\omega \approx 2 \sin \omega = \Delta t \left(\frac{\partial u}{\partial z} - \frac{\partial v}{\partial r}\right) \qquad (25)$$

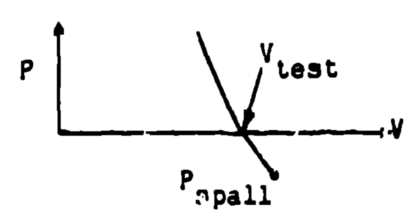
SPALL, MELTING AND FRACTURE

Material failure can be considered under a number of different conditions. However, under intense, short-duration tensile loading, a particular type of fracture called "spall" is frequently produced. For the problems of our current interest, the material failure is likely to occur in this form. When spalled, small, independent cracks or voids are produced, and usually an extensive crack propagation does not take place. The shape of voids thus produced, may depend on material structure. However, effects of crystallographic orientation on grossdamage, and also the stress distribution relative to the shape of the void seems to be insignificant.

Considering these characteristics of spall, and also considering that our problems do not require much computation once a material is significantly fractured, a simplistic model seems to be adequate. Therefore, for the present code, the following criteria are used to check material failure and phase transition.

When I > melt energy, the material is melted and subsequently is treated as a pure hydrodynamic fluid.

When pressure gets down to a certain specified spall pressure ($P \le P_{spall}$) the material is assumed to be spalled.



Once spalled, the material cannot support any stress, and P and S^{ij} are set to be zero until re-combined.

For re-combining, v is compared to V_{test}, and if $V \le V_{test}$, the material is regarded as recombined.

Presently the fracture criterion is based on tensile strength, namely if principal stresses, σ_I > tensile strength, c, the material is assumed to be fractured. A fractured cell is treated as a spalled cell. A detail description of the procedure to solve the pertinent conservation equations and the equation of state is given in Reference [10].

CALCULATIONS OF THE HEMISPHERICAL COPPER-SHAPED CHARGE PROBLEM

To demonstrate the present code capability, we choose the hemispherical copper liner shaped charge problem which was also calculated by Harrison (11). Fig. 1 shows the initial dimension of the test problem with the hollow hemispherical copper liner of thickness 0.206 cm and outside diameter of 6.35 cm. The bare 75/25 OCTOL high explosive has an outside diameter of 6.985 cm and was detonated by single point initiated at point A. We use a 2-D Lagrangian code to setup the input and run the problem up to 15 μsec when the liner becomes about 0.52 cm thick. The present code calculations start at 15 μsec and stop at 90 μsec using a window of 7.5 cm (r-direction) x 30 cm (z-direction). The grid size is 0.15 cm square mesh that is equivalent to have a grid number of 50 x 200. For 75/25 OCTOL, we use the JWL-EOS for the pressure which has the form

$$P = A\left(1 - \frac{\omega}{R_1 V}\right) e^{-R_1 V} + B\left(1 - \frac{\omega}{R_2 V}\right) e^{-R_2 V} + (\varepsilon - \varepsilon_1)\frac{\omega}{V}$$

where A = 7.486 MBar, B = 0.1338 MBar, R_1 = ?.5, R_2 = 1.2, ω = 0.38, ε_1 = 0.272 MBar - cm^3/cm^3, V is the specific volume and ε the detonation energy. For the Chapman-Jouguet parameters: ρ_o = 1.821 g/cm^3, detonation velocity, D = 0.849 cm/μsec, ε_o = 0.098 MBar - cm^3/cm^3 and $\varepsilon_{chemical} = \varepsilon_o + \varepsilon_1$ = 0.37 MBar - cm^3/cm^3. For the copper liner, we use a quadratic form such as:

$$P(\text{MBar}) = \left[A_1\mu + A_2\,\mu|\mu| + (B_o + B_1\mu + B_2\mu^2)\,\varepsilon + (C_o + C_1\mu)\,\varepsilon^2\right]/(\varepsilon + D_o)$$

where $\mu = \rho/\rho_o - 1$, $\varepsilon = \rho_o I$ (MBar - cm^3/cm^3), A_1 = 4.9578323, A_2 = 3.6883726, B_o = 7.4727361, B_1 = 11.519148, B_2 = 5.5251138, C_o = 0.39492613, C_1 = 0.52883412, D_o = 3.6000001, and ρ_o = 8.899 (g/cm^3). Fig. 2 shows the initial grid setup for the 2-D Lagrangian code with 31 zones in the HE Region and 11 in liner along the z axis and 90 sectors (1° in one sector) for the first quadrant. At t = 15 μsec, the liner has become about 0.52 cm thick near the z axis as shown in Fig. 3, while the HE region has slid way below the liner wing. The geometry of the collapsing copper liner and the jet formations at time t = 20, 30, 40, and 50 μsec are given in Fig. 4. The vel y distributions along the z-axis for the liner is given in Fig. 5 which shows that the jet slug section is moving into the positive z-direction and many velocity fluctuations exist inside the jet between the slug and tip. The observed cumulative mass versus jet velocity is plotted in Fig. 6 along with the computer simulations of HOIL Code [11] and the present study. Experimental data shows that the tip velocity is 0.422 cm/μsec compared to the present code of 0.43 cm/μsec.

CONCLUSIONS

A second order PIC method is used for computing hydro-elastic-plastic flow. Although there remains the question of how to treat the advection of the stresses correctly in the Eulerian code, present study does give good numerical results for the explosive-pushing metal problems. There are at least eight shaped charge and self-forging fragment problems have been run using the present code that produces excellent numerical results compared with experimental data. The authors believe that a combination of the 2-D Lagrangian and the present 2-D Eulerian codes can become a very useful engineering design tool for explosive-metal interaction problems.

REFERENCES

1. Wilkins, M. L., "Calculation of Elastic-Plastic Flow," in Alder, B. et. al. (eds.) Methods in Computational Physics, (Academic Press, NY) pp. 211-264 (1964).

2. Swegle, J. W., "TOODY IV - A Computer Program for Two-Dimensional Wave Propagation," Sandia National Laboratory, SAND-78-0552, Sept. 1978.

3. Kolsky, H. G., "A Method for the Numerical Solution of Transient Hydrodynamic Shock Problems in Two Space Dimensions, "Los Alamos National Laboratory, Report LA-1867 (1955).

4. Mader, C. L., "Numerical Modeling of Detonations," University of California Press, pp. 333-352 (1979).

5. Harlow, F. H., "The Particle-in-Cell Computing Method for Fluid Dynamics," in Method in Computational Physics, Vol. III, Academic Press, New York, 1964.

6. Johnson, Wallace E. "Modifications of OIL-Type Computer Programs," BRL Contract Report ARBRL-CR-0476, Ballistic Research Laboratory (January 1982).

7. Hageman, L. J., et. al., "HELP, A Multi-material Eulerian Program for Compressible Fluid and Elastic-Plastic Flows in Two-Dimensions and Time," Systems, Science and Software Report SSS-R-75-2654, July 1975.

8. Thompson, S. L., "CSQII - An Eulerian Finite Difference Program for Two-Dimensional Material Response - Part I. Material Sections," SAND77-1339, Sandia National Laboratories, Albuquerque, NM (1977).

9. Clark, R. A., "Second-order Particle-in-cell Computing Method," Los Alamos National Laboratory Report LA-UR-79-1947 (1979).

10. Lee, W. H. and Kwak, D., "Elastic-Plastic Flow Using Operator Splitting and PIC Method in a 2-Dimensional Eulerian Hydrodynamic Code," Los Alamos National Laboratory Report LA-UR-85-3537 (1985).

11. Harrision, J. T., "A Two Stage, Hydrodynamic, Numerical Technique, "HOIL" and an Analysis of the Results of a Hemispherical, Shaped Charge Liner Collapse," at Eighth International Symposium on Ballistics, Orlando, Florida, Oct. 23-25, 1984.

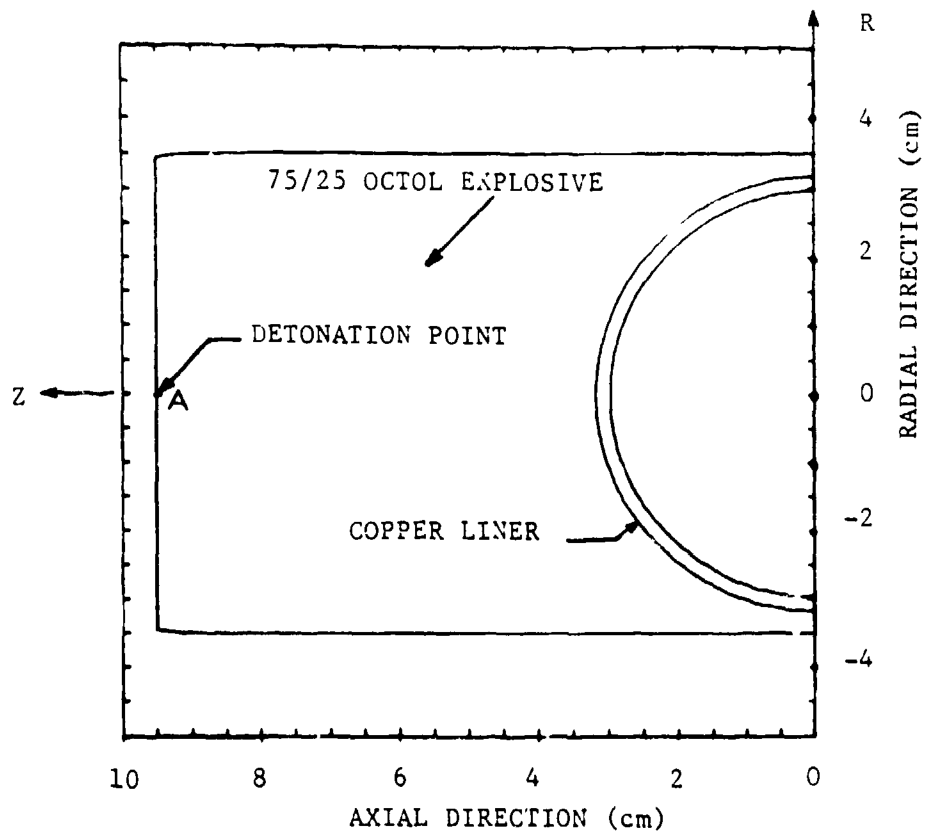


Fig. 1 THE INITIAL CONDITIONS WITH 75/25 OCTOL AS HE AND COPPER LINER OF 0.206 cm THICKNESS

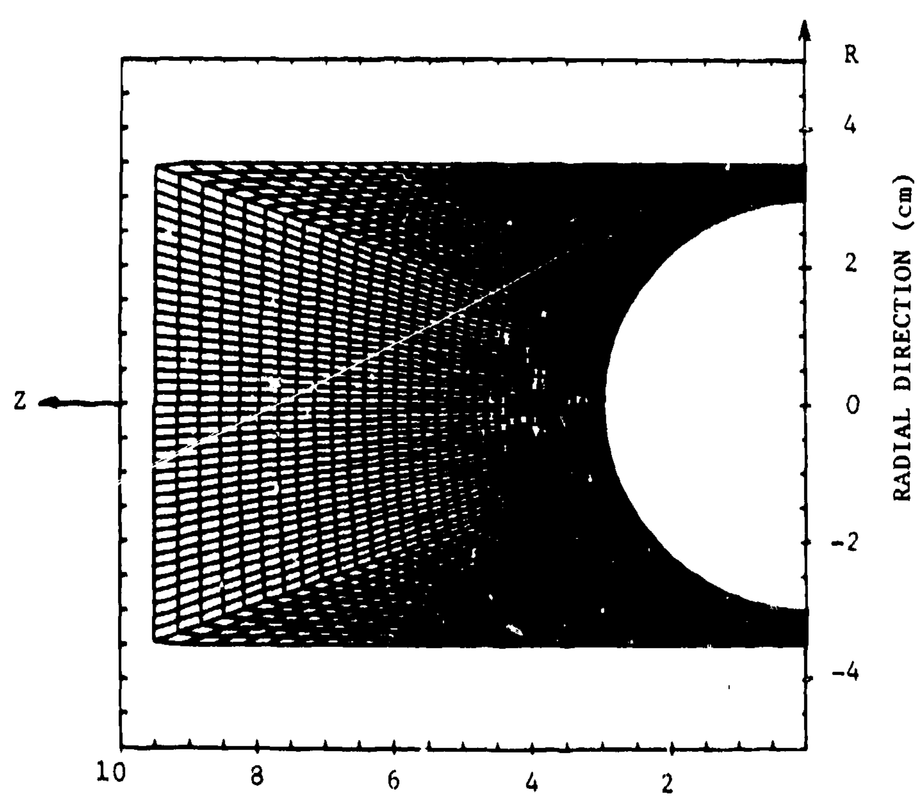


Fig. 2 THE INITIAL GRID SETUP FOR THE 2-D LAGRANGIAN CODE WITH 31 ZONES IN HE, 11 IN COPPER LINER AND 90 SECTORS IN THE FIRST QUADRANT.

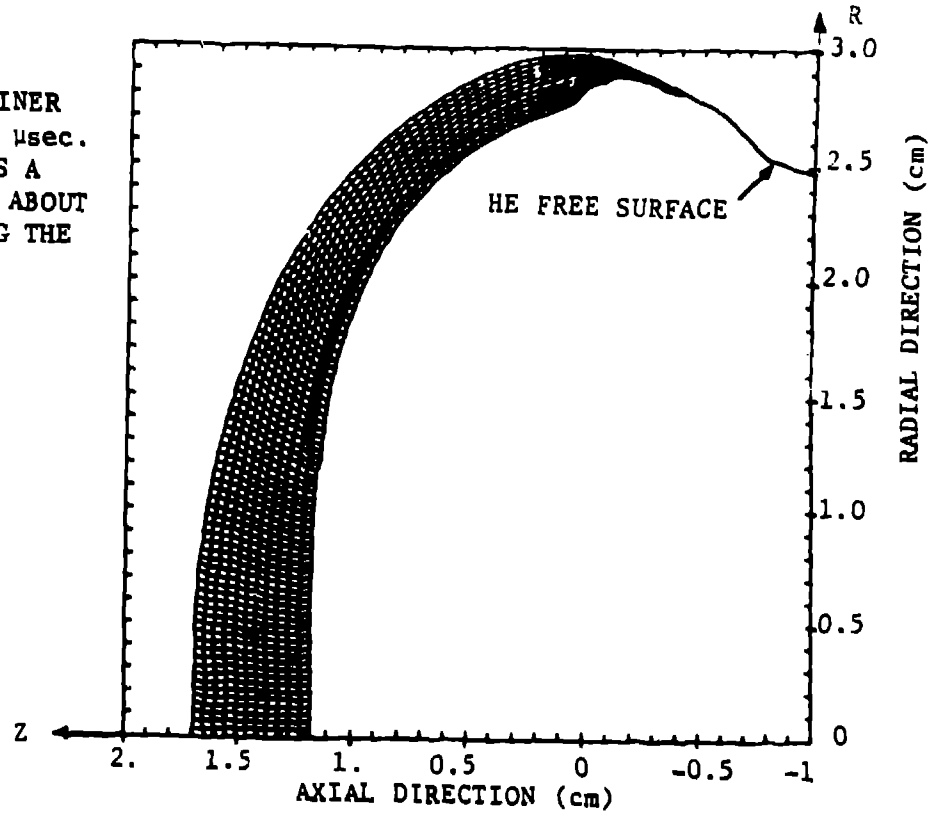


Fig. 3 THE COPPER LINER AT TIME = 15 µsec. THE LINER HAS A THICKNESS OF ABOUT 0.52 cm ALONG THE Z-AXIS

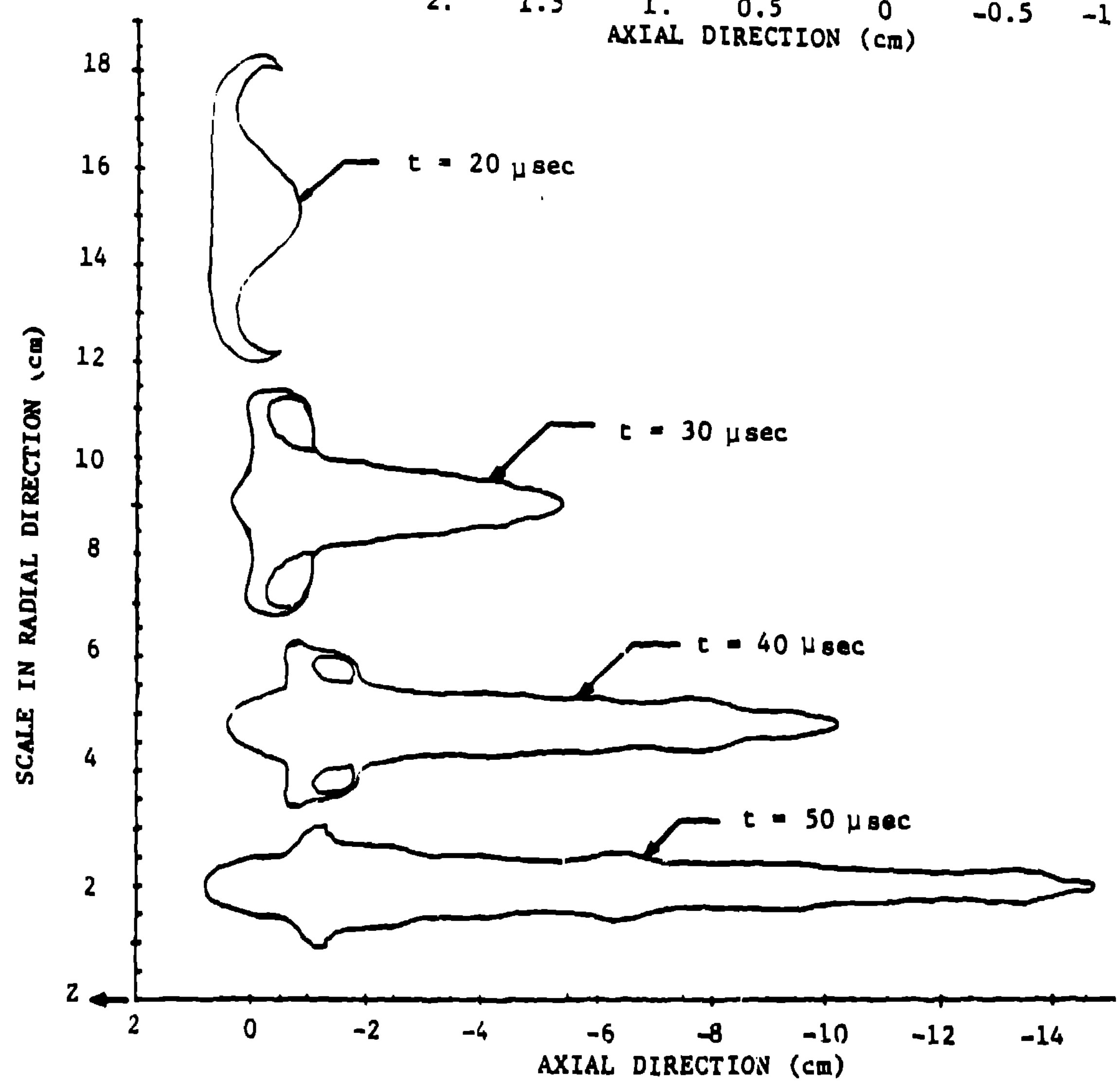


Fig. 4. THE SHAPES OF THE COPPER JET AT t = 20, 30, 40, and 50 µsec.

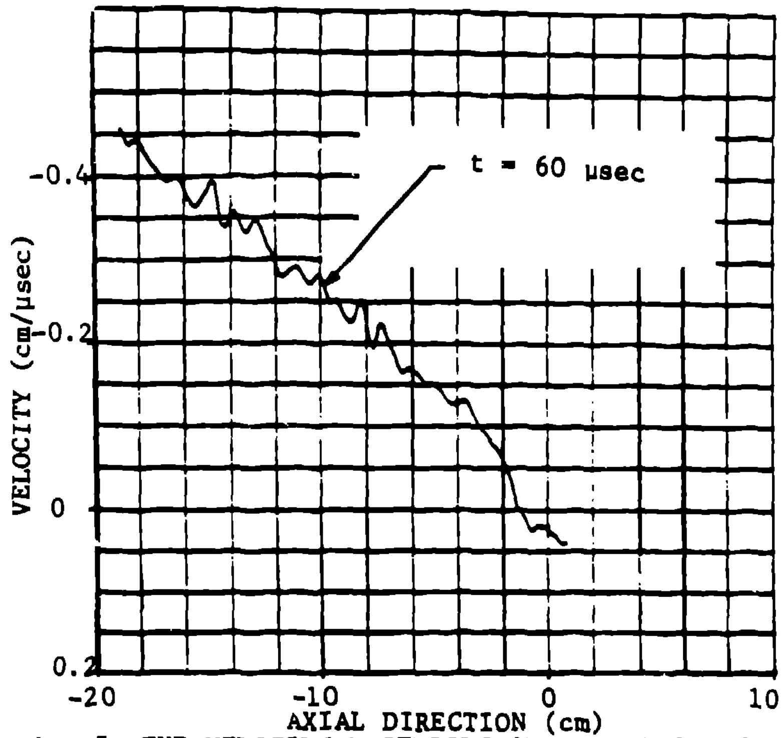


Fig. 5 THE VELOCITY DISTRIBUTIONS FOR THE LINER ALONG THE Z-AXIS.

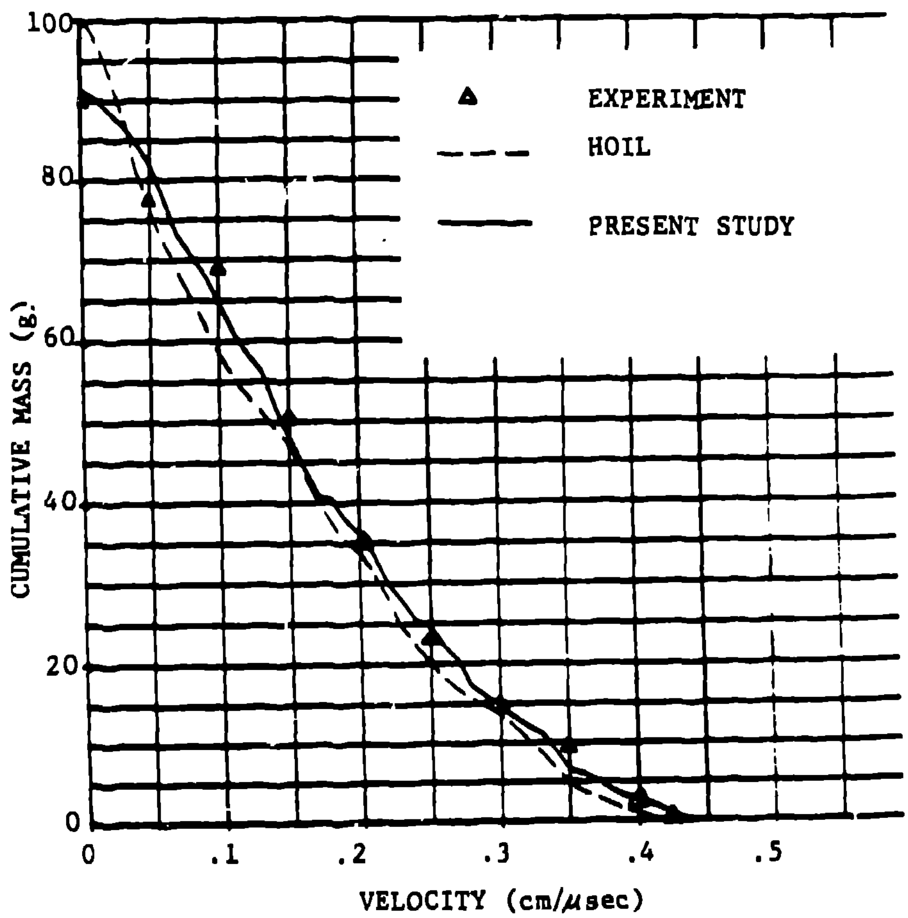


FIG. 6 COMPARISON OF CUMULATIVE MASS vs. VELOCITY AMONG EXPERIMENT, HOIL AND PRESENT CODE CALCULATIONS.