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by

James D. Kershner
Charles L. Mader

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2DE: A TWO-DIMENSIONAL CONTINUOUS EULERIAN HYDRODYNAMIC CODE FOR COMPUTING MULTICOMPONENT REACTIVE HYDRODYNAMIC PROBLEMS

by

James D. Kershner and Charles L. Mader

ABSTRACT

This report describes a code called 2DE that computes two-dimensional reactive multicomponent hydrodynamic problems in slab or cylindrical geometry using continuous Eulerian equations of motion.

Realistic equation-of-state treatments for mixed cells are combined with the donor-acceptor-cell method to calculate mixed cell fluxes.

The calculated results using the 2DE code are compared with Lagrangian calculations for several one- and two-dimensional problems.

I. INTRODUCTION

The finite difference analogs of the Eulerian equations of motion have been studied at the Los Alamos Scientific Laboratory (LASL) for more than ten years. The initial work of Rich[1] was followed by that of Gentry, Martin, and Daly,[2] which resulted in the FLIC method. A one-component Eulerian hydrodynamic code written by Gage and Mader[3] in STRETCH machine language used the features of the FLIC method and the OIL method[4] developed at General Atomic Division of General Dynamics Corporation. The 2DE code was used to solve reactive hydrodynamic problems that required high resolution of highly distorted flows. Results of the detonation physics studies using the code are described in Refs. 5 through 9.

The study described in this report was undertaken to determine whether or not the continuous Eulerian approach to reactive hydrodynamic problems, where severe distortions prevent solution by Lagrangian methods, could be extended to multicomponent problems in reactive hydrodynamics. Also, because of the untimely death of STRETCH, a FORTRAN version of the one-component Eulerian code was needed.

Multicomponent Eulerian calculations require equations of state for mixed cells and methods for moving mass and its associated state values into and out of mixed cells. The particle-in-cell (PIC) method uses particles for this movement. We previously had developed realistic equation-of-state treatments for mixed cells using the PIC method described in Ref. 10. We have extended the mixed equation-of-state treatments to include several cases not considered previously and have used the donor-acceptor method for moving mass and its associated state values as determined by the mixed equations of state.

The donor-acceptor method developed by Johnson[11] has been used by several investigators to solve a variety of problems. The donor-acceptor method for determining the mass flux was chosen over other methods, such as those proposed by Hirt[12] and developed by Hageman and Walsh,[13] only because of its ease of application. Ideally, several methods for mass flux calculations should be available in a general-purpose Eulerian code so that the best method for a particular problem can be used.

Because reactive hydrodynamic problems require as much numerical resolution as possible, the 2DE code (named after its STRETCH father) was written to make maximum use of the large capacity memory devices on the CDC 7600 data processing system.

This report describes the method in complete detail. It also presents sufficient details to enable the reader to follow and modify the code. The latter information is not of interest to the casual reader; therefore, the more tedious descriptions of the mixture equation-of-state treatments and derivations of the various equations are described in Appendixes A, B, and C.

II. THE HYDRODYNAMIC EQUATIONS.

The partial differential equations for nonviscous, nonconducting, compressible fluid flow in cylindrical coordinates are

$$\frac{\partial \rho}{\partial t} + U\frac{\partial \rho}{\partial R} + V\frac{\partial \rho}{\partial Z} = -\rho\left(\frac{\partial U}{\partial R} + \frac{\partial V}{\partial Z} + \frac{U}{R}\right) \qquad \text{Mass,}$$

$$\left.\begin{aligned}\rho\left(\frac{\partial U}{\partial t} + U\frac{\partial U}{\partial R} + V\frac{\partial U}{\partial Z}\right) &= -\frac{\partial P}{\partial R}\\ \rho\left(\frac{\partial V}{\partial t} + U\frac{\partial V}{\partial R} + V\frac{\partial V}{\partial Z}\right) &= -\frac{\partial P}{\partial Z}\end{aligned}\right\} \qquad \text{Momentum,}$$

and

$$\rho\left(\frac{\partial I}{\partial t} + U\frac{\partial I}{\partial R} + V\frac{\partial I}{\partial Z}\right) = -P\left(\frac{\partial U}{\partial R} + \frac{\partial V}{\partial Z} + \frac{U}{R}\right) \quad \text{Energy.}$$

The equations, written in finite-difference form appropriate to a fixed (Eulerian) mesh, are used to determine the dynamics of the fluid. The fluid is moved by a continuous mass transport method.

The first of the above equations, that of mass conservation, is automatically satisfied. The momentum and energy equations are treated as follows. In the first step, contributions to the time derivatives which arise from the terms involving pressure are calculated. Mass is not moved at this step; thus, the transport terms are dropped. Tentative new values of velocity and internal energy are calculated for each cell.

In the second step, the mass is moved according to the cell velocity. The mass crossing cell boundaries carries with it into the new cells appropriate fractions of the mass, momentum, and energy of the cells from which it came. This second step accomplishes the transport that was neglected in the first step.

In the third step, the amount of chemical reaction is determined, and the new cell pressure is computed using the HOM equations of state.

The equations we shall difference are of the form

$$\rho\frac{\partial U}{\partial t} = -\frac{\partial(P+q)}{\partial R} \; ,$$

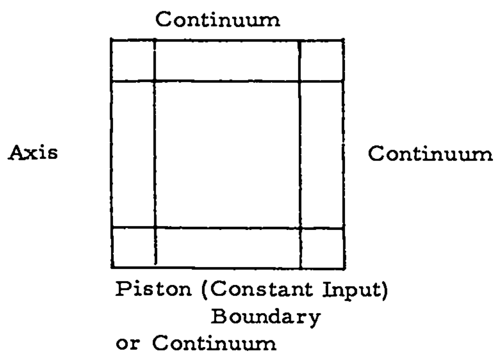
$$\rho\frac{\partial V}{\partial t} = -\frac{\partial(P+q)}{\partial Z} \; ,$$

and

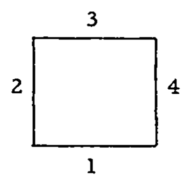
$$\rho\frac{\partial I}{\partial t} = -\frac{P}{R}\frac{\partial(UR)}{\partial R} - \frac{1}{R}\frac{\partial(qUR)}{\partial R} + U\frac{\partial q}{\partial R} - P\frac{\partial V}{\partial Z} - \frac{\partial qV}{\partial Z} + V\frac{\partial q}{\partial Z} \; .$$

III. THE CODING EQUATIONS AND TECHNIQUES

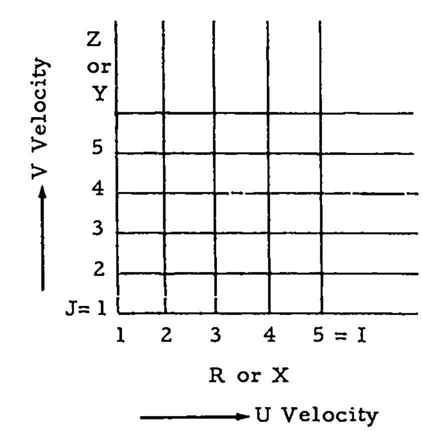
Problem Boundaries



Cell Sides



The Initial Problem Setup



Cell quantities:

ρ - CM - Cell density

I - CI - Cell internal energy

P - CP - Cell pressure

T - CT - Cell temperature

W - CW1 - Cell mass fraction for unburned explosive

U - CU - Cell r or x velocity

V - CV - Cell z velocity

$\hat{\rho}$ - RHOT - Tilde density

q - Q1, Q2, Q3, Q4 - Viscosities

$\tilde{U}$ - CUB - Cell R velocity tilde

$\tilde{V}$ - CVB - Cell Z velocity tilde

ΔM - DMASS - Density increment for mass movement

ΔE - DE - Energy increment

ΔW - DW - Mass fraction increment

ΔPU - DPU - Momentum in R direction increment

ΔPV - DPV - Momentum in Z direction increment

ID - CID - Cell identification word

The cell ID word contains a material identifier, mixed cell pointers, flags for spall, tension, and material type. It also carries temporary flags which are set when DE or DW is calculated by the mixed cell routine.

A. Phase I. Equation of State and Reaction

The pressure and temperature are calculated from the density, internal energy, and cell mass fractions using the subroutines HOM, HOM2S, HOMSG, HOM2G, or HOM2SG described in Appendix A. Mixed cells carry the individual component densities and energies as calculated from mixture equation of state.

If $\Delta V'/V'$ ($V' = \frac{1}{\rho}$), and $\Delta I/I$, from the neighboring cell and the present cell are less than 0.0005, the previous cell P and T are used, i.e., $P_{i,j} = P_{i-1,j}$ and $T_{i,j} = T_{i-1,j}$.

Knowing T, we calculate W using the Arrhenius rate law

$$\frac{\delta W}{\delta t} = -Z\ W e^{-E^*/R_g T} ,$$

where Z is the frequency factor, E^* is the activation energy, R_g is the gas constant, and

δt is the time increment. In difference form this is

$$W^{n+1} = W^n - \delta t\, Z\, W^n e^{-E^*/R_g T^{n+1}} .$$

1. If cell temperature is less than MINWT (1000), reaction is not permitted.

2. If CW1 is less than GASW (0.02), set CW 1 = 0.

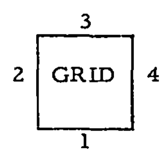
3. Do not react for first VCNT (25) cycles.

4. If CT is less than TO, CT = TO and if CP is less than PO and tension flag is O, set CP = PO.

Phases I and II are skipped if $\rho^n_{i,j} \leq$ MINGRHO + (ρ_o - MINGRHO) ($W^n_{i,j}$). This is for handling free surfaces to eliminate false diffusion. MINGRHO = 0.5. For gases at free surfaces $W^n_{i,j}$ is replaced by one.

B. Phase II. Viscosity and Velocity

1. Viscosity Equations



$$Q1_{i,j} = q^n_{i,j-\frac{1}{2}} = Q3_{i,j-1}$$

except on boundary 1 when $Q1_{i,1} = 0.0$ or on piston boundary when

$$Q1_{i,1} = K(\rho^n_{i,j} + \text{MAPP})(\text{VAPP} - V^n_{i,1}) \qquad \text{if VAPP} > V^n_{i,1}$$

$$= 0.0 \qquad \text{if VAPP} \leq V^n_{i,1} .$$

$$Q2_{i,j} = q^n_{i-\frac{1}{2},j} = Q4_{i-1,j}$$

except on axis boundary 2 when

$$Q2_{1,j} = 2Q4_{1,j} - Q4_{2,j} .$$

$$Q3_{i,j} = q^n_{i,j+\frac{1}{2}} = K(\rho^n_{i,j} + \rho^n_{i,j+1})(V^n_{i,j} - V^n_{i,j+1}) \qquad \text{if } V^n_{i,j} \geq V^n_{i,j+1}$$

$$= 0.0 \qquad \text{if } V^n_{i,j} < V^n_{i,j+1}$$

except $Q3_{i,JMAX} = 0.0$ on continuative boundary 3.

$$Q4_{i,j} = q^n_{i+\frac{1}{2},j} = K(\rho^n_{i,j} + \rho^n_{i+1,j})(U^n_{i,j} - U^n_{i+1,j}) \qquad \text{if } U^n_{i,j} \geq U^n_{i+1,j}$$

$$= 0.0 \qquad \text{if } U^n_{i,j} < U^n_{i+1,j}$$

except on continuative boundary 4 when $Q4_{IMAX,j} = 0.0$

2. Velocity Equations

$P1 = P^n_{i,j-1}$

except on piston boundary 1, P1 = PAPP or on continuative boundary 1, $P1 = P^n_{i,1}$.

$P2 = P^n_{i-1,j}$

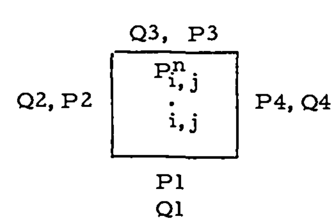
except on axis boundary 2, $P2 = P^n_{1,j}$.

$P3 = P^n_{i,j+1}$

except on continuative boundary 3, $P3 = P^n_{i,JMAX}$.

$P4 = P^n_{i+1,j}$

except on continuative boundary 4, $P4 = P^n_{i,IMAX}$.



$$\tilde{U}^n_{i,j} = U^n_{i,j} - \frac{\delta t}{\rho^n_{i,j}\,\delta R}\left(\left\{\frac{(i-1)(P4-P2) + P4-P^n_{i,j}}{2i-1}\right\} + Q4_{i,j} - Q2_{i,j}\right).$$

$$\tilde{V}^n_{i,j} = V^n_{i,j} - \frac{\delta t}{\rho^n_{i,j}\,\delta Z}\left(\frac{P3-P1}{2} + Q3_{i,j} - Q1_{i,j}\right).$$

where

$i = 1, 2, \cdots, IMAX$

$j = 1, 2, \cdots, NJMAX*JMAX$ (for NJMAX core increments containing JMAX rows each).

In slab geometry, the quantity in { } = $\frac{P4-P2}{2}$ for $\tilde{U}^n_{i,j}$.

C. Phase III. Internal Energy and $\hat{\rho}$ Calculation

1. $\hat{\rho}$ Calculation

$$\hat{\rho}^n_{i,j} = \rho^n_{i,j}\left\{1.0 - \frac{\delta t}{2\delta R}\left(U^n_{i+1,j} - U^n_{i-1,j}\right) - \frac{\delta t}{2\delta Z}\left(V^n_{i,j+1} - V^n_{i,j-1}\right)\right\}.$$

Exceptions:

Piston boundary, $V_{i,j-1} = VAPP$

Axis boundary, $U_{i-1,j} = -U_{i+1,j} + 2U_{i,j}$

boundary 3, $V_{i,j+1} = V_{i,j}$

boundary 4, $U_{i+1,j} = U_{i,j}$

2. Piston Energy Constraints

For the first VCNT cycles,

$$\bar{I}^n_{i,j} = \begin{cases} 1/2\,(P^n_{i,j} + Q3_{i,j})\,(V'_o - 1/\rho^n_{i,j}) + KE_{i,j} & \text{if } V'_o \geq 1/\rho^n_{i,j} \\ I^n_{i,j} & \text{if } V'_o < 1/\rho^n_{i,j}\,, \end{cases}$$

where $KE_{i,j} = 1/2\left(\tilde{U}^{n^2}_{i,j} + \tilde{V}^{n^2}_{i,j}\right)$.

3. Internal Energy Calculation

For $\rho^n_{i,j} <$ MINGRHO + $(\rho_o$ - MINGRHO$)(W^n_{i,j})$, $E^n_{i,j} = I^n_{i,j}$ and the rest of Phase III is skipped.

$U1 = (U^n_{i-1,j} + \tilde{U}^n_{i-1,j})$.

$U2 = (U^n_{i+1,j} + \tilde{U}_{i+1,j})$.

$V1 = (V^n_{i,j-1} + \tilde{V}^n_{i,j-1})$.

$V2 = (V^n_{i,j+1} + \tilde{V}^n_{i,j+1})$.

$T3 = (U^n_{i,j} + \tilde{U}^n_{i,j})$.

$T1 = (V^n_{i,j} + \tilde{V}^n_{i,j})$.

Exceptions:

Axis boundary, $U1 = 2(U^n_{1,j} + \tilde{U}^n_{1,j}) - U2$

Continuative boundary 4,
$U2 = (U^n_{IMAX,j} + \tilde{U}^n_{IMAX,j})$

Piston boundary, $V1 = 2VAPP$

Continuative boundary 1, $V1 = (V^n_{i,1} + \tilde{V}_{i,1})$

Continuative boundary 3,
$V2 = (V^n_{i,JMAX} + \tilde{V}^n_{i,JMAX})$.

$$\bar{I}^n_{i,j} = I^n_{i,j} - \frac{\delta t}{4\rho_{i,j}}\left(\frac{P^n_{i,j}}{\delta R}\left[U2 - U1 + \left\{\frac{U2 + 2\,T3 + U1}{2i-1}\right\}\right] + \frac{Q4_{i,j}}{\delta R}\left[U2 - T3 + \left\{\frac{2U2}{2i-1}\right\}\right] - \frac{Q2_{i,j}}{\delta R}\left[U1 - T3 - \left\{\frac{2U1}{2i-1}\right\}\right] + \frac{1}{\delta Z}\left[P^n_{i,j}\,(V2 - V1) + Q3_{i,j}\,(V2 - T1) + Q1_{i,j}\,(T1 - V1)\right]\right).$$

In slab geometry the quantities in { } are set equal to zero.

4. Total Energy Calculation

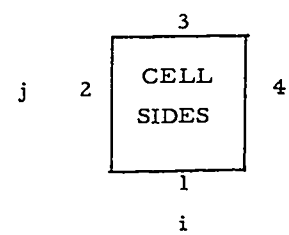
$$E^n_{i,j} = \tilde{I}^n_{i,j} + 1/2 \left[(\tilde{V}^n_{i,j})^2 + (\tilde{U}^n_{i,j})^2 \right] .$$

D. Phase IV. Mass Movement

Mass is not moved unless the pressure of the cell from which it moves is greater than FREPR (0.0005) or if the tension flag is on.

Nomenclature for Phase IV and V:

DE	Change in energy
DW	Change in mass fraction
DPU	Change in U momentum
DPV	Change in V momentum
DMASS	Change in density



1. Mass Movement Across Side 2

a. For axis boundary DMASS = 0, otherwise

$$\Delta = \frac{1/2\,(\tilde{U}^n_{i,j} + \tilde{U}^n_{i-1,j})\,(\delta t/\delta R)}{1 + (\tilde{U}^n_{i,j} - \tilde{U}^n_{i-1,j})(\delta t/\delta R)} .$$

b. If $\Delta \geq 0$ the mass moves from donor cell i-1, j to cell i, j .

$$\text{Cylindrical DMASS} = \hat{\rho}_{i-1,j} \left(\frac{2i - 2 - \Delta}{2i - 3} \right) (\Delta) .$$

$$\text{Slab DMASS} = (\hat{\rho}_{i-1,j})\,(\Delta) .$$

$$DE_{i,j} = E^n_{i-1,j}\,(\text{DMASS}) \qquad DE_{i-1,j} = DE_{i-1,j} - E^n_{i-1,j}\,(\text{DMASS}) .$$

Mixed-cell modification of DMASS and DE occurs if required as described in mixed-cell section.

$$DW_{i,j} = W^n_{i-1,j}\,(\text{DMASS}) \qquad DW_{i-1,j} = DW_{i-1,j} - W^n_{i-1,j}\,(\text{DMASS}) .$$

$$DPU_{i,j} = \tilde{U}_{i-1,j}\,(\text{DMASS}) \qquad DPU_{i-1,j} = DPU_{i-1,j} - \tilde{U}^n_{i-1,j}\,(\text{DMASS}) .$$

$$DPV_{i,j} = \tilde{V}_{i-1,j}\,(\text{DMASS}) \qquad DPV_{i-1,j} = DPV_{i-1,j} - \tilde{V}_{i-1,j}\,(\text{DMASS}) .$$

$$\text{Cylindrical} \quad DM_{i,j} = \text{DMASS} \left(\frac{2i-3}{2i-1} \right) \qquad DM_{i-1,j} = DM_{i-1,j} - \text{DMASS} .$$

$$\text{Slab} \quad DM_{i,j} = \text{DMASS}.$$

c. If $\Delta < 0$, the mass moves from the donor cell i, j to acceptor cell i-1, j.

$$\text{Cylindrical DMASS} = \hat{\rho}^n_{i,j} \frac{(2i - 2 - \Delta)}{(2i - 1)} \Delta, \quad \text{slab DMASS} = \hat{\rho}^n_{i,j} \Delta .$$

$$DE_{i,j} = E^n_{i,j} \text{ (DMASS)} \qquad DE_{i-1,j} = DE_{i-1,j} - E^n_{i,j} \text{ (DMASS)} .$$

Mixed-cell modification of DMASS and DE occurs if required,

$$DW_{i,j} = W^n_{i,j} \text{ (DMASS)} \qquad DW_{i-1,j} = DW_{i-1,j} - W^n_{i,j} \text{ (DMASS)}.$$

$$DPU_{i,j} = \tilde{U}^n_{i,j} \text{ (DMASS)} \qquad DPU_{i-1,j} = DPU_{i-1,j} - \tilde{U}_{i,j} \text{ (DMASS)} .$$

$$DPV_{i,j} = \tilde{V}^n_{i,j} \text{ (DMASS)} \qquad DPV_{i-1,j} = DPV_{i-1,j} - \tilde{V}_{i,j} \text{ (DMASS)} .$$

$$DM_{i,j} = \text{DMASS} \qquad \text{Cylindrical} \quad DM_{i-1,j} = DM_{i-1,j} - \text{DMASS}\left(\frac{2i-1}{2i-3}\right) .$$

$$\text{Slab } DM_{i-1,j} = \text{DMASS} .$$

2. Mass Movement Across Side 1

a. For a piston boundary

$$\Delta = 1/2 \; \frac{(\text{VAPP} + \tilde{V}^n_{i,j})\,(\delta t/\delta Z)}{(\tilde{V}^n_{i,j} - \text{VAPP})\,(\delta t/\delta Z) + 1} .$$

For $\Delta < 0$, DMASS = 0.

For $\Delta > 0$, DMASS = (MAPP) (Δ), and the mass moves from the piston to cell i, j.

$$DE_{i,j} = DE_{i,j} + \text{DMASS (EAPP)} .$$

$$DW_{i,j} = DW_{i,j} + \text{DMASS (WAPP)} .$$

$$DPV_{i,j} = DPV_{i,j} + \text{DMASS (VAPP)} .$$

$$DPU_{i,j} = DPU_{i,j} + \text{DMASS (UAPP)} .$$

$$DM_{i,j} = DM_{i,j} + \text{DMASS} .$$

b. For continuative boundary 1 cell,

$$\Delta = (\tilde{V}^n_{i,j})\,(\partial t/\partial Z)\ .$$

$$DMASS = (\hat{\rho}^n_{i,j})\,(\Delta)\ .$$

$$DE_{i,j} = DE_{i,j} + E^n_{i,j}\,(DMASS)\ .$$

Mixed-cell modifications of DMASS and DE occurs if required.

$$DW_{i,j} = DW_{i,j} + W^n_{i,j}\,(DMASS)\ .$$

$$DPV_{i,j} = DPV_{i,j} + \tilde{V}_{i,j}\,(DMASS)\ .$$

$$DPU_{i,j} = DPU_{i,j} + \bar{U}_{i,j}\,(DMASS)\ .$$

$$DM_{i,j} = DM_{i,j} + DMASS\ ,$$

otherwise

$$\Delta = \frac{1/2\,(\tilde{V}^n_{i,j} + \tilde{V}^n_{i,j-1})\,(\delta t/\delta Z)}{1 + (\tilde{V}^n_{i,j} - \tilde{V}^n_{i,j-1})\,(\delta t/\delta Z)}\ .$$

c. If $\Delta \geq 0$, the mass moves from donor cell i, j-1 to acceptor cell i, j.

$$DMASS = (\hat{\rho}_{i,j-1})\,(\Delta)\ .$$

$$DE_{i,j} = DE_{i,j} + E^n_{i,j-1}\,(DMASS) \qquad DE_{i,j-1} = DE_{i,j-1} - E^n_{i,j-1}\,(DMASS)\ .$$

Mixed-cell modification of DMASS and DE occurs if required.

$$DW_{i,j} = DW_{i,j} + W^n_{i,j-1}\,(DMASS) \qquad DW_{i,j-1} = DW_{i,j-1} - W_{i,j-1}\,(DMASS)\ .$$

$$DPV_{i,j} = DPV_{i,j} + \tilde{V}^n_{i,j-1}\,(DMASS) \qquad DPV_{i,j-1} = DPV_{i,j-1} - \tilde{V}_{i,j-1}\,(DMASS)\ .$$

$$DPU_{i,j} = DPU_{i,j} + \bar{U}^n_{i,j-1}\,(DMASS) \qquad DPU_{i,j-1} = DPU_{i,j-1} - \tilde{U}_{i,j-1}\,(DMASS)\ .$$

$$DM_{i,j} = DM_{i,j} + DMASS \qquad DM_{i,j-1} = DM_{i,j-1} - DMASS\ .$$

d. If $\Delta < 0$, the mass moves from donor cell i, j to acceptor cell i, j-1.

$$DMASS = (\hat{\rho}^n_{i,j})\,(\Delta)\;.$$

$$DE_{i,j} = DE_{i,j} + E^n_{i,j}\,(DMASS) \qquad DE_{i,j-1} = DE_{i,j-1} - E^n_{i,j}\,(DMASS)\;.$$

Mixed-cell modification of DMASS and DE occurs if required.

$$DW_{i,j} = DW_{i,j} + W^n_{i,j}\,(DMASS) \qquad DW_{i,j-1} = DW_{i,j-1} - W^n_{i,j}\,(DMASS)\;.$$

$$DPV_{i,j} = DPV_{i,j} + \bar{V}_{i,j}\,(DMASS) \qquad DPV_{i,j-1} = DPV_{i,j-1} - \tilde{V}^n_{i,j}\,(DMASS)\;.$$

$$DPU_{i,j} = DPU_{i,j} + \tilde{U}_{i,j}\,(DMASS) \qquad DPU_{i,j-1} = DPU_{i,j-1} - \tilde{U}_{i,j}\,(DMASS)\;.$$

$$DM_{i,j} = DM_{i,j} + DMASS \qquad DM_{i,j-1} = DM_{i,j-1} - DMASS\;.$$

3. Mass Movement Across Side 3

Except on continuative boundary 3, this mass movement is taken care of by the mass movement across side 1 of the cell directly above.

On the boundary 3,

$$\Delta = (\bar{V}^n_{i,j})\,(\delta t/\delta Z)\;.$$

$$DMASS = (\hat{\rho}^n_{i,j})\,(\Delta)\;.$$

$$DE_{i,j} = DE_{i,j} - E_{i,j}\,(DMASS)\;.$$

Mixed-cell modification of DMASS and DE occurs if required.

$$DW_{i,j} = DW_{i,j} - W_{i,j}\,(DMASS)\;.$$

$$DPV_{i,j} = DPV_{i,j} - \bar{V}_{i,j}\,(DMASS)\;.$$

$$DPU_{i,j} = DPU_{i,j} - \tilde{U}_{i,j}\,(DMASS)\;.$$

$$DM_{i,j} = DM_{i,j} - DMASS\;.$$

4. Mass Movement Across Side 4

Except on the continuative boundary 4, this mass movement is taken care of by the mass movement across side 2 of the cell on its right.

For i = IMAX

$$\Delta = 0.5\,(3\,\tilde{U}^n_{i,j} - \tilde{U}^n_{i-1,j})\,(\partial t/\partial R)\ .$$

a. $\Delta \geq 0$ mass moves out of cell i, j.

$$\text{Cylindrical DMASS} = (\hat{\rho}_{i,j})\,\frac{(2i-\Delta)(\Delta)}{(2i-1)}\ .$$

b. $\Delta \leq 0$ mass moves into cell i, j .

$$\text{Cylindrical DMASS} = (\hat{\rho}_{i,j})\,\frac{(2i-\Delta)}{(2i+1)}\,(\Delta)$$

for either a. or b. Slab DMASS = $(\hat{\rho}_{i,j})\,(\Delta)$.

$$DE_{i,j} = DE_{i,j} - E^n_{i,j}\,(\text{DMASS})\ .$$

Mixed-cell modification of DMASS and DE occurs if required.

$$DW_{i,j} = DW_{i,j} - W^n_{i,j}\,(\text{DMASS})\ .$$

$$DPV_{i,j} = DPV_{i,j} - \tilde{V}_{i,j}\,(\text{DMASS})\ .$$

$$DPU_{i,j} = DPU_{i,j} - \tilde{U}_{i,j}\,(\text{DMASS})\ .$$

$$DM_{i,j} = DM_{i,j} - \text{DMASS}\ .$$

5. Mixed Cells

The composition of the mass to be moved from the donor to the acceptor cell is determined as follows. Materials common to both the donor and acceptor cells are moved according to the mass fractions of common materials in the acceptor cell. If the donor and acceptor cell have no common materials, then mass is moved according to the mass fractions of the donor cell. The mass to be moved from the donor cell has the density and energy determined for that component or components by the mixture equation-of-state calculation in Phase I.

1. Therefore, the DMASS term is corrected by dividing by cell ρ used in Phase IV and replacing it with the ρ of the material being moved from the donor cell (ρ_k).

$$\text{DMASS} = \text{DMASS}\ \frac{\rho_k}{\rho}\ .$$

If the mass of the material in the donor cell is less than the total mass to be moved, the remainder of the mass moved has the remaining donor-cell composition density and energy.

2. The DE term is calculated using the internal energy of the component being moved from the donor cell as calculated from the mixture equation-of-state routines in Phase I.

$$DE^{n+1}_{\text{DONOR}} = DE^{n}_{\text{DONOR}} - (\text{DMASS})\,(\text{Donor Component I} + \text{Donor K.E.})\ .$$

$$DE^{n+1}_{\text{ACCEPTOR}} = DE^{n}_{\text{ACCEPTOR}} + (\text{DMASS})\,(\text{Donor Component I} + \text{Donor K.E.})\ .$$

The mass fraction of decomposing explosive between a mixed and unmixed cell is treated as follows. If the donor cell is mixed and explosive is being moved to an acceptor cell, the donor cell CW is not changed. If the acceptor cell is mixed and explosive is being moved into the acceptor cell the acceptor cell W is calculated by

$$CW^{n+1}_{\text{ACCEPTOR}} = \frac{\left(CW^n_{\text{ACCEPTOR}}\right)\left(\rho^n_{\substack{\text{ACCEPTOR}\\ \text{EXPLOSIVE}}}\right) + (\text{DMASS})\left(CW^n_{\text{DONOR}}\right)}{\rho^n_{\substack{\text{ACCEPTOR}\\ \text{EXPLOSIVE}}} + \text{DMASS}}$$

By convention CW is set to equal 1.0 for an inert or 0.0 for a gas if the donor or acceptor does not contain an explosive.

E. Phase V. Repartition

Add on mass moved quantities.

For $\rho^n_{i,j} > \text{MINGRHO} + (\rho_o - \text{MINGRHO})\,(W^n_{i,j})$,

$$\rho^{n+1}_{i,j} = \rho^n_{i,j} + DM_{i,j} .$$

$$W^{n+1}_{i,j} = \frac{1}{\rho^{n+1}_{i,j}} (\rho^n_{i,j} W^n_{i,j} + DW_{i,j}).$$

$$V^{n+1}_{i,j} = \frac{1}{\rho^{n+1}_{i,j}} (\bar{V}^n_{i,j} \rho^n_{i,j} + DPV_{i,j}) .$$

$$U^{n+1}_{i,j} = \frac{1}{\rho^{n+1}_{i,j}} (\bar{U}^n_{i,j} \rho^n_{i,j} + DPU_{i,j}) .$$

$$I^{n+1}_{i,j} = \frac{1}{\rho^{n+1}_{i,j}} (\rho^n_{i,j} E^n_{i,j} + DE_{i,j}) - \frac{1}{2} \left((V^{n+1}_{i,j})^2 + (U^{n+1}_{i,j})^2 \right) .$$

For $\rho^n_{i,j} \le \text{MINGRHO} + (\rho_o - \text{MINGRHO})\,(W^n_{i,j})$,

$$\rho^{n+1}_{i,j} = \rho^n_{i,j} + DM_{i,j} .$$

$$W^{n+1}_{i,j} = \frac{1}{\rho^{n+1}_{i,j}} (\rho^n_{i,j} W^n_{i,j} + DW_{i,j}) .$$

$$V^{n+1}_{i,j} = \frac{1}{\rho^{n+1}_{i,j}} (V^n_{i,j} \rho^n_{i,j} + DPV_{i,j}) .$$

$$U^{n+1}_{i,j} = \frac{1}{\rho^{n+1}_{i,j}} (U^n_{i,j} \rho^n_{i,j} + DPU_{i,j}).$$

$$I^{n+1}_{i,j} = 0.0 .$$

IV. TEST PROBLEMS

The 2DE code has been used to calculate one-component, two-dimensional problems of a shock in nitromethane interacting with a rectangular or a cylindrical void. The results agreed with those published in Ref. 6.

The 2DE code has been used to calculate the one-dimensional, multicomponent problem of an 85 kbar shock in 0.04 cm of nitromethane described by 100 cells in the Z direction, interacting with a 0.016-cm slab of aluminum described by 40 cells, which had as its other interface 0.016 cm of air at 1 atm initial pressure described by 40 cells. The equation of state for nitromethane and aluminum were identical to those described in Ref. 10. The calculated pressure, energy, and particle velocity profiles are shown in Fig. 1. The results were compared with SIN[14] one-dimensional Lagrangian calculations for the same problem. A comparison of the average results of the calculations is shown below. The units are mbar, cm^3/g, mbar-cm^3/g, degrees Kelvin, and cm/μsec respectively for pressure, specific volume, energy, temperature and particle velocity.

	Eulerian	Lagrangian
Nitromethane Shock		
Pressure	0.0858	0.0857
Specific Volume	0.5455	0.5455
Energy	0.0146	0.0146
Temperature	1146.2	1181.9
Particle Velocity	0.171	0.171
Reflected Shock (Nitromethane)		
Pressure	0.178	0.1787
Specific Volume	0.4686	0.4858
Energy	0.02248	0.0225
Temperature	1365.5	1436.1
Particle Velocity	0.0967	0.0964
Aluminum Shock		
Pressure	0.1785	0.1786
Specific Volume	0.3071	0.3070
Energy	0.0047	0.0046
Temperature	487.1	518.3
Particle Velocity	0.0964	0.0964
Aluminum Rarefaction		
Pressure	0.008	0.0004
Specific Volume	0.3561	0.3603
Energy	0.0007	0.0005
Temperature	384.0	355.5
Particle Velocity	0.1873	0.1932

The agreement between the Lagrangian and Eulerian calculations is adequate except at the nitromethane-aluminum interface. In the Eulerian calculation, the internal energy is 11% too high in the nitromethane cell next to the interface and is

10% too low in the aluminum cell next to the interface. Such an error is in the expected direction because the reflected shock Hugoniot has less energy than the single shock Hugoniots used to partition the energy between the doubly shocked nitromethane and the singly shocked aluminum in the mixture equation-of-state routines. This suggests that an improved mixture equation-of-state treatment could be accomplished by keeping track of whether the component had been previously shocked and by partitioning the energy accordingly.

Of course, it is not correct to assume that the Lagrangian calculation treated the boundary in an exact manner. Because of the large density difference, the Lagrangian calculation had nitromethane energies that were 6.6% too high at the interface and aluminum energies that were 2.4% too low.

The 2DE code has been used to calculate the two-dimensional, multicomponent problem of an 85-kbar shock in a cylinder of nitromethane interacting with a 0.025-cm radius aluminum sphere and an 85-kbar shock in a slab of nitromethane interacting with an aluminum rod. The calculation was performed with 100 cells in the Z direction and 50 cells in the R direction of 0.001 cm. The results compared well with those obtained previously using the PIC technique in the EIC[10] code which were compared with PHERMEX radiographs of the interaction of shocks in water with aluminum rods (Ref. 15).

The isoplots for the aluminum rod being shocked in nitromethane are shown at various times in Fig. 2.

The results of these and other test problems support our conclusion that the continuous Eulerian approach to reactive hydrodynamic problems can be used to solve multicomponent problems involving reactive flow. Further improvement is possible in the treatment of the mixture equations of state. The mass flux treatment from mixed cells could be improved by including more constraints on the donor-acceptor method, and by including some interface following technique such as those used by Hageman and Walsh[13] and proposed by Hirt.[12]

We plan to use the code in its present form to study several reactive and nonreactive flow problems of current interest. We also plan to include into the code the capability to describe elastic-plastic and viscous flow similar to that used in our two-dimensional reactive Lagrangian code 2DL. We plan to include other methods for describing the decomposition of the explosive such as C-J volume burn, sharp-shock burn, heterogeneous sharp-shock partial reaction burn and Dremin burn.

It is already apparent that a three-dimensional version of the 2DE code would be a useful tool and would probably be more useful than a three-dimensional particle Eulerian code such as the one we studied in Ref. 16. Such a capability would permit more realistic modeling of the reactive fluid dynamics problems discussed in Refs. 6, 7, and 9. It would, of course, be useful for studying many other problems.

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PRESSURE

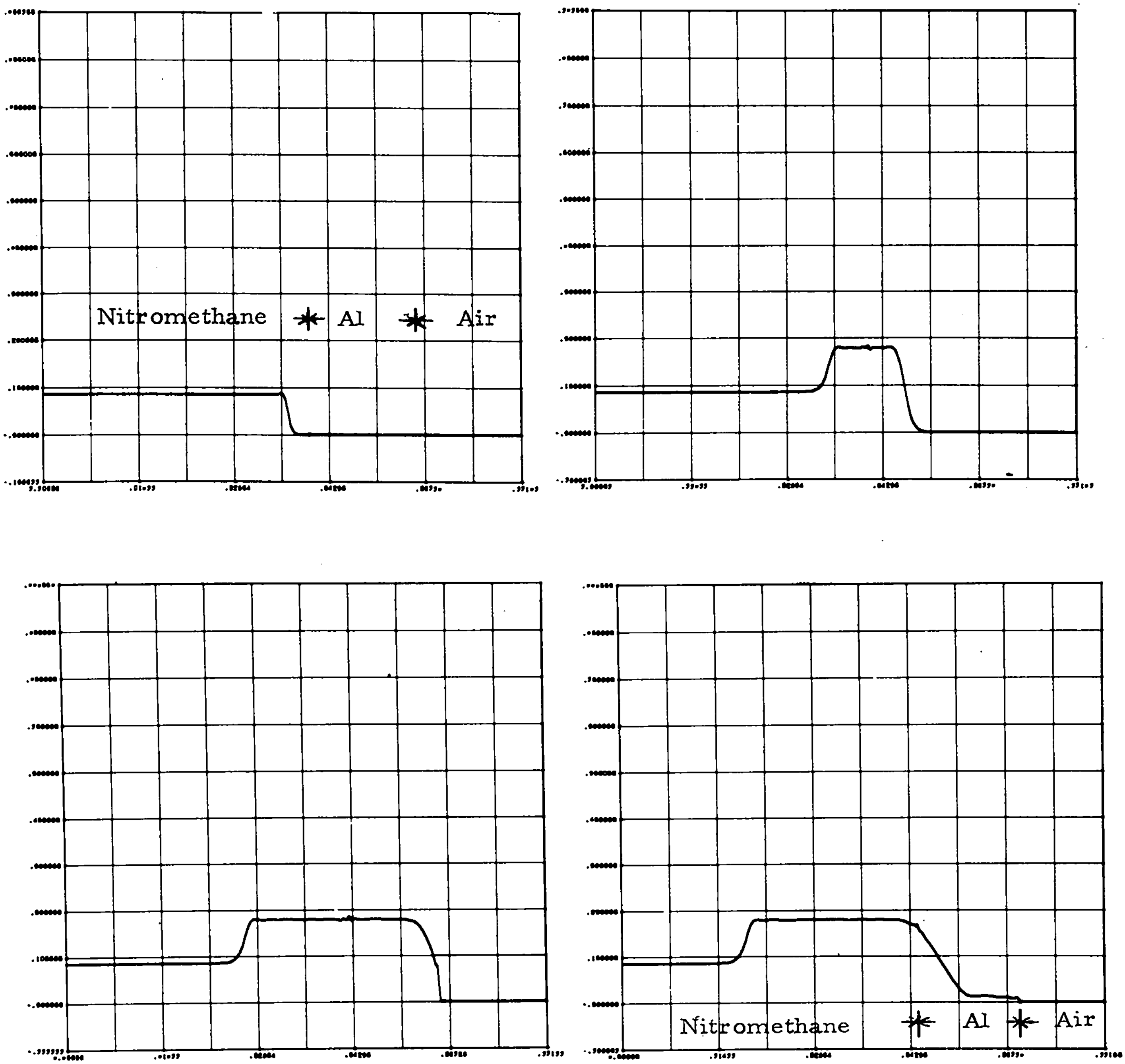


Fig. 1. The pressure, internal energy, and particle velocity profiles as a function of distance at 0.080, 0.096, 0.112, and 0.128 μsec for an 85-kbar shock in nitromethane interacting with a 0.016-cm-thick aluminum plate and then with air are shown. The pressure scale is 0.1 mbar, the internal energy scale is 0.01 mbar-cm^3/g and the particle velocity scale is 0.2 cm/μsec.

INTERNAL ENERGY

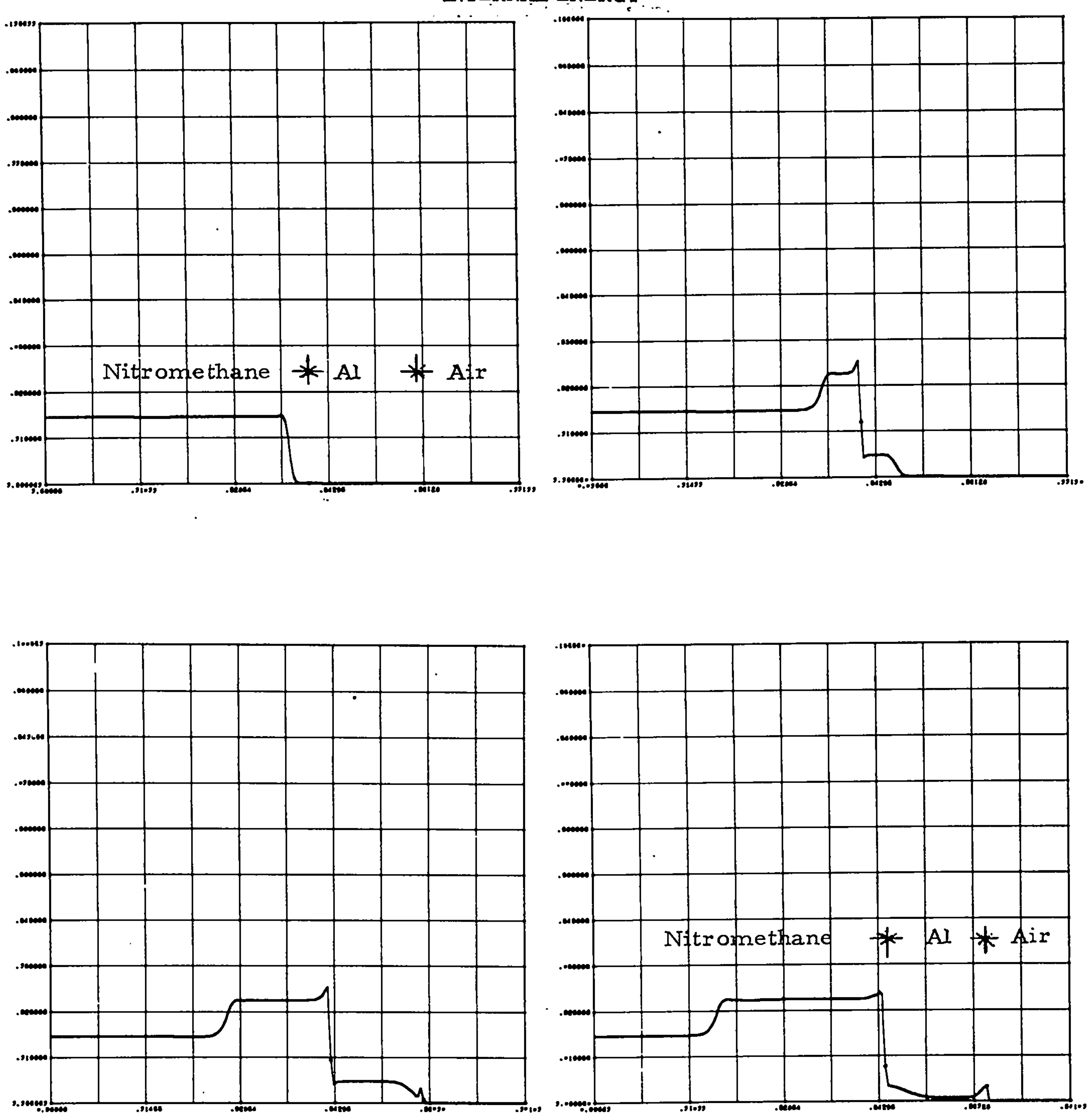


Fig. 1. (cont)

PARTICLE VELOCITY

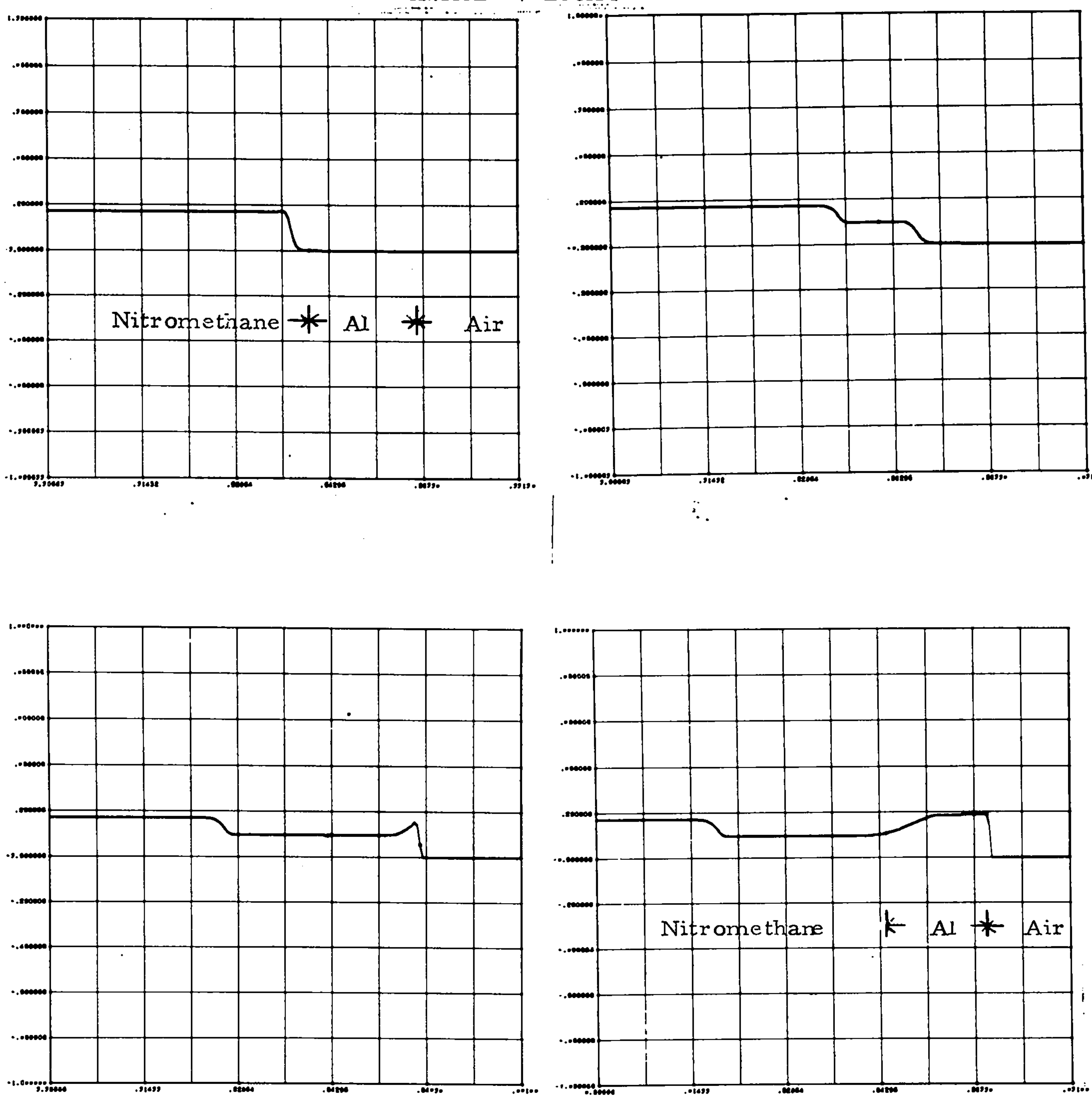


Fig. 1. (cont)

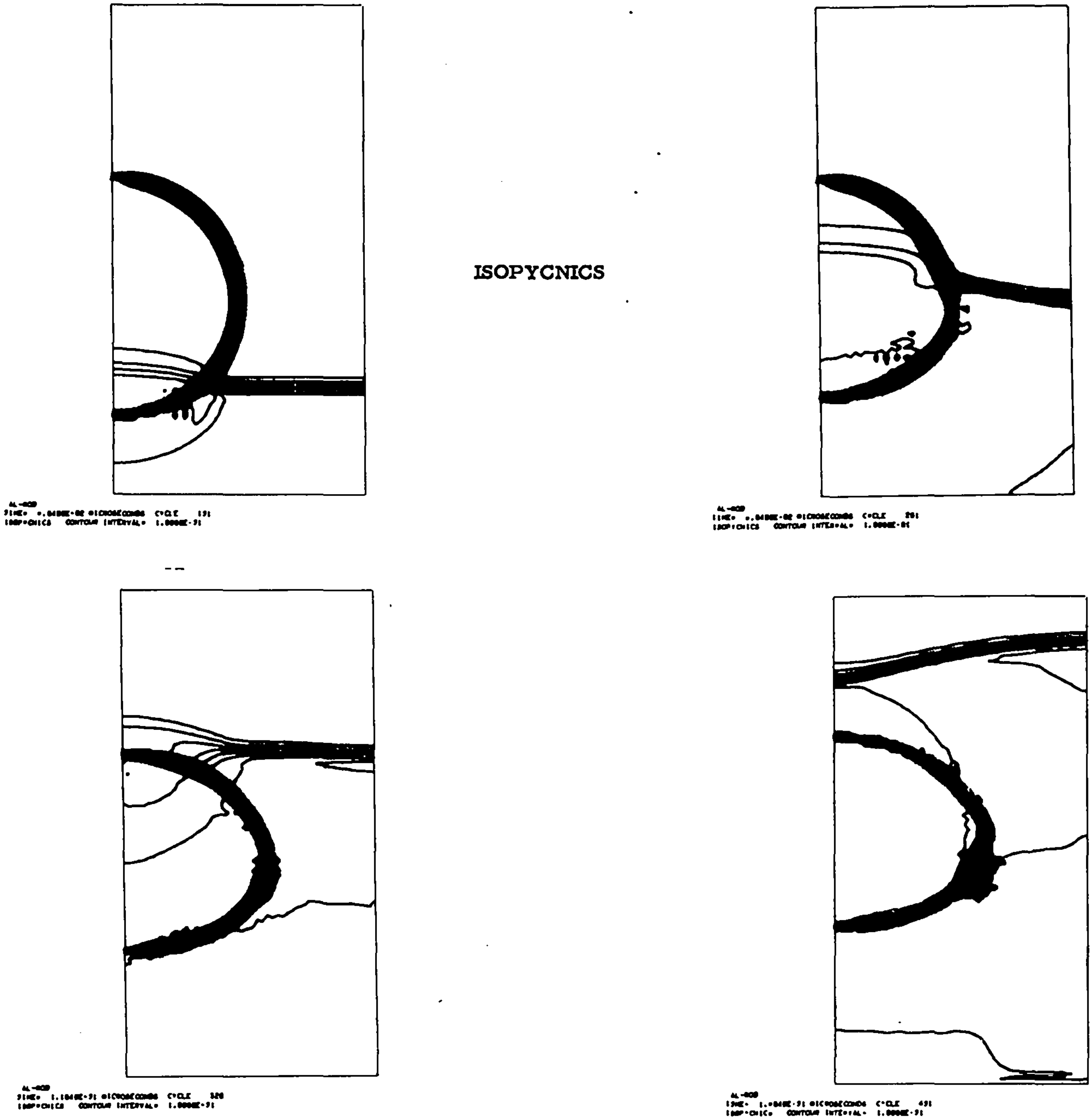


Fig. 2. The isopycnics, isobars, isotherms, isoenergy, and isovelocity in the X direction and isovelocity in Y direction profiles at 0.04, 0.08, 0.13, and 0.18 μsec for an 85-kbar shock in nitromethane interacting with a 0.025-cm-radius aluminum rod are shown. The contour intervals are 0.1 g/cm^3, 0.01 mbar, 200° K, 0.005 mbar-cm^3/g, and 0.01 cm/μsec. The locations of the mixed cells are shown with an "*".

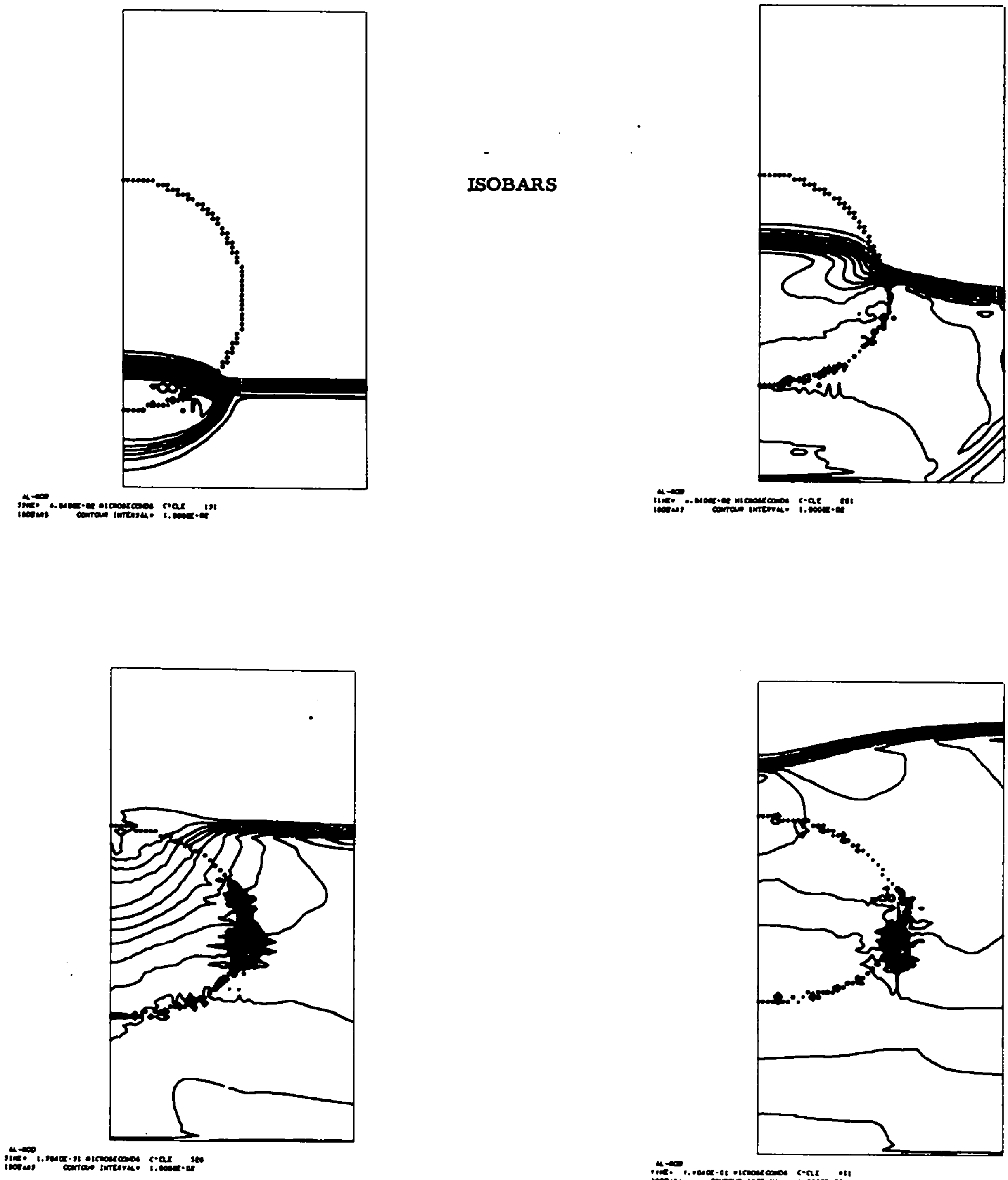


Fig. 2. (cont)

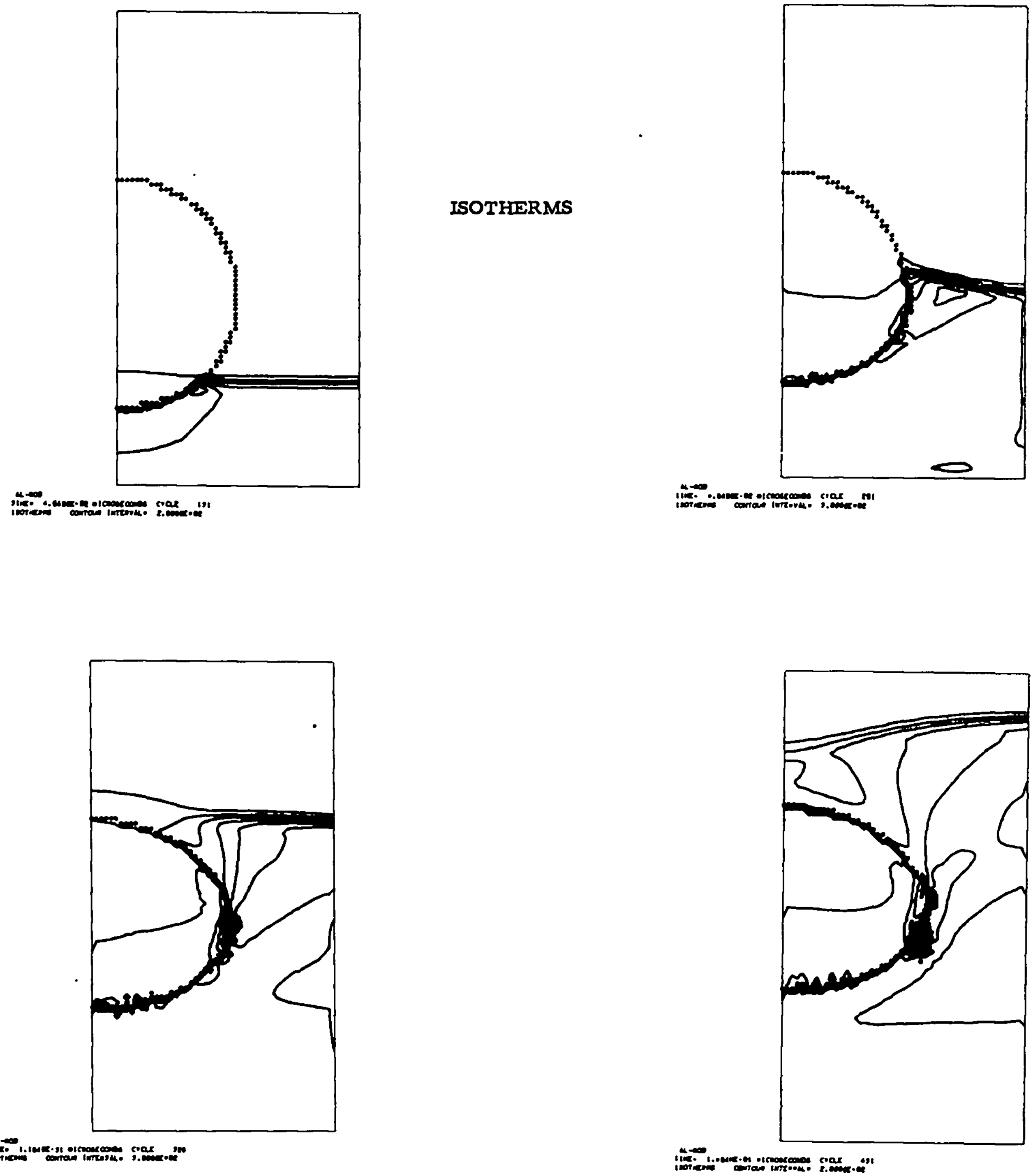


Fig. 2. (cont)

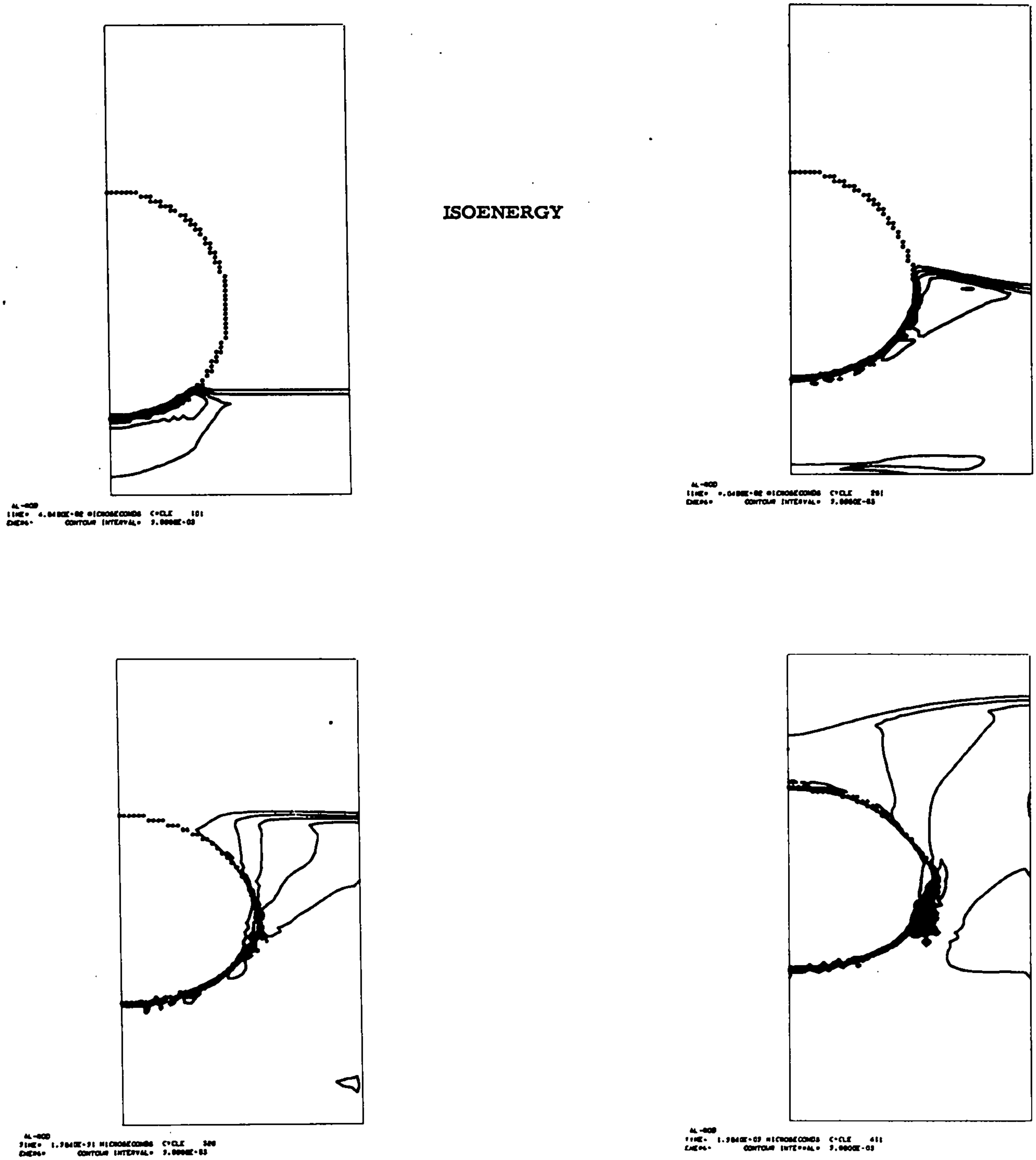


Fig. 2. (cont)

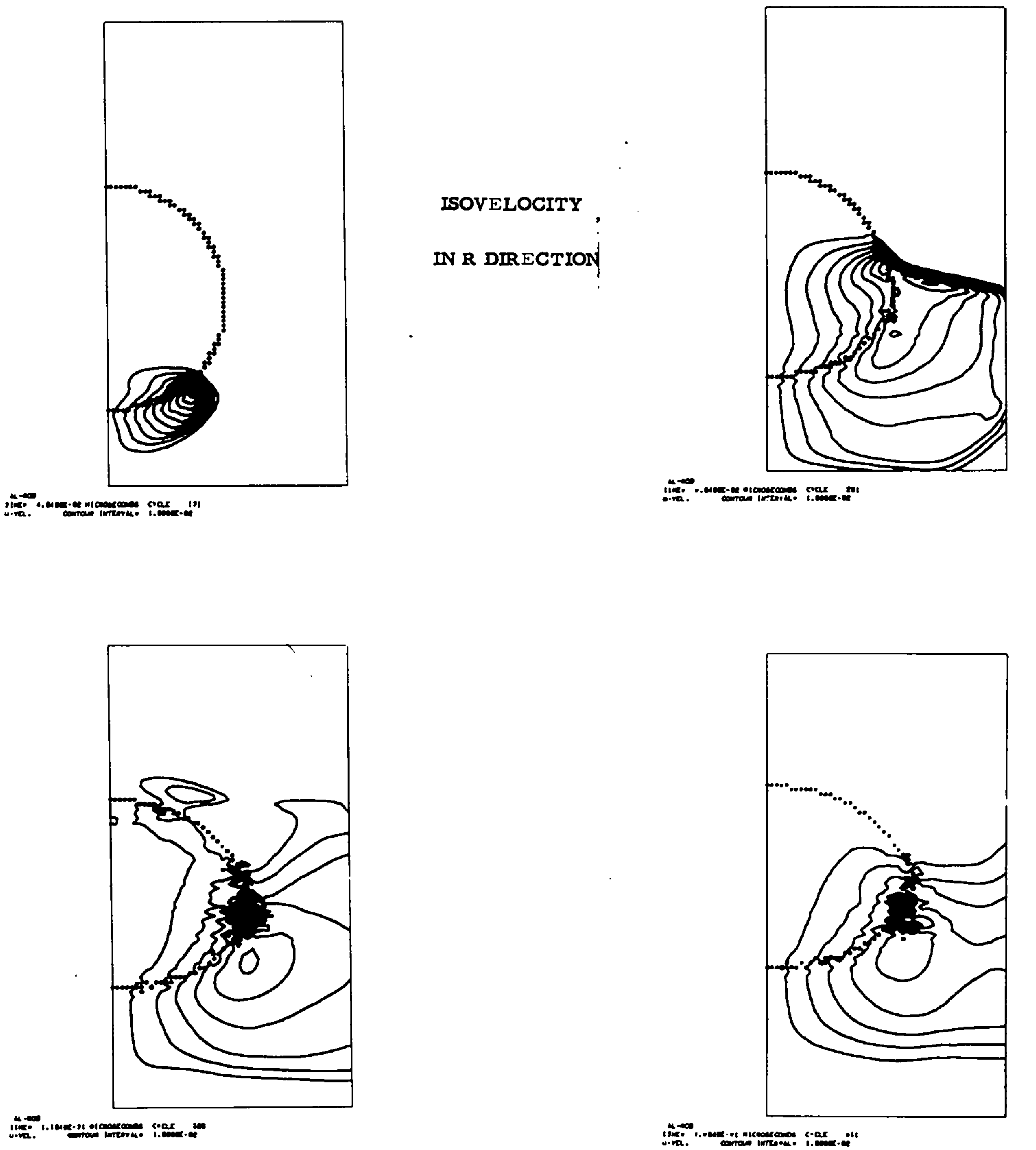


Fig. 2. (cont)

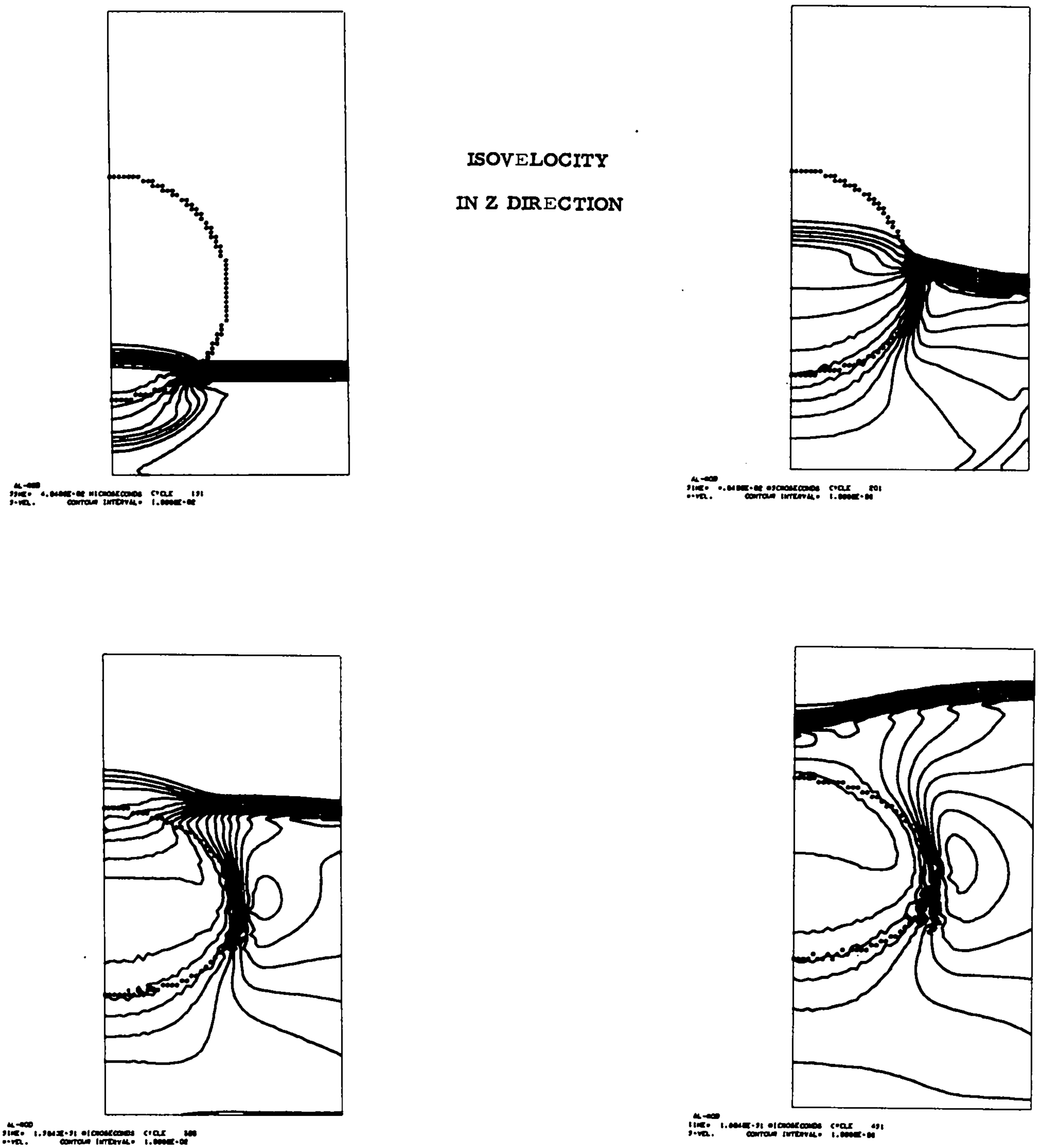


Fig. 2. (cont)

APPENDIX A
EQUATIONS OF STATE

The HOM equation of state was used for a cell containing a single component or any mixture of condensed explosive and detonation products. Temperature and pressure equilibrium was assumed for any mixture of detonation products and condensed explosive in a cell.

When there are two components present in a cell, separated by a boundary and not homogeneously mixed, it is reasonable to assume pressure equilibrium, but the temperatures may be quite different. For these systems we assumed that the difference between the total Hugoniot energy and the total cell energy was distributed between the components according to the ratio of the Hugoniot energies of the components for two solids or liquids. For two gases we assumed that the difference between the total isentrope energy and the total cell energy was distributed between the components according to the ratio of the isentrope energies of the components. For a solid and a gas we assumed that the difference between the sum of the gas isentrope energy and the solid Hugoniot energy and the total cell energy was distributed between the components according to the ratio of the gas isentrope energy and the solid Hugoniot energy of the components.

When there are three components present in a cell, an explosive, its detonation products, and a third solid or liquid nonreactive component, the equation of state is computed assuming temperature and pressure equilibrium for the detonation products and condensed explosive, and pressure equilibrium with the nonreactive component.

The equation-of-state subroutines require the specific volume, internal energy, and mass fractions of the components as input and iterate to give the pressure, the individual densities, temperatures, and energies of the components.

This treatment of the equation of state of mixtures is attractive because if the state values of the components are reasonably close to the state value for the standard curve (the Hugoniot for the solid or the isentrope for the gas), one can have considerable confidence in the calculated results. For the gases it would be best to choose a state value near those expected in the problem to use for forming the isentrope.

Nomenclature:

C, S	coefficients to a linear fit of U_s and U_p
C1, S1	second set of coefficients to a linear fit of U_s and U_p
C_V	heat capacity of condensed component (cal/g/deg)
C'_V	heat capacity of gaseous component (cal/g/deg)
I	total internal energy (Mbar-cm^3/g)
P	pressure (Mbar)
SPA	spalling constant to relate spall pressure and tension rate
SPALL P	interface spalling pressure
T	temperature (^{o}K)
USP	ultimate spalling pressure
U_p	particle velocity
U_s	shock velocity
V	total volume (cm^3/g).
V_o	initial volume of condensed component (cm^3/g)
W	mass fraction of undecomposed explosive
X or χ	mass fraction of solid or gaseous component

Subscripts:

g	gaseous component
H	Hugoniot
i	isentrope
s	condensed component
A	component A
B	component B

I. HOM

HOM is used for a single solid or gas component and for mixtures of solid and gas components in pressure and temperature equilibrium.

The Method

A. Condensed Components

(The mass fraction, W, is 1; the internal energy, I, is I_s; and the specific volume, V, is V_s.) For volumes less than V_o, the experimental Hugoniot data are expressed as a linear fit of the shock and particle velocities. The Hugoniot temperatures are computed using the Walsh and Christian technique.

$$U_s = C + SU_P$$

$$P_H = \frac{C^2(V_o - V_s)}{[V_o - S(V_o - V_s)]^2} \ .$$

$$\ln T_H = F_s + G_s \ln V_s + H_s (\ln V_s)^2 + I_s(\ln V_s)^3 + J_s (\ln V_s)^4 \ . \tag{A-1}$$

$$I_H = \frac{1}{2} P_H (V_o - V_s) \ .$$

$$P_s = \frac{\gamma_s}{V_s} (I_s - I_H) + P_H, \text{ where } \gamma_s = V\left(\frac{\partial P}{\partial E}\right)_V \ . \tag{A-2}$$

$$T_s = T_H + \frac{(I_s - I_H)(23,890)}{C_V} \ . \tag{A-3}$$

Two sets of C and S coefficients may be given. For V_s < MINV, the fit $U_s = C1 + S1\,(U_p)$ is used with the corresponding changes to the above equations. Between MINV and VSW, the volume is set equal to MINV, and $U_s = C1 + S1\,(U_p)$ is used. For volumes greater than V_o, we use the Grüneisen equation of state and the P = 0 line as the standard curve.

$$P_s = \left[I_s - \frac{C_V}{(3)(23890)(\alpha)}\left(\frac{V_s}{V_o} - 1\right)\right]\frac{\gamma_s}{V_s} \ .$$

$$T_s = \frac{(I_s)(23,890)}{C_V} + T_o \ .$$

The spalling option is not used if SPA < 0.0001. If $P_s \le$ USP, set P_s = SPALL P and set the spall indicator. If $P_s \le \text{SPA}\sqrt{\Delta P/\Delta X}$ ($\Delta P/\Delta X$ is the tension rate), and $P_s \le$ SPMIN (5×10^{-3}) set P_s = SPALL P and set the spall indicator. Do not spall if neither of the above conditions is satisfied.

B. Gas Components

(Mass Fraction, W, is 0; the internal energy, I, is I_g; and the specific volume, V, is V_g.) The pressure, volume, temperature, and energy values of the detonation products are computed using FORTRAN BKW and are fitted by a method of least squares to Eqs. (4) through (6). A gamma-law gas may also be fit to these equations as a special case.

$$\ln P_i = A + B\ln V_g + C(\ln V_g)^2 + D(\ln V_g)^3 + E(\ln V_g)^4 . \tag{A-4}$$

$$\ln I_i = K + L\ln P_i + M(\ln P_i)^2 + N(\ln P_i)^3 + O(\ln P_i)^4 \ . \tag{A-5}$$

$I_i = I_i - Z$ (where Z is a constant used to change the standard state to be consistent with the solid explosive standard state, and if the states are the same, Z is used to keep I positive when making a fit).

$$\ln T_i = Q + R\ln V_g + S(\ln V_g)^2 + T(\ln V_g)^3 + U(\ln V_g)^4 . \tag{A-6}$$

$$-\frac{1}{\beta} = R + 2S\ln V_g + 3T(\ln V_g)^2 + 4U(\ln V_g)^3 \ .$$

$$P = \left(\frac{1}{\beta V_i}\right)(I_g - I_i) + P_i \ . \tag{A-7}$$

$$T = T_i + \frac{(I_g - I_i)(23,890)}{C'_V} \ . \tag{A-8}$$

C. Mixture of Condensed and Gaseous Components

$(0 < W < 1)$

$V = WV_s + (1 - W)V_g$.

$I = WI_s + (1 - W)I_g$.

$P = P_g = P_s$.

$T = T_g = T_s$.

Multiplying Eq. (3) by (W/C_V) and Eq. (8) by $(1 - W)/C_V$ and adding, we get, after substituting T for T_s and T_g and I for $WI_s + (1 + W)I_g$,

$$T = \frac{23,890}{C_V W + C'_V(1 - W)} \left\{ I - \left[WI_H - I_i(1 - W) \right] + \frac{1}{23,890} \left[T_H C_V W + T_i C'_V (1 - W) \right] \right\} . \qquad (A\text{-}9)$$

Equating Eq. (2) and (7) and substituting from Eq. (9), we get

$$P_H - P_i + \left(\frac{\gamma_s C_V}{V_s} - \frac{C'_V}{\beta V_g} \right) \left(\frac{1}{C_V W + C'_V(1-W)} \left\{ I - \left[WI_H + I_i (1-W) \right] + \frac{1}{23,890} \left[T_H C_V W + T_i C'_V (1-W) \right] \right\} \right) - \frac{1}{23,890} \left(\frac{\gamma_s C_V T_H}{V_s} - \frac{C'_V T_i}{\beta V_g} \right) = 0 . \qquad (A\text{-}10)$$

Knowing V, I, and W, one may use the linear feedback to iterate on either V_s or V_g until Eq. (10) is satisfied.

For $V < V_o$, we iterate on V_s with an initial guess of $V_s = V_o$ and a ratio to get the second guess of 0.999. For $V \geq V_o$, we iterate on V_g with an initial guess of $V_g = (V - 0.9\, V_o W)(1 - W)$ and a ratio to get the second guess of 1.002.

If the iteration goes out of the physical region ($V_g \leq 0$ to $V_s \leq 0$), that point is replaced by $V_s = V_g = V$. Then knowing V_s and V_g, we calculate P and T.

The Calling Sequence

CALL HOM (V, S, G, IND)

V, S, and G are dimensioned arrays of size 5, 23, and 17 numbers, respectively.

V(1)	specific volume V
V(2)	internal energy I
V(3)	mass fraction W
V(4)	$- \lvert \frac{\Delta P}{\Delta x} \rvert$ input; pressure P output
V(5)	temperature T output
S(1)	C
S(2)	S
S(3)	VSW
S(4)	C1
S(5)	S1
S(6)	F
S(7)	G
S(8)	H
S(9)	I
S(10)	J
S(11)	γ_s
S(12)	C_V
S(13)	V_o
S(14)	α
S(15)	SPA
S(16)	USP

S(17)	T_o
S(18)	P_o
S(22)	SPALL P
S(23)	MINV
G(1)	A
G(2)	B
G(3)	C
G(4)	D
G(5)	E
G(6)	K
G(7)	L
G(8)	M
G(9)	N
G(10)	O
G(11)	Q
G(12)	R
G(13)	S
G(14)	T
G(15)	U
G(16)	C'_V
G(17)	Z

IND is set to 0 for normal exit, to -1 for iteration error in mixture calculations, and to +1 for a spalled solid.

II. HOM2S

HOM2S is used for two solids or liquids that are in pressure, but not for temperature equilibrium.

The Method

Knowing total energy I, total volume V, and the mass fraction X of component A present, we iterate for the volume of A, V^A, if X is greater than 0.5 and for the volume of B, V^B, if X is less than 0.5.

To obtain our first guess we assume that the volumes of A and B are proportional to the initial specific volumes of the components. So

$$V^A = \frac{V}{X + \frac{V_o^B}{V_o^A}(1-X)}$$

or

$$V^B = \frac{V}{W\left(\frac{V_o^A}{V_o^B}\right) + 1 - W} \quad .$$

We have the following relationships.

$$\text{(a)} \quad V = X\,(V^A) + (1 - X)\,(V^B)$$

$$\text{(b)} \quad P = P^A = P^B \quad . \qquad \text{(A-11)}$$

Knowing V^A and V^B, we calculate I_H^A and I_H^B from Eq. (1).

$$\text{(c)} \quad I_H = X\,(I_H^A) + (1 - X)\,(I_H^B) \;,$$

$$\text{(d)} \quad I^A = (I_H^A) + (I - I_H)\left(\frac{X(I_H^A)}{I_H}\right) \;,$$

and

$$\text{(e)} \quad I^B = (I_H^B) + (I - I_H)\left(\frac{(1-X)\,(I_H^B)}{I_H}\right) .$$

Using the Grüneisen Eq. (2) and Eq. (11), we find

$$\text{(f)} \quad \frac{\gamma_S^A}{V^A}\,(I^A - I_H^A) + P_H^A - \frac{\gamma_S^B}{V^B}\,(I^B - I_H^B) - P_H^B \approx 0. \qquad \text{(A-12)}$$

Knowing V, I, and X, one may use linear feedback to iterate on either V^A or V^B until Eq. (12) is satisfied. The pressure and temperatures may be calculated as in HOM.

<u>The Calling Sequence</u>

CALL HOM2S (V, S^A, S^B, IND) V, S^A, and S^B are dimensioned arrays of size 10, 23, and 23 numbers, respectively. S^A and S^B have the same values as S described in HOM.

V(1)	specific volume V	Input
V(2)	internal energy I	Input
V(3)	mass fraction X	Input
V(4)	P	Output
V(5)	T^A	Output
V(6)	T^B	Output
V(7)	I^A	Output
V(8)	I^B	Output
V(9)	V^A	Output
V(10)	V^B	Output

IND = 0 for normal exit

= -2 for iteration error.

III. HOMSG

HOMSG is used when there is one solid or liquid and one gas in pressure but not temperature equilibrium.

<u>The Method</u>

Knowing total energy I, total volume V, and the mass fraction X of the solid present, we iterate on the solid volume V^S. To obtain our first guess we use V if it is less than V_o^S, otherwise we use 0.99 V_o^S. We have the following relationships.

$$\text{(a)} \quad V = X\,(V^S) + (1 - X)\,(V^G)$$

and

$$\text{(b)} \quad P = P^S = P^G \,. \qquad \text{(A-13)}$$

Knowing V^S and V^G, we calculate I_H from Eq. (2) and I_i^G from Eq. (5).

$$\text{(c)} \quad I' = X\,(I_H^S) + (1 - X)\,(I_i^G) \,,$$

$$\text{(d)} \quad I'' = X\,(I_H^S) + (1 - X)\,(|I_i^G|) \,,$$

$$\text{(e)} \quad I^S = I_H^S + (I - I')\left(X(I_H^S)\right)/I'' \,,$$

and

$$\text{(f)} \quad I^G = I_i^G + (I - I')\left((1 - X)\,(|I_i^G|)\right)/I'' \,.$$

From Eq. (13) we equate Eqs. (2) and (7) to obtain

$$\text{(g)} \quad \frac{\gamma_S}{V^S}\,(I^S - I_H^S) + P_H^S - \frac{1}{\beta V^G}\,(I^G - I_i^G) - P_i^G = 0 \,. \qquad \text{(A-14)}$$

Knowing V, I, and X, one may use linear feedback to iterate on V^S until Eq. (14) is satisfied. The pressure and temperatures may be calculated as in HOM.

The Calling Sequence

CALL HOMSG (V, S, G, IND) V, S, and G are dimensioned arrays of size 10, 23, and 17 numbers, respectively.

S and G have the same values as S and G described in HOM.

V(1)	V	Input
V(2)	I	Input
V(3)	X	Input
V(4)	P	Output
V(5)	T^S	Output
V(6)	T^G	Output
V(7)	I^S	Output
V(8)	I^G	Output
V(9)	V^S	Output
V(10)	V^G	Output

IND = 0 for normal exit

= -3 for iteration error.

IV. HOM2G

HOM2G is used for two gases that are in pressure but not temperature equilibrium.

The Method

Knowing total energy I, total volume V, and the mass fraction X of gas A present, we iterate on V^A. To obtain our first guess we assume that the volumes of A and B are proportional to the initial specific volumes of the components with the limitation that the ratio of the initial specific volumes is less than 10 or greater than 0.1.

$$V^A = \frac{V}{X + \frac{V_o^B}{V_o^A}(1 - X)} .$$

We have the following relationships.

(a) $V = X\,(V^A) + (1 - X)\,V^B$

and

(b) $P = P^A = P^B$. (A-15)

Knowing V^A and V^B, we calculate I_i^A and I_i^B using Eq. (5).

(c) $I' = X\,(I_i^A) + (1 - X)\,(I_i^B)$,

(d) $I'' = X\,(|I_i^A|) + (1 - X)\,(|I_i^B|)$,

(e) $I^A = I_i^A + (I - I')\left(X(|I_i^A|)\right)/I''$,

and

(f) $I^B = I_i^B + (I - I')\left((1 - X)\,(|I_i^B|)\right)/I''$.

Using Eqs. (15) and (7), we find

$$\frac{1}{\beta^A V^A}\,(I^A - I_i^A) + P_i^A - \frac{1}{\beta^B V^B}\,(I^B - I_i^B) - P_i^B = 0 . \qquad \text{(A-16)}$$

Knowing V, I, and X, linear feedback can be used to iterate on V^A until Eq. (16) is satisfied. The pressures and temperatures may be calculated as in HOM.

The Calling Sequence

CALL HOM2G (V, SA, GA, SB, GB, IND) V, S, and G are dimensioned arrays of size 10, 23, and 17 numbers, respectively. S and G have the same values as described in HOM.

V(1)	V	Input
V(2)	I	Input
V(3)	X	Input
V(4)	P	Output
V(5)	T^A	Output
V(6)	T^B	Output
V(7)	I^A	Output
V(8)	I^B	Output
V(9)	V^A	Output
V(10)	V^B	Output

INP = 0 for normal exit

= -5 for iteration error.

V. HOM2SG

HOM2SG is used for mixtures of an undecomposed explosive, detonation products, and a nonreactive component that is in pressure; but not thermal equilibrium with the explosive and its products that are assumed to be in pressure and thermal equilibrium.

To obtain the initial guess for the volume of the undecomposed explosive $V^{(1)}$, the volume of the detonation products $V^{(2)}$, and the volume of the nonreactive component $V^{(3)}$, we guess a volume for $V^{(2)}$ of 0.9 of $V_o^{(1)}$ and then estimate $V^{(1)}$ and $V^{(3)}$, assuming the remaining volume is partitioned proportional to the initial specific volumes of components (1) and (3). Given reasonable initial guesses, the iteration is successful; however, unreasonable guesses result in iteration failure. We have the following relationships.

(a) $P = P^{(1)} = P^{(2)} = P^{(3)}$, (A-17)

(b) $T^{(1)} = T^{(2)}$, (A-18)

(c) $V^{(1+2)} = W(V^{(1)}) + (1-W)(V^{(2)})$, (A-19)

(d) $V = \chi(V^{(3)}) + (1-\chi)(V^{(1+2)})$, (A-20)

(e) $I^{(1+2)} = W(I^{(1)}) + (1-W)(I^{(2)})$,

(f) $I_H^{(1+2)} = W(I_H^{(1)}) + (1-W)(I_i^{(2)})$,

(g) $I_H = \chi(I_H^{(3)}) + (1-\chi)(I_H^{(1+2)})$,

(h) $I^{(3)} = (I_H^{(3)}) + (I-I_H)\left(\dfrac{(\chi)(I_H^{(3)})}{I_H}\right)$, (A-21)

(i) $I^{(1+2)} = (I_H^{(1+2)}) + (I-I_H)\left(\dfrac{1-\chi)(I_H^{(1+2)})}{I_H}\right)$, (A-22)

and

(j) $I = I^{(3)} - I_H^{(3)} + I^{(1+2)} - I_H^{(1+2)} + I_H$

From Eqs. (19) and (20), one obtains

(k) $V = \chi(V^{(3)}) + (1-\chi)\left[W(V^{(1)}) + (1-W)(V^{(2)})\right]$.

From Eq. 2,

(l) $P^{(3)} = P_H^{(3)} + \dfrac{Y^{(3)}}{V^{(3)}}\left[I^{(3)} - I_H^{(3)}\right]$, (A-23)

and from Eqs. (17) and (21), one obtains

(m) $f_1 = P = P_H^{(3)} + \dfrac{Y^{(3)}}{V^{(3)}}\left[(I-I_H)\dfrac{(\chi)(I_H^{(3)})}{I_H}\right]$. (A-24)

From Eq. (7),

(n) $P^{(2)} = P_i^{(2)} + \dfrac{1}{\beta V^{(2)}}\left[I^{(2)} - I_i^{(2)}\right]$, (A-25)

and from Eqs. (23), (21), and (22), one obtains

$$f_2 = P = \left[I - I_H + \frac{V^{(3)}\,P_H^{(3)}}{Y^{(3)}} + \frac{V^{(1)}P_H^{(1)}W}{Y^{(1)}} + (1-W)\,P_i^{(2)}\,\beta V^{(2)}\right] \cdot \left[\frac{V^{(3)}}{Y^{(3)}} + \frac{W(V^{(1)})}{Y^{(1)}} + (1-W)V^{(2)}\beta\right]^{-1} . \quad \text{(A-26)}$$

From Eq. (3),

$$T^{(1)} = T_H^{(1)} + \frac{(I^{(1)} - I_H^{(1)})\,(23,890)}{C_V} ,$$

and from Eqs. (18), (23), and (25), one obtains

$$f_3 = P = \left[\frac{T_i^{(2)} - T_H^{(1)}}{23,890} + \frac{P_H^{(1)}V^{(1)}}{C_V^{(1)}\,Y^{(1)}} - \frac{P_i^{(2)}\,\beta V^{(2)}}{C_V^{(2)}}\right]\left[\frac{V^{(1)}}{C_V^{(1)}Y^{(1)}} - \frac{\beta(V^{(2)})}{C_V^{(2)}}\right]^{-1} . \quad \text{(A-27)}$$

To keep I_i positive the energy base for all the components is raised by Z for the iteration procedure.

Taking

and $F = f_1 - f_3 = 0$

$G = f_2 - f_3 = 0$,

one may solve for $V^{(1)}$ and $V^{(2)}$ by the Newton-Raphson method. These equations were first derived by W. Gage.

The Celling Sequence

CALL HOM2SG (V, S3, S1, G2, IND)

V, S3, S1, and G2 are dimensioned arrays of size 14, 23, 23, and 17, respectively. S3 is the nonreactive component, S1 is the undecomposed explosive, and G2 is its detonation products. S3, S1 have the same values as S in HOM, and G2 has the same values as G in HOM.

V(1)	V	Input
V(2)	I	Input
V(3)	X (S3 mass fraction relative to S1 + G2 + S3)	
V(4)	W (S1 mass fraction relative to S1 + G2)	
V(5)	P	Output
V(6)	V(3)	Output
V(7)	V(1)	Output
V(8)	V(2)	Output
V(9)	I(3)	Output
V(10)	I(1)	Output
V(11)	I(2)	Output
V(12)	T(3)	Output
V(13)	T(1)	Output
V(14)	T(2)	Output

IND = 0 for normal exit

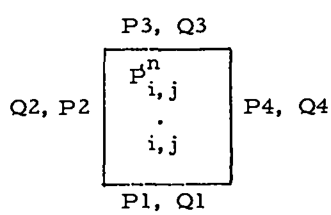
= -4 for iteration error.

APPENDIX B
DERIVATIONS OF MOMENTUM, ENERGY, AND MASS MOVEMENT EQUATIONS

In this appendix we present the derivations of the difference approximations used to describe the momentum and energy equations with the transport terms dropped. The method used for mass movement is also described in detail. This is the OIL method described in Refs. 4 and 11.

I. DERIVATION OF MOMENTUM EQUATIONS

$$\rho \frac{\partial V}{\partial t} = - \frac{\partial(P+q)}{\partial Z}$$



$$\tilde{V}^n_{i,j} = V^n_{i,j} - \frac{\delta t}{\rho^n_{i,j}\delta Z}\left[(P+q)^n_{i,j+\frac{1}{2}} - (P+q)^n_{i,j-\frac{1}{2}}\right]$$

$$= V^n_{i,j} - \frac{\delta t}{\rho_{i,j}\delta Z}\left[P^n_{i,j+\frac{1}{2}} + q^n_{i,j+\frac{1}{2}} - P_{i,j-\frac{1}{2}} - q_{i,j-\frac{1}{2}}\right]$$

$$P^n_{i,j+\frac{1}{2}} = \frac{(P^n_{i,j} + P^n_{i,j+1})}{2} = \frac{(P^n_{i,j} + P3)}{2}$$

$$P^n_{i,j-\frac{1}{2}} = \frac{(P^n_{i,j} + P1)}{2}$$

$$\tilde{V}^n_{i,j} = V^n_{i,j} - \frac{\delta t}{\rho_{i,j}\delta Z}\left[\frac{P3 - P1}{2} + Q3_{i,j} - Q1_{i.j}\right]$$

$$\rho\frac{\partial U}{\partial t} = -\frac{\partial(P+q)}{\partial R}$$

$$\tilde{U}^n_{i,j} = U^n_{i,j} - \frac{\delta t}{\rho^n_{i,j}}\left\{\frac{1}{2V_i}\left[S^r_{i+\frac{1}{2}}\left(P^n_{i+1,j} - P^n_{i,j}\right) - S^r_{i-\frac{1}{2}}\left(P^n_{i-1,j} - P^n_{i,j}\right)\right] + \frac{1}{\delta R}\left[q^n_{i+\frac{1}{2},j} - q^n_{i-\frac{1}{2},j}\right]\right\}$$

$$S^r_{i+\frac{1}{2}} = 2\pi(i)\,\delta R\delta Z \qquad V'_i = 2\pi(i-\tfrac{1}{2})\,\delta R^2\,\delta Z$$

$$\tilde{U}^n_{i,j} = U^n_{i,j} - \frac{\delta t}{\rho^n_{i,j}\delta R}\left\{\frac{1}{2i-1}\left[(i)(P^n_{i+1,j} - P^n_{i,j}) - (i-1)(P^n_{i-1,j} - P^n_{i,j})\right] + q^n_{i+\frac{1}{2},j} - q^n_{i-\frac{1}{2},j}\right\}$$

$$= U^n_{i,j} - \frac{\delta t}{\rho^n_{i,j}\delta R}\left\{\frac{(i-1)(P4-P2) + P4 - P^n_{i,j}}{2i-1} + Q4_{i,j} - Q2_{i,j}\right\} .$$

II. DERIVATION OF ENERGY EQUATION

$$\rho\left(\frac{\partial I}{\partial t} + U\frac{\partial I}{\partial R} + V\frac{\partial I}{\partial Z}\right) = -P\left(\frac{\partial U}{\partial R} + \frac{\partial V}{\partial Z} + \frac{U}{R}\right)$$

$$\rho\left(\frac{\partial I}{\partial t} + U\frac{\partial I}{\partial R} + V\frac{\partial I}{\partial Z}\right) = -P\left(\frac{1}{R}\frac{\partial UR}{\partial R} + \frac{\partial V}{\partial Z}\right),$$

eliminating the transport terms

$$\rho\frac{\partial I}{\partial t} = -\frac{P}{R}\frac{\partial UR}{\partial R} - P\frac{\partial V}{\partial Z} .$$

Add on viscosity to P.

$$\rho\frac{\partial I}{\partial t} = -\frac{(P+q)}{R}\frac{\partial UR}{\partial R} - (P+q)\frac{\partial V}{\rho Z}$$

$$= -\frac{P}{R}\frac{\partial UR}{\partial R} - q\frac{\partial UR}{\partial R} - P\frac{\partial V}{\partial Z} - q\frac{\partial V}{\partial Z} .$$

$$\rho\frac{\partial I}{\partial t} = -\frac{P}{R}\frac{\partial UR}{\partial R} - \frac{1}{R}\frac{\partial qUR}{\partial R} + U\frac{\partial q}{\partial R} - p\frac{\partial V}{\partial Z} - \frac{\partial qV}{\partial Z} + V\frac{\partial q}{\partial Z} .$$

The above equation is known as the ZIP energy equation and is differenced as follows.

$$\tilde{I}^n_{i,j} = I^n_{i,j} - \frac{\delta t}{\rho^n_{i,j}V'_i}\left\{P^n_{i,j}\left(S^r_{i+\frac{1}{2}}\overline{U}^n_{i+\frac{1}{2},j} - S^r_{i-\frac{1}{2}}\overline{U}^n_{i,j-\frac{1}{2}}\right) + \tfrac{1}{2}q^n_{i+\frac{1}{2},j}\left(S^r_{i+1}\overline{U}^n_{i+1,j} + S^r_i\overline{U}^n_{i,j}\right) - \tfrac{1}{2}q^n_{i-\frac{1}{2},j}\right.$$

$$\left(S^r_i\overline{U}^n_{i,j} + S^r_{i-1}\overline{U}^n_{i-1,j}\right) - \overline{U}^n_{i,j}S^r_i\left(q^n_{i+\frac{1}{2},j} - q^n_{i-\frac{1}{2},j}\right) - \overline{V}^n_{i,j}S^Z_i\left(q^n_{i,j+\frac{1}{2}} - q^n_{i,j-\frac{1}{2}}\right) + S^Z_i$$

$$\left.\left[\overline{V}^n_{i,j+\frac{1}{2}}\left(P^n_{i,j} + q^n_{i,j+\frac{1}{2}}\right) - \overline{V}^n_{i,j-\frac{1}{2}}\left(P^n_{i,j} + q^n_{i,j-\frac{1}{2}}\right)\right]\right\} ,$$

where

$$\overline{U}^n_{i+\frac{1}{2},j} = \frac{1}{4}\left(U^n_{i,j} + \tilde{U}^n_{i,j} + U^n_{i+1,j} + \tilde{U}_{i+1,j}\right)$$

$$\overline{V}^n_{i,j+\frac{1}{2}} = \frac{1}{4}\left(V^n_{i,j} + \tilde{V}^n_{i,j} + V^n_{i,j+1} + \tilde{V}^n_{i,j+1}\right)$$

$$\overline{U}^n_{i,j} = \frac{1}{2}\left(U^n_{i,j} + \tilde{U}^n_{i,j}\right)$$

$$\overline{V}^n_{i,j} = \frac{1}{2}\left(V^n_{i,j} + \tilde{V}^n_{i,j}\right)$$

$$\tilde{I}^n_{i,j} = I^n_{i,j} - \frac{\delta t}{\rho^n_{i,j}\, V'_i}\left\{P^n_{i,j}\left(S^r_{i+\frac{1}{2}}\,\overline{U}^n_{i+\frac{1}{2},j} - S^r_{i-\frac{1}{2}}\,\overline{U}^n_{i,j-\frac{1}{2}}\right) + \frac{1}{2}\,q^n_{i+\frac{1}{2},j}\left(S^r_{i+1}\,\overline{U}^n_{i+1,j} - S^r_i\,\overline{U}^n_{i,j}\right) - \frac{1}{2}\,q^n_{i-\frac{1}{2},j}\right.$$

$$\left(S^r_{i-1}\,\overline{U}^n_{i-1,j} - S^r_i\,\overline{U}^n_{i,j}\right) + S^Z_i\left[P^n_{i,j}\left(\overline{V}^n_{i,j+\frac{1}{2}} - \overline{V}^n_{i,j-\frac{1}{3}}\right) + q^n_{i,j+\frac{1}{2}}\left(\overline{V}^n_{i,j+\frac{1}{2}} - \overline{V}^n_{i,j}\right) + q^n_{i,j-\frac{1}{2}}\right.$$

$$\left.\left.\left(\overline{V}^n_{i,j} - \overline{V}^n_{i,j-\frac{1}{2}}\right)\right]\right\}.$$

$$S^r_i = 2\pi\,(i - \tfrac{1}{2})\,\delta R\,\delta Z$$

$$V'_i = 2\pi\,(i - \tfrac{1}{2})\,\delta R^2\,\delta Z$$

$$S^Z_i = 2\pi\,(i - \tfrac{1}{2})\,\delta R^2$$

$$U1 = \left(U^n_{i-1,j} + \overline{U}^n_{i-1,j}\right)$$

$$U2 = \left(U^n_{i+1,j} + \tilde{U}^n_{i+1,j}\right)$$

$$V1 = \left(V^n_{i,j-1} + \overline{V}^n_{i,j-1}\right)$$

$$V2 = \left(V^n_{i,j+1} + \tilde{V}_{i,j+1}\right)$$

$$T3 = \left(U^n_{i,j} + \overline{U}^n_{i,j}\right)$$

$$T1 = \left(V^n_{i,j} + \tilde{V}^n_{i,j}\right).$$

$$\tilde{I}^n_{i,j} + I_{i,j} - \frac{\delta t}{\rho^n_{i,j}}\left\{\frac{P^n_{i,j}}{2(2i-1)\delta R}\left[(i)\,(T3 + U2) - (i - 1)\,(T3 - U1)\right] + \frac{Q4_{i,j}}{2(2i-1)\delta R}\left[(i + \tfrac{1}{2})\,U2 - (i - \tfrac{1}{2})T3\right]\right.$$

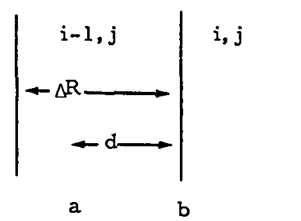
$$\left. - \frac{Q\,2_{i,j}}{2(2i-1)\delta R}\left[(i - 1\tfrac{1}{2})U1 - (i - \tfrac{1}{2})T3\right] + \frac{1}{4\delta Z}\left[P^n_{i,j}(V2 - V1) + Q3_{i,j}(V2 - T1) + Q1_{i,j}(T1 - V1)\right]\right\}.$$

$$\tilde{I}^n_{i,j} = I^n_{i,j} - \frac{\delta t}{4\rho_{i,j}}\left(\frac{P^n_{i,j}}{\delta R}\left[U_2 - U_1 + \frac{U_2 + 2T3 + U1}{2i - 1}\right] + \frac{Q4_{i,j}}{\delta R}\left[U_2 - T3 + \frac{2U2}{2i - 1}\right]\right.$$

$$\left. - \frac{Q2_{i,j}}{\delta R}\left[U1 - T3 - \frac{2U1}{2i - 1}\right] + \frac{1}{\delta Z}\left[P^n_{i,j}(V_2 - V1) + Q3_{i,j}(V_2 - T1) + Q1_{i,j}(T1 - V1)\right]\right).$$

III. DERIVATION OF MASS MOVEMENT EQUATION

The Oil method[4, 11] for velocity weighting is derived below.



The mass to move across b is between a and b where $d = b - a$; thus, $d = \tilde{u}\Delta t$ where $\tilde{u}$ is the weighted velocity at d. Using the first two terms of the Taylor series at a distance - d from b, we expand

$$u_{(b)} = \frac{u_{i-1,j} + u_{i,j}}{2}$$

$$\tilde{u} = \frac{u_{i-1,j} + u_{i,j}}{2} + (-\Delta)\left(\frac{u_{i-1,j} - u_{ij}}{\Delta R}\right).$$

Substitute $\Delta = \bar{u}\Delta t$ and solve for $\bar{u}$.

$$\bar{u} = \frac{u_{i-1,j} + u_i}{2} \bigg/ \left(1 + \frac{\Delta t}{\Delta R}\left(- U_{i-1,j} + U_{i,j}\right)\right).$$

<u>Mass moved</u> $= S_{d/2}\hat{\rho}_{i,j}\,\bar{u}\,\Delta t$ where S_d is surface area at $i\Delta R - \frac{1}{2}d$, so for cylindrical geometry $S_{d/2} = 2\pi(i\Delta R - \frac{1}{2}d)\Delta Z$.

We define $\Delta = d/\Delta R = \frac{\tilde{u}\Delta t}{\Delta R}$ for convenience; therefore,

$$S_{d/2} = 2\pi\left(i\Delta R - \tfrac{1}{2}(\Delta)(\Delta R)\right)\Delta Z$$

$$= 2\pi\Delta R\,(i - \tfrac{1}{2}\Delta)\,\Delta Z$$

$$= \pi\Delta R\,(2i - \Delta)\,\Delta Z\,.$$

Mass Moved $= \pi\Delta R\,(2i - \Delta)\,\Delta Z\,\hat{\rho}_{i-1,j}\,\bar{u}\,\Delta t$.

The volume of cell i-1, j is

$$V_{i-1,j} = \pi(i\Delta R)^2\,\Delta Z - \pi\left((i-1)\,\Delta R\right)^2\Delta Z$$

$$= \pi(2i - 1)\,\Delta R^2\Delta Z$$

$$DM = \frac{\text{Mass Moved}}{\text{Unit Volume}} = \frac{\pi \Delta R\ (2i - \Delta)\, \Delta Z\ \hat{\rho}_{i-1,j}\ \tilde{u}\, \Delta t}{\pi (2i - 1)\, \Delta R^2 \Delta Z} .$$

$$DM = \frac{(2i - \Delta)}{(2i - 1)}\ \hat{\rho}_{i-1,j} \left(\frac{\tilde{u} \Delta t}{\Delta R}\right)$$

$$= \hat{\rho}_{i-1,j}\ \frac{(2i - \Delta)}{(2i - 1)}\ \hat{\rho}_{i-1,j} \Delta$$

for slab geometry $\frac{(2i - \Delta)}{(2i - 1)} = 1.0$, which can be shown by letting $S_{d/2} = \Delta R \Delta Z$ and $V_{i-1,j} = \Delta R^2 \Delta Z$ or $S_{d/2} = \Delta Z$ and $V_{i-1,j} = \Delta R \Delta Z$.

APPENDIX C

2DE CODE DETAILS

I. COMPUTER TIME

The time required to run a calculation is useful in evaluating a numerical technique. Because the computer time will vary with the details of the calculation, it is instructive to have the times from several sample problems.

The problem of an 85-kbar shock in nitromethane interacting with an aluminum rod was calculated using 100 cells in the Z direction and 50 cells in the R direction. The aluminum rod had a radius of 25-cell widths. The calculation required 9.64 min of CDC 7600 time to complete the calculation to 446 cycles. The average time per cycle was 1.297 sec, and the average time per cell per cycle was 0.00026 sec.

The problem of an 85-kbar shock in nitromethane interacting with an aluminum slab and then the aluminum interacting with air was calculated using 180 cells in the Z direction and 3 cells in the R direction. The calculation required 4.916 min of CDC 7600 time to complete the calculation to 2323 cycles. The average time per cycle was 0.127 sec and the average time per cell per cycle was 0.000235 sec.

A reasonable estimate of the computer time required for the 2DE code is between 0.0002 and 0.0003 sec per cell per cycle.

II. MIXED-CELL TREATMENT

Up to 15 materials can be accommodated by the code. However, at present, equation-of-state routines allow only two materials in a cell simultaneously.

Each mixed cell (cell containing more than one material) is flagged in its cell identification word (CID) by an index pointer, which is the FORTRAN index of a material identification word in the mixed-cell table (CMT or MT). A material identification word exists in the CMT table for each material in a mixed cell. This word contains (1) an integer that identifies the material and (2) index values that determine subsequent and previous material identification words for other materials in the mixed cell. Quantities associated with a given material are indexed relative to material identification words. When mixed-cell information is used or modified, it is first moved into smaller processing arrays and, if modified, moved back into the CMT tables. When a material is depleted from a mixed cell, the space in the mixed-cell table is made available for further use. Formats for the cell identification word and the mixed-cell table are documented in the code listing. Mass is moved from the donor cell to the acceptor cell on the basis of the fraction of material in the acceptor cell, which is common to the donor cell. If the acceptor and donor cells do not contain any common materials, then mass is moved according to the mass fractions of materials in the donor cell. Energy and specific volumes are partitioned by the mixed-cell equations of state. If the acceptor cell contains only one material and the donor cell also contains this material, then the amount of mass moved is done on the basis of this partitioning. The internal energy is similarly handled.

This calculation and storage of the results is handled by the subroutine "CMXD" which requires the indices of the donor and acceptor cells and the amount of mass moved per unit volume of the donor cell in its calling sequence. This routine deals with absolute mass movement and because other routines deal with the change in mass per unit volume, this mass is calculated using the donor cell volume.

III. DATA PROCESSING

Storage requirements for individual problems are minimized by a preprocessing routine called VARYDIM. This routine processes generalized FORTRAN common, dimension, equivalence and data statements. These statements have the same format as ordinary FORTRAN statements except that integer quantities may be replaced by either a variable or an arithmetic statement. The result of an arithmetic statement being a simple left-to-right evaluation of the operations in the statement. The operands may be either integers or variable names that represent integer values. The results of this routine are output to a file of compilable FORTRAN statements and update control cards. The FORTRAN statements are distributed throughout the code by CDC system update routine. In general, only a small number of changes are required to completely modify the storage requirements for a specific problem.

Preprocessing dimensions before the code is compiled allows flexibility in the size of arrays that must be maintained in addressable memory. Because the row R dimension can be set before the code is compiled, processing of arrays that contain cell and intermediate quantities are on the basis of this dimension being fixed at execution time. These quantities are maintained in external storage and moved into core for processing and/or output. The problem grid is divided into NJMAX core increments for a fixed number of rows in the Z direction at the discretion of the user.

The routines RDCELLS and WCELLS handle I/O on the basis of reading or writing rows in the Z direction for a specified core increment. These routines are programmed for the CDC 6600 or 7600 using extended core storage or large core memory. Disk can also be used.

Processing control for the five phases of the code is accomplished by subroutine CONTROL. The grid is processed from left to right, bottom to top. Because the processing of a row often requires information contained in a previous row, reading, processing, and storing the results are staggered.

Rows are indexed from J = 1 to JMAX in addressable storage. Initially, the first two rows are read into core and the first row is processed (case 1). Then rows 3 through JMAX are read and rows 2 through JMAX-1 are processed (case 2). The first JMAX-2 rows are written to external storage, and two rows from the next core increment are read into rows 1 and 2 of core allowing processing of row JMAX and row 1 of the next core increment (case 3). After rows JMAX and JMAX-1 are written to external storage, the process is looped back through cases 2 and 3 until the final core increment where the last row of the grid is processed and written as a special case (case 4).

IV. PROCESSOR INPUT

Generalized FORTRAN statements prepared for the preprocessing routine VARYDIM modify storage requirements for the code 2DE. The user must define the preprocessor variables used in these statements. Preprocessor variables are input to the routine VARYDIM in a format-free fashion by the specification of the variable name, an equal sign, and the integer value of the variable. All 80 columns of the card are used. A $ terminates processing allowing the remainder of the card for comments. Since variables are used in left-to-right arithmetic, their values must be defined before they are used to define other variables.

The following preprocessor variables must have values.

For cell storage:

IMAX	Number of cells in the R direction.
JMAX	Number of cells in the Z direction.
NJMAX	Number of core increments.

For material storage:

NM	Number of materials.
NMH	Number of materials requiring HOM equation of state parameters (usually equal to NM).

For rectangular storage:

NRI	Number of rectangular intervals on the R axis.
NZJ	Number of rectangular intervals on the Z axis.

For mixed-cell information storage:

NTRYS	Estimated total number of materials for all cells containing more than one material. (Note that when a material is depleted in a cell, storage is again available for more information.) Example: If there are N mixed cells and each of these contain two materials, then NTRYS = 2*N

For circular input storage:

NCIR	Number of circles.

For two-dimensional plot storage:

NGRPHS	Total number of graph types available (default = 8).
NPLØTS	Number of plots produced each time cycle.
NTYPES	Number of graph types used by the code. (default = 8).
NCØNL	Maximum number of contour lines allowed in a given cell at the same time (default = 20).

For one-dimensional plot storage:

KPLØTS	Number of plots produced each time cycle.
IXZ	Number of cross-sections parallel to the Z axis.
JXR	Number of cross-sections parallel to the R axis.

All of the above must have a value of at least one because they are used to form dimension and common statements.

V. INPUT AND OUTPUT

Except for input required to define storage, problem input is accomplished using the system NAMELIST input.

The two NAMELIST names "Dump" and "General" pertain to input required by the dump routine and the general input for the problem. "Dump" input is read by routine EULER2D. "General" input is read by subroutine INPUT.

A. General Input

The following FORTRAN variables are used for the problem input. The integer subscript K must be consistent for each material and must not exceed the value of the preprocessor variable (NM) that defines storage.

Problem identification:

ID	Contains up to 70 Hollerith characters printed on the output listing, film listing, and graph titles.

Material descriptions:

NAME(K)	Material names, each name consisting of up to 10 Hollerith characters.
KMH(K)	Assigned material number.
VISC(K)	Viscosity constant.
IREACT(K)	.T. or .F. reaction flag for the Arrhenius rate law.

IHE(K)	.T. or .F. flag for a high explosive.
S(1, K)	Equation-of-state parameters for the solid.
G(1, K)	Equation-of-state parameters for the detonation products.
RHØO(K)	Initial density, used only for skipping tests.
ACTE(K)	Activation energy.
FREQ(K)	Frequency factor.
MTYPE(K)	3HGAS for a gas, 4HSØLID for a solid, 2HHE for an explosive. These flags are initialized for a solid.
DICE	.T. allows the code to eliminate a component from a cell if the component is isolated.

Problem description: Cells are processed using either slab or cylindrical geometry. Boundary types are numbered starting at the bottom of the grid and increasing in a clockwise direction for the four grid boundaries.

SLAB	.T. indicates slab geometry. (Default value = .F. for cylindrical geometry.)

Boundary types:

B1	Boundary 1 (default value = 6 HPISTØN).
B2	Boundary 2 (default value = 4HAXIS).
B3	Boundary 3 (default value = 9HCØNTINUUM).
B4	Boundary 4 (default value = 9HCØNTINUUM).

Piston applied values:

PAPP	Applied pressure.
WAPP	Applied mass fraction.
EAPP	Applied energy.
VAPP	Applied velocity.
MAPP	Applied mass.

Miscellaneous:

MINWT	Minimum cell reaction temperature (default value = 1000).
MINGRHØ	Constant for handling free surfaces, eliminating false diffusion (default value = 0.5).
FREPR	Mass is not moved unless the pressure of the cell from which mass moves is greater than this variable (default value = 0.0005). or a tension flag has been set.

B. Rectangular Input

The problem grid is divided into NR rectangles indexed from left to right, bottom to top. All cell quantities are initialized from this rectangular input.

Rectangles are formed by dividing the R and Z problem directions into NRI and NZJ intervals. If M and N index these intervals, then

NR	Number of rectangles.
RW(M)	Width of the M th interval.
ZW(N)	Width of the N th interval.
IR(M)	Number of cells in the M th interval.
JZ(N)	Number of cells in the N th interval.
DELR(M)	Cell width in the M th interval (currently the same for all intervals).
DELZ(N)	Cell width in the N th interval (currently the same for all intervals).

For the L th rectangle:

KMAT(L)	Material K for the rectangle.
RHØ(L)	Initial cell density.
PO(L)	Initial cell pressure.
TO(L)	Initial cell temperature.
UO(L)	Initial cell velocity in the U direction.
VO(L)	Initial cell velocity in the V direction.

WO(L)	Initial cell mass fraction.
DELT(L)	Time increment.

C. Circular Input

Cells can be initialized by defining NCIR concentric circles. The radial difference between circles must be at least larger than the largest diagonal of any cells contained between the difference.

RO	R coordinate for the circle centers.
ZO	Z coordinate for the circle centers.

For the L th circle, indexed from the largest to the smallest,

RAD(L)	Radius of the L th circle.
RHØOC(L)	Density of the L th circle.
KCIR(L)	Material K for the L th circle.
IOC(L)	Energy of L th circle.
UOC(L)	U velocity of L th circle.
VOC(L)	V velocity of L th circle.
WOC(L)	W of L th circle.

D. Output

Output for specific cycles is directed to both the printer and to film. This output is controlled by the specification of an initial cycle, an increment between cycles and a terminating cycle. Input information is output unless the print or film terminating cycle is set to zero.

PCS	Starting print cycle (default value = 1).
PCI	Print cycle increment (default value = 50).
PCE	Terminating print cycle (default value = 5000).
FCS	Starting film cycle (default value = 1).
FCI	Film cycle increment (default value = 25).
FCE	Terminating film cycle (default value = 5000).

Plot cycles are specified by the above film cycle specifications unless specified by the following variables:

PLTS	Plot cycle start.
PLTI	Plot cycle increment.
PLTE	Plot cycle end.

2DE is programmed to produce isoplots (contour plots) of values associated with each cell. At present eight isoplots are allowed. Up to 10 individual plots per problem time cycle can be produced by input control. Any or all of the isoplots associated with cell quantities can be plotted on an individual plot frame. Contour intervals, grid maximum, and grid minimum can be modified. Default values are documented in the code. If L indexes the plot frame, then

ISØPLØT(L)	Determines which isoplots will be produced on the L th plot frame.

1 = isotherm, 2 = isobar, 4 = isopycnic, 8 = energy, 16 = cell U velocity, 32 = cell V velocity, 64 = W mass fraction.

To get more than one plot per frame, values are added together for ISØPLØT(L).

If M indexes the isoplot type, then

GMAX(M)	Maximum value plotted for the M th isoplot type.
GMIN(M)	Minimum value plotted for the M th isoplot type.
GDELTA(M)	Contour interval for the M th isoplot type.
NPLØTS	Number of two-dimensional plots. This variable is set by the preprocessor; however, if it is modified here by being set equal to zero, all two-dimensional plots will be eliminated from the output.

NTRFCE	If .T., positions of mixed cells are plotted with an asterisk.

2DE produces one-dimensional cross-section plots of the cell quantities as a function of R or Z. The total number of one-dimensional plots, the number of cross sections parallel to the Z axis (IXZ), and the number of cross sections parallel to the R axis (JXR) are fixed by the preprocessor. Default values that determine which cell quantities are plotted, and the location of cross sections on the grid are documented in the code. A cross section parallel to an axis is specified by a cell index on the other axis. If M indexes plots and L indexes cross sections, then

ICØN(L)	Contains IXZ indices that define cross sections parallel to the Z axis.
JCØN(L)	Contains JXR indices that define cross sections parallel to the R axis.
PTYPE(M)	Determines which cell quantity is plotted.
KPLØTS	Number of one-dimensional plots. This variable is set by the preprocessor; however, if it is modified here by being set equal to zero, all one-dimensional plots will be eliminated from the output.

Scaling of plotted output: 4020 grid coordinates can be used to scale graph output. Default values are for a square grid.

IXL	Grid left coordinate (default value = 120).
IXR	Grid right coordinate (default value = 980).
IYT	Grid top coordinate (default value = 50).
IYB	Grid bottom coordinate (default value = 910).

E. Debug Features

Debug routines display the results of each phase of the code, mixed cell processing, and the dump routine. The following variables control the output.

DEBUG(L)	For the logical variables L = 1 through 5, phases 1 through 5 are debugged. Flags 6 and 7 produce dump information for the mixed-cell and dump routine.
DBS	Cycle control starting the debug dump.
DBI	Cycle increment for dumping.
DBE	Terminating cycle for dumping.

Unless specific cells are designated, the entire grid calculation is printed for a debug cycle. The following variables restrict printing to particular cells.

IGS	Starting radial or I index.
IGE	Ending radial or I index.
JGS	Starting Z or J index.
JGE	Ending Z or J index.

F. Restart Features

The user has the option of dumping at specified running time increments or of dumping at specified problem cycles. Uses the NAMELIST name "Dump."

DCYCLE	Initially zero. Set to the problem cycle for picking up dumps.
COMMENT	Up to 70 Hollerith characters that go to the printer and express file.
TAPE	Up to 10 Hollerith characters for a dump tape label.
DTI	Dump time increment (default value = 300 sec).
SECS	Tolerance that allows time for the last dump before

the problem is terminated by a time limit.

For the optional method of dumping, the following variables must be specified.

DMPS	Starting dump cycle. (If DMPI = 0 the alternate method of time increment dumping is used.)
DMPI	Dump cycle increment.

G. Time Step Modification

At specified cycles the time step (DELT) can be modified by a multiplication factor (TFCT). Up to 5 modifications are allowed.

NTCY	Problem cycle at which the time step is modified.
TFCT	Multiplication factor.

H. NAMELIST Types

NAMELIST input requires that input variables and input values agree in type. The types are listed below.

INTEGER

MTYPE	PLTI	IYB	DMPE
KMAT	PLTE	DBS	NR
IR	ISØPLØT	DBI	NRI
JZ	NPLØTS	DBE	NZJ
KCIR	ICØN	IGS	KMH
PCS	JCØN	NCYLIM	NTCY
PCI	PTYPE	IGE	KCIR
PCE	VCNT	JGS	NCØNL
FCS	KPLØTS	JGE	IXL
FCI	IXL	DCYCLE	IXR
FCE	IXR	DMPS	IYT
PLTS	IYT	DMPI	IYB

FLOATING POINT

VISC	PO	UOC	PAPP
S	TO	RG	VOC
G	UO	DELT	RW
RHØO	VO	GMAX	EAPP
ACTE	WO	GMIN	WAPP
FREQ	IO	GDELTA	VAPP
RHØ	DELR	DTI	MAPP
IOC	DELZ	SECS	MINWT
MINGRHØ	WOC	RHØOC	ZO
FREPR	ZW	RO	RAD
TFCT	DTI		

LOGICAL

IHE	SLAB
IREACT	NTRFCE
DEBUG	DICE

HOLLERITH

ID	B1
NAME	B2
CØMMENT	B3
TAPE	B4
MTYPE	

VI. STORAGE REQUIRMENTS

On the CDC 7600 computer the 512,000 words available in large core memory (LCM) are shared by the user, the program file set buffers, and the system monitors. Because the system requirements are subject to change, only rough estimates can be given for the problem storage limitations.

The code can process approximately 20,100 cells if the buffers are set to minimum values.

If more cells are needed, the disk can be used.

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