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by

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This report supersedes LA-3629-MS.
2DE: A TWO-DIMENSIONAL CONTINUOUS EULERIAN HYDRODYNAMIC CODE FOR COMPUTING MULTICOMPONENT REACTIVE HYDRODYNAMIC PROBLEMS

by

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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 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 and developed by Hageman and Walsh, 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 Appendices A, B, and C.

II. THE HYDRODYNAMIC EQUATIONS

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

\[
\frac{\partial \rho}{\partial t} + U \frac{\partial \rho}{\partial R} + V \frac{\partial \rho}{\partial Z} = -\rho \left( \frac{\partial U}{\partial R} + \frac{\partial V}{\partial Z} + \frac{U}{R} \right)
\]

Mass,

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

Momentum,

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

and

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

Energy.

The equations, written in finite-difference form appropriate to a fixed (Eulerian) mesh, are used to determine the fixed (Eulerian) mesh. 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

\[
\frac{\partial \rho}{\partial t} = \frac{\partial (\rho u)}{\partial R},
\]

\[
\frac{\partial \rho}{\partial t} = \frac{\partial (\rho v)}{\partial Z},
\]

and

\[
\frac{\partial}{\partial t} \left( \rho \left( \frac{\partial U}{\partial R} + \frac{\partial V}{\partial Z} \right) \right) = -\frac{\partial P}{\partial R} - \frac{1}{R} \frac{\partial (qU)}{\partial R} + U \frac{\partial I}{\partial R} - \frac{\partial V}{\partial Z}.
\]
III. THE CODING EQUATIONS AND TECHNIQUES

Cell quantities:

- $p$ - 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
- $\rho$ - RHOT - Tilde density
- $q$ - Q1, Q2, Q3, Q4 - Viscosities
- $\tilde{U}$ - CUB - Cell R velocity tilde
- $\tilde{V}$ - CVB - Cell Z velocity tilde
- $\Delta M$ - D MASS - Density increment for mass movement
- $\Delta E$ - DE - Energy increment
- $\Delta W$ - DW - Mass fraction increment
- $\Delta PU$ - DPU - Momentum in R direction increment
- $\Delta PV$ - 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 $\Delta V'/V' \left( \frac{V'}{=1} \right)$, and $\Delta/I$, 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

$$\frac{\Delta W}{\Delta t} = Z \cdot Z \cdot W \cdot \frac{e^{E^{*}/RT}}{r^{E}}$$

where $Z$ is the frequency factor, $E^{*}$ is the activation energy, $R$ is the gas constant, and...
\( \delta t \) is the time increment. In difference form this is
\[
W_{n+1}^n = W^n - \delta t Z \frac{W^n e^{-E^*/R_T}}{T_n}.
\]

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

2. If CW1 is less than GASW (0.02), set CW1 = 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 0, set CP = PO.

Phases I and II are skipped if \( n \leq \text{MINGRHO} \) + (\( p_o - \text{MINGRHO} \)). This is for handling free surfaces to eliminate false diffusion. MINGRHO = 0.5. For gases at free surfaces \( W_{n+1}^n \) is replaced by one.

B. Phase II: Viscosity and Velocity

1. Viscosity Equations

\[
Q_{1_{i,j}}=q_{i,j-\delta_s} = \frac{Q_3}{i,j-1}
\]

except on boundary 1 when \( Q_{1_{i,j}} = 0.0 \) or on piston boundary when
\[
Q_{1_{i,j}} = K \left( \rho_{i,j}^n + \text{MAPPP} \right) \left( V_{\text{APP}} - V_{i,j}^n \right)
\]
if \( V_{\text{APP}} > V_{i,j}^n \)
\[
= 0.0
\]
if \( V_{\text{APP}} < V_{i,j}^n \).

\[
Q_{2_{i,j}}=q_{i-\delta_s,j} = \frac{Q_4}{i-1,j}
\]

except on axis boundary 2 when
\[
Q_{2_{i,j}} = 2Q_{4_{i,j}} - Q_{4_{i-1,j}}.
\]

2. Velocity Equations

\[
P_1 = P^n_{i,j-1}
\]

except on piston boundary 1, \( P_1 = \text{PAPP} \) or on continuative boundary 1, \( P_1 = P^n_{i,j} \).

\[
P_2 = P^n_{i-1,j}
\]

except on axis boundary 2, \( P_2 = P^n_{i,j} \).

\[
P_3 = P^n_{i,j+1}
\]

except on continuative boundary 3, \( P_3 = P^n_{i,j+1} \).

\[
P_4 = P^n_{i+1,j}
\]

except on continuative boundary 4, \( P_4 = P^n_{i,j+1} \).

\[
Q_3_{i,j} = q^n_{i,j} = K \left( \rho_{i,j}^n + \rho_{i,j+1}^n \right) \left( V_{i,j}^n - V_{i,j+1}^n \right)
\]
if \( V_{i,j}^n > V_{i,j+1}^n \)
\[
= 0.0
\]
if \( V_{i,j}^n < V_{i,j+1}^n \)

except \( Q_{3_{i,j+1}} \) on continuative boundary 3.

\[
Q_4_{i,j} = q^n_{i+1,j} = K \left( \rho_{i,j}^n + \rho_{i+1,j}^n \right) \left( U_{i,j}^n - U_{i,j+1}^n \right)
\]
if \( U_{i,j}^n > U_{i,j+1}^n \)
\[
= 0.0
\]
if \( U_{i,j}^n < U_{i,j+1}^n \)

except on continuative boundary 4 when
\( Q_{4_{i,j+1}} = 0.0 \)
\[ \ddot{u}^{n}_{i,j} = u^{n}_{i,j} - \frac{\partial t}{\partial t} \left( \left\{ (i-1)(P_4-P_2) + P_4-P_2^{n} \right\}_{i,j} \right) \]
\[ + q_{4,i,j} - q_{2,i,j} \).

\[ \ddot{v}^{n}_{i,j} = v^{n}_{i,j} - \frac{\partial t}{\partial t} \left( \left\{ P_3-P_1 + q_{3,i,j} - q_{1,i,j} \right\}_{i,j} \right). \]

where
\[ i = 1, 2, \ldots, \text{IMAX} \]
\[ j = 1, 2, \ldots, \text{NJMAX} \times \text{JMAX} \text{ (for NJMAX core increments containing JMAX rows each).} \]

In slab geometry, the quantity in \{ \} is \( \frac{P_4-P_2}{2} \)
for \( \ddot{u}^{n}_{i,j} \).

C. Phase III. Internal Energy and \( \tilde{\gamma} \) Calculation

1. \( \tilde{\gamma} \) Calculation
\[ \ddot{\gamma}^{n}_{i,j} = \gamma^{n}_{i,j} \left\{ \frac{1}{2} - \frac{\partial t}{2\partial t} \left( u^{n}_{i+1,j} - u^{n}_{i-1,j} \right) \right\} \]
\[ - \frac{\partial t}{2\partial t} \left( v^{n}_{i,j+1} - v^{n}_{i,j-1} \right) \}

Exceptions:

Piston boundary, \( v^{n}_{i,j-1} = \text{VAPP} \).

Axis boundary, \( u^{n}_{i-1,j} = u^{n}_{i+1,j} + 2u^{n}_{i,j} \).

boundary 3, \( v^{n}_{i,j+1} = v^{n}_{i,j} \).

boundary 4, \( u^{n}_{i+1,j} = u^{n}_{i,j} \).

2. Piston Energy Constraints

For the first VCNT cycles,
\[ \ddot{\rho}^{n}_{i,j} = \rho^{n}_{i,j} \left\{ \begin{array}{l} 1/2 (P^{n}_{i,j} + Q^{n}_{3,i,j}) (V^{n}_{i,j} - 1/\rho^{n}_{i,j}) + \frac{KE^{n}_{i,j}}{2} \\
\text{if } V^{n}_{i,j} > 1/\rho^{n}_{i,j} \\
\ddot{u}^{n}_{i,j} \\
\text{if } V^{n}_{i,j} < 1/\rho^{n}_{i,j} \end{array} \right. \]

where \( KE^{n}_{i,j} = 1/2 \left( \ddot{u}^{n}_{i,j} + \ddot{v}^{n}_{i,j} \right). \)

3. Internal Energy Calculation

For \( \tilde{\gamma}^{n}_{i,j} < \text{MINRHO} + (\rho^{n}_{i,j} - \text{MINRHO})(W^{n}_{i,j}) \), \( E^{n}_{i,j} = \tilde{\gamma}^{n}_{i,j} \) and the rest of Phase III is skipped.

\[ U^{n}_{1} = (U^{n}_{i=1,j} + \ddot{u}^{n}_{i=1,j}) \]
\[ U^{n}_{2} = (U^{n}_{i=1,j} + \ddot{u}^{n}_{i=1,j}) \]
\[ V^{n}_{1} = (V^{n}_{i=1,j} + \ddot{v}^{n}_{i=1,j}) \]
\[ V^{n}_{2} = (V^{n}_{i=1,j} + \ddot{v}^{n}_{i=1,j}) \]
\[ T^{n}_{3} = (U^{n}_{i=1,j} + \ddot{u}^{n}_{i=1,j}) \]
\[ T^{n}_{1} = (V^{n}_{i=1,j} + \ddot{v}^{n}_{i=1,j}) \]

Exceptions:

Axis boundary, \( U^{n}_{i=1,j} = 2(U^{n}_{i=1,j} + \ddot{u}^{n}_{i=1,j}) - U^{n}_{2} \).

Continuative boundary 4, \( U^{n}_{i=1,j} = (U^{n}_{i=1,j} + \ddot{u}^{n}_{i=1,j}) \).

Piston boundary, \( V^{n}_{i=1,j} = 2V^{n}_{APP} \).

Continuative boundary 1, \( V^{n}_{1} = (V^{n}_{i=1,j} + \ddot{v}^{n}_{i=1,j}) \).

Continuative boundary 3, \( V^{n}_{2} = (V^{n}_{i=1,j} + \ddot{v}^{n}_{i=1,j}) \).

In slab geometry the quantities in \{ \} are set equal to zero.
4. Total Energy Calculation

\[ E_{i,j}^n = \bar{E}_{i,j}^n + 1/2 \left[ (\bar{V}_{i,j}^n)^2 + (\bar{R}_{i,j}^n)^2 \right] \]

D. Phase IV. Mass Movement

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

Nomenclature for Phase IV and V:

- \( \Delta \) Change in energy
- \( \Delta W \) Change in mass fraction
- \( \Delta \text{PU} \) Change in U momentum
- \( \Delta \text{PV} \) Change in V momentum
- \( \Delta \text{MASS} \) Change in density

1. Mass Movement Across Side 2

a. For axis boundary \( \Delta \text{MASS} = 0 \), otherwise

\[ \Delta = \frac{1/2 (\bar{U}_{i,j}^n + \bar{U}_{i-1,j}^n) (\rho / \rho R)}{1 + (\bar{U}_{i,j}^n - \bar{U}_{i-1,j}^n) (\rho / \rho R)} \]

b. If \( \Delta > 0 \) the mass moves from donor cell \( i-1, j \) to cell \( i, j \).

Cylindrical \( \Delta \text{MASS} = \Delta t_{1-1,j} \left( \frac{2i - 2 - \Delta}{2i - 3} \right) (\rho) \)

Slab \( \Delta \text{MASS} = \Delta t_{1-1,j} (\rho) \)

\[ \Delta E_{i,j} = E_{i,j}^n (\Delta \text{MASS}) \]

Mixed-cell modification of \( \Delta \text{MASS} \) and \( \Delta E \) occurs if required as described in mixed-cell section.

\[ \Delta W_{i,j} = W_{i,j}^n (\Delta \text{MASS}) \]

\[ \Delta \text{PU}_{i,j} = \hat{U}_{i,j}^n (\Delta \text{MASS}) \]

\[ \Delta \text{PV}_{i,j} = \hat{V}_{i,j}^n (\Delta \text{MASS}) \]

Cylindrical \( \Delta M_{i,j} = \text{MASS} \left( \frac{2i-3}{2i-1} \right) \)

Slab \( \Delta M_{i,j} = \text{MASS} \)
c. If $\Delta < 0$, the mass moves from the donor cell $i, j$ to acceptor cell $i-1, j$.

\[
\text{Cylindrical } \text{DMASS} = \frac{\tilde{\rho}^n_{i, j}}{(2i - 2 - \Delta)} \Delta, \text{ slab } \text{DMASS} = \tilde{\rho}^n_{i, j} \Delta.
\]

\[
\text{DE}_{i, j} = E^n_{i, j} \text{(DMASS)} \quad \text{DE}_{i-1, j} = \text{DE}_{i-1, j} - E^n_{i, j} \text{(DMASS)}.
\]

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

\[
\text{DW}_{i, j} = w^n_{i, j} \text{(DMASS)} \quad \text{DW}_{i-1, j} = \text{DW}_{i-1, j} - w^n_{i, j} \text{(DMASS)}.
\]

\[
\text{DPU}_{i, j} = \tilde{u}^n_{i, j} \text{(DMASS)} \quad \text{DPU}_{i-1, j} = \text{DPU}_{i-1, j} - \tilde{u}^n_{i, j} \text{(DMASS)}.
\]

\[
\text{DPV}_{i, j} = \tilde{v}^n_{i, j} \text{(DMASS)} \quad \text{DPV}_{i-1, j} = \text{DPV}_{i-1, j} - \tilde{v}^n_{i, j} \text{(DMASS)}.
\]

\[
\text{DM}_{i, j} = \text{DMASS} \quad \text{Cylindrical } \text{DM}_{i-1, j} = \text{DMASS} \left( \frac{2i-1}{2i-3} \right).
\]

\[
\text{Slab } \text{DM}_{i-1, j} = \text{DMASS}.
\]

2. Mass Movement Across Side 1

a. For a piston boundary

\[
\Delta = \frac{1}{2} \frac{(V\text{APP} + \tilde{V}^n_{i, j})(\xi/\xi Z)}{(\tilde{V}^n_{i, j} - V\text{APP})(\xi/\xi Z) + 1}.
\]

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

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

\[
\text{DE}_{i, j} = \text{DE}_{i, j} + \text{DMASS (EAPP)}.
\]

\[
\text{DW}_{i, j} = \text{DW}_{i, j} + \text{DMASS (WAPP)}.
\]

\[
\text{DPV}_{i, j} = \text{DPV}_{i, j} + \text{DMASS (VAPP)}.
\]

\[
\text{DPU}_{i, j} = \text{DPU}_{i, j} + \text{DMASS (UAPP)}.
\]

\[
\text{DM}_{i, j} = \text{DM}_{i, j} + \text{DMASS}.
\]
b. For continuative boundary 1 cell,

\[ \Delta = (\bar{V}_{i,j}^n) \left( \frac{\partial f}{\partial z} \right) \]

DMASS = \left( n_{i,j}^n \right) (\Delta) .

DE_{i,j} = DE_{i,j} + E_{i,j}^n (DMASS) .

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

\[ DW_{i,j} = DW_{i,j}^n + W_{i,j}^n (DMASS) . \]

\[ DPV_{i,j} = DPV_{i,j} + \bar{V}_{i,j}^n (DMASS) . \]

\[ DPU_{i,j} = DPU_{i,j} + \bar{U}_{i,j}^n (DMASS) . \]

\[ DM_{i,j} = DM_{i,j} + DMASS , \]

otherwise

\[ \Delta = \frac{1}{2} \left( \bar{V}_{i,j}^n + \bar{V}_{i,j-1}^n \right) \left( \frac{\partial f}{\partial z} \right) \]

\[ 1 + \left( \bar{V}_{i,j}^n - \bar{V}_{i,j-1}^n \right) \left( \frac{\partial f}{\partial z} \right) \]

\[ A = 1 + \left( s_{i,j} - s_{i,j-1} \right) \left( \frac{\partial f}{\partial z} \right) \]

\[ c. \text{ If } \Delta \geq 0, \text{ the mass moves from donor cell } i,j-1 \text{ to acceptor cell } i,j. \]

\[ DMASS = \left( n_{i,j}^{n-1} \right) (\partial f/\partial z) . \]

DE_{i,j} = DE_{i,j} + E_{i,j-1}^n (DMASS) \quad DE_{i,j-1} = DE_{i,j-1} - E_{i,j-1}^n (DMASS) .

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

\[ DW_{i,j} = DW_{i,j}^n + W_{i,j-1}^n (DMASS) . \]

\[ DPV_{i,j} = DPV_{i,j} + \bar{V}_{i,j-1}^n (DMASS) . \]

\[ DPU_{i,j} = DPU_{i,j} + \bar{U}_{i,j-1}^n (DMASS) . \]

\[ DM_{i,j} = DM_{i,j} + DMASS . \]
d. If $\Delta < 0$, the mass moves from donor cell $i, j$ to acceptor cell $i, j-1$.

$$\text{DMASS} = (\phi_{i,j}^n)(\phi).$$

$$\text{DE}_{i,j} = \text{DE}_{i,j} + E_{i,j}^n (\text{DMASS}) \quad \text{DE}_{i,j-1} = \text{DE}_{i,j-1} - E_{i,j}^n (\text{DMASS}).$$

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

$$\text{DW}_{i,j} = \text{DW}_{i,j} + W_{i,j}^n (\text{DMASS}) \quad \text{DW}_{i,j-1} = \text{DW}_{i,j-1} - W_{i,j}^n (\text{DMASS}).$$

$$\text{DPV}_{i,j} = \text{DPV}_{i,j} + \tilde{V}_{i,j}^n (\text{DMASS}) \quad \text{DPV}_{i,j-1} = \text{DPV}_{i,j-1} - \tilde{V}_{i,j}^n (\text{DMASS}).$$

$$\text{DPU}_{i,j} = \text{DPU}_{i,j} + \tilde{U}_{i,j}^n (\text{DMASS}) \quad \text{DPU}_{i,j-1} = \text{DPU}_{i,j-1} - \tilde{U}_{i,j}^n (\text{DMASS}).$$

$$\text{DM}_{i,j} = \text{DM}_{i,j} + \text{DMASS} \quad \text{DM}_{i,j-1} = \text{DM}_{i,j-1} - \text{DMASS}.$$  

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,

$$\Delta = \frac{\nabla^n}{\tilde{\phi} \phi_{i,j}} (\phi/\phi Z).$$

$$\text{DMASS} = (\phi_{i,j}^n)(\phi).$$

$$\text{DE}_{i,j} = \text{DE}_{i,j} - E_{i,j} (\text{DMASS}).$$

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

$$\text{DW}_{i,j} = \text{DW}_{i,j} - W_{i,j} (\text{DMASS}).$$

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

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

$$\text{DM}_{i,j} = \text{DM}_{i,j} - \text{DMASS}.$$
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
\[ \Delta = 0.5 \left( 3 \bar{U}_{i,j} - \bar{U}_{i-1,j} \right) \left( \frac{\partial t}{\partial R} \right) . \]

a. \( \Delta > 0 \) mass moves out of cell \( i,j \).

Cylindrical DMASS = \( (c_{i,j} \bar{U}_{i,j}) \left( \frac{2i+1}{2i-1} \right) (\Delta) \).

b. \( \Delta < 0 \) mass moves into cell \( i,j \).

Cylindrical DMASS = \( (c_{i,j} \bar{U}_{i,j}) \left( \frac{2i+1}{2i-1} \right) (\Delta) \)

for either a. or b. Slab DMASS = \( (c_{i,j} \bar{U}_{i,j}) (\Delta) \).

\[ DE_{i,j} = DE_{i+1,j} + \frac{E_{i,j} (\Delta)}{\rho_{i,j}} (DMASS) . \]

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

\[ DW_{i,j} = DW_{i,j} - \frac{W_{i,j} (\Delta)}{\rho_{i,j}} (DMASS) . \]

\[ DPV_{i,j} = DPV_{i,j} - \frac{v_{i,j} (\Delta)}{\rho_{i,j}} (DMASS) . \]

\[ DPU_{i,j} = DPU_{i,j} - \frac{U_{i,j} (\Delta)}{\rho_{i,j}} (DMASS) . \]

\[ DM_{i,j} = DM_{i,j} - DMASS . \]

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 \( \rho \) used in Phase IV and replacing it with the \( \rho \) of the material being moved from the donor cell (\( \rho_k \)).

\[ DMASS = DMASS \frac{\rho_k}{\rho} . \]

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.

\[ DE_{i,j}^{n+1} = DE_{i,j}^n + DMASS (\Delta) (Donor Component I + Donor K.E.) . \]

\[ DE_{i,j}^{n+1} = DE_{i,j}^n + DMASS (\Delta) (Donor Component I + Donor K.E.) . \]

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 \( CW \) is calculated by

\[ CW_{i,j} = \begin{cases} \left( CW_{i,j}^n \right) & \text{for unmixed acceptor} \\ \left( CW_{i,j}^n + DMASS \right) (\Delta) & \text{for mixed acceptor} \end{cases} \]

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 $\rho, j > MINGRHO + (\rho_0 - MINGRHO) (W_{i,j})^n$,

$$\rho_{i,j}^{n+1} = \rho_{i,j}^n + DM_{i,j}^n.$$  

$$W_{i,j}^{n+1} = \frac{1}{n_{i,j}^n} (\rho_{i,j}^n W_{i,j}^n + DW_{i,j}^n).$$  

$$V_{i,j}^{n+1} = \frac{1}{\rho_{i,j}^n} (n_{i,j}^n V_{i,j}^n + DPV_{i,j}).$$  

$$U_{i,j}^{n+1} = \frac{1}{\rho_{i,j}^n} (U_{i,j}^n \rho_{i,j}^n + DPU_{i,j}).$$  

$$\tau_{i,j}^{n+1} = \frac{1}{\rho_{i,j}^n} (n_{i,j}^n \rho_{i,j}^n + DE_{i,j}).$$

$$= \frac{1}{2} \left( (V_{i,j}^n)^2 + (U_{i,j}^n)^2 \right).$$

For $\rho, j > MINGRHO + (\rho_0 - MINGRHO) (W_{i,j})^n$,

$$\rho_{i,j}^{n+1} = \rho_{i,j}^n + DM_{i,j}^n.$$  

$$W_{i,j}^{n+1} = \frac{1}{n_{i,j}^n} (\rho_{i,j}^n W_{i,j}^n + DW_{i,j}^n).$$  

$$V_{i,j}^{n+1} = \frac{1}{\rho_{i,j}^n} (n_{i,j}^n V_{i,j}^n + DPV_{i,j}).$$  

$$U_{i,j}^{n+1} = \frac{1}{\rho_{i,j}^n} (U_{i,j}^n \rho_{i,j}^n + DPU_{i,j}).$$  

$$\tau_{i,j}^{n+1} = 0.0.$$  

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 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 SINE 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.

<table>
<thead>
<tr>
<th>Nitromethane Shock</th>
<th>Eulerian</th>
<th>Lagrangian</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pressure</td>
<td>0.0858</td>
<td>0.0857</td>
</tr>
<tr>
<td>Specific Volume</td>
<td>0.5455</td>
<td>0.5455</td>
</tr>
<tr>
<td>Energy</td>
<td>0.0146</td>
<td>0.0146</td>
</tr>
<tr>
<td>Temperature</td>
<td>1146.2</td>
<td>1181.9</td>
</tr>
<tr>
<td>Particle Velocity</td>
<td>0.171</td>
<td>0.171</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Reflected Shock (Nitromethane)</th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Pressure</td>
<td>0.178</td>
<td>0.1787</td>
</tr>
<tr>
<td>Specific Volume</td>
<td>0.4686</td>
<td>0.4858</td>
</tr>
<tr>
<td>Energy</td>
<td>0.02248</td>
<td>0.0225</td>
</tr>
<tr>
<td>Temperature</td>
<td>1365.5</td>
<td>1436.1</td>
</tr>
<tr>
<td>Particle Velocity</td>
<td>0.0967</td>
<td>0.0964</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Aluminum Shock</th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Pressure</td>
<td>0.1785</td>
<td>0.1786</td>
</tr>
<tr>
<td>Specific Volume</td>
<td>0.3071</td>
<td>0.3070</td>
</tr>
<tr>
<td>Energy</td>
<td>0.0047</td>
<td>0.0046</td>
</tr>
<tr>
<td>Temperature</td>
<td>487.1</td>
<td>518.3</td>
</tr>
<tr>
<td>Particle Velocity</td>
<td>0.0964</td>
<td>0.0964</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Aluminum Rarefaction</th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Pressure</td>
<td>0.008</td>
<td>0.0004</td>
</tr>
<tr>
<td>Specific Volume</td>
<td>0.3561</td>
<td>0.3603</td>
</tr>
<tr>
<td>Energy</td>
<td>0.0007</td>
<td>0.0005</td>
</tr>
<tr>
<td>Temperature</td>
<td>384.0</td>
<td>355.5</td>
</tr>
<tr>
<td>Particle Velocity</td>
<td>0.1873</td>
<td>0.1932</td>
</tr>
</tbody>
</table>

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 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\textsuperscript{13} and proposed by Hirt,\textsuperscript{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.

ACKNOWLEDGMENTS

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-cm³/g and the particle velocity scale is 0.2 cm/μsec.
Fig. 1. (cont)
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/cm³, 0.01 mbar, 200° K, 0.005 mbar·cm³/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)
ISO VELOCITY
IN Z DIRECTION

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 isentrope energies 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:

- \( C_s \), \( S \): coefficients to a linear fit of \( U_s \) and \( U_p \)
- \( C_{l_s} \), \( S_l \): second set of coefficients to a linear fit of \( U_s \) and \( U_p \)
- \( C_V \): heat capacity of condensed component (cal/g/deg)
- \( C_{l_V} \): heat capacity of gaseous component (cal/g/deg)
- \( I \): total internal energy (Mbar-cm\(^3\)/g)
- \( P \): pressure (Mbar)
- \( S \): spalling constant to relate spall pressure and tension rate
- \( S \): interface spalling pressure
- \( T \): temperature (°K)
- \( USP \): ultimate spalling pressure
- \( U_p \): particle velocity
- \( U_s \): shock velocity
- \( V \): total volume (cm\(^3\)/g)
- \( V_i \): initial volume of condensed component (cm\(^3\)/g)
- \( W \): mass fraction of undecomposed explosive
- \( X \) or \( x \): 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 Christians technique.

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

\[
\ln T_H = F_s + G_s \ln V_s + H_s (\ln V_s)^2 + I_s (\ln V_s)^3 \\
+ J_s (\ln V_s)^4.
\] (A-1)

\[
L_H = \frac{1}{2} P_H (V_o - V_s') .
\]

\[
P_s = \frac{V_s}{V_s} (I_s - I_H') + P_H', \text{ where } V_s = \frac{3P}{3P/V} .
\] (A-2)

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

Two sets of \( C \) and \( S \) coefficients may be given.

For \( V_s < \text{MINV} \), the fit \( U_s = C_l + S_l (U_P) \) is used with the corresponding changes to the above equations. Between \( \text{MINV} \) and \( \text{VSW} \), the volume is set equal to \( \text{MINV} \), and \( U_s = C_l + S_l (U_P) \) is used. For volumes greater than \( V_o' \), we use the Grüneisen equation of state and the \( P = 0 \) line as the standard curve.

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

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

The spalling option is not used if \( \text{SPA} < 0.0001 \).

If \( P_s < \text{USP} \), set \( P_s = \text{SPALL} P \) and set the spall indicator. If \( P_s < \text{SPA} \sqrt{\frac{\beta}{\alpha}} \frac{\partial P}{\partial X} \) (\( \frac{\partial P}{\partial X} \) is the tension rate), and \( P_s < \text{SPMIN} (5 \times 10^{-3}) \) set \( P_s = \text{SPALL} P \) 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.

\[
\ln P_i = A + B \ln V_g + C(\ln V_g)^2 + D(\ln V_g)^3 + E(\ln V_g)^4.
\] (A-4)

\[
\ln I_i = K + L \ln P_i + M(\ln P_i)^2 + N(\ln P_i)^3 + O(\ln P_i)^4 .
\] (A-5)

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

\[
\ln T_i = Q + R \ln V_g + S(\ln V_g)^2 + T(\ln V_g)^3 + U(\ln V_g)^4 .
\] (A-6)

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

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

\[
T = T_i + \frac{(I_g - I_i) (23,890)}{C_i V} .
\] (A-8)
C. Mixture of Condensed and Gaseous Components

\((0 < W < 1)\)

\[
V = W V_s + (1 - W) V_g.
\]

\[
I = W I_s + (1 - W) I_g.
\]

\[
P = P_g = P_s.
\]

\[
T = T_g = T_s.
\]

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 \(W I_s + (1 + W) I_g\),

\[
T = \frac{23,890}{C_V w + C_I V (1 - W)} I - \left[ W I_H - I_H (1 - W) \right] + \frac{1}{23,890} \left[ T_H C_V w + T_I C_I V (1 - W) \right].
\]

\((A-9)\)

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

\[
P_H - P = \left( \frac{V_s C_V}{V_s} - \frac{C_I V}{C_V w} \right) \left( \frac{1}{C_V w + C_I V (1 - W)} \right) \left[ I - \left[ W I_H + I_H (1 - W) \right] + \frac{1}{23,890} \left[ T_H C_V w + T_I C_I V (1 - W) \right] \right] - \frac{1}{23,890} \left( \frac{V_s C_V T_H}{V_s} - \frac{C_I V T_I}{C_V w} \right) = 0.
\]

\((A-10)\)

Knowing \(V_s\), \(I\), 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 \((V_g \leq 0 \text{ to } V_s \leq 0)\), 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 \((V, S, G, \text{IND})\)

\(V, S, \text{and } G\) 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 \(W\)

\(V(4)\) \(- \frac{\partial P}{\partial X}\) input;

\(V(5)\) temperature \(T\) output

\(S(1)\) \(C\)

\(S(2)\) \(S\)

\(S(3)\) VSW

\(S(4)\) Cl

\(S(5)\) S1

\(S(6)\) F

\(S(7)\) G

\(S(8)\) H

\(S(9)\) I

\(S(10)\) J

\(S(11)\) \(\gamma_s\)

\(S(12)\) \(C_V\)

\(S(13)\) \(V_o\)

\(S(14)\) \(a\)

\(S(15)\) 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

\[
V^A = \frac{V}{V^B} \frac{V^B}{V^A} \frac{X}{1-X}.
\]
or
\[ V^B = -\frac{V}{W \left( \frac{V^A_o}{V^B_o} \right) + 1 - W} \]

We have the following relationships.

(a) \[ V = X (V^A) + (1 - X) (V^B) \]
(b) \[ P = P^A = P^B \]  \hspace{1cm} (A-11)

Knowing \( V^A \) and \( V^B \), we calculate \( I^A_H \) and \( I^B_H \) from Eq. (1).

(c) \[ I^A_H = X \left( I^A_H \right) + (1 - X) \left( I^B_H \right) \]

(d) \[ I^A_H = (I^A_H) + (1 - I^H) \left( \frac{X(I^A_H)}{I^H} \right) \]
and

(e) \[ I^B_H = (I^B_H) + (1 - I^H) \left( \frac{(1-X)(I^B_H)}{I^H} \right) \]

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

(f) \[ \frac{Y_s^A}{V^A} (I^A - I^A_H) + P^A_H - \frac{Y_s^B}{V^B} (I^B - I^B_H) \]

\[ - P^H = 0, \] \hspace{1cm} (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.

The Calling Sequence

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 \( V \) \hspace{2cm} Input
V(2) internal energy \( I \) \hspace{2cm} Input
V(3) mass fraction \( X \) \hspace{2cm} Input
V(4) \( P \) \hspace{2cm} Output
V(5) \( T^A \) \hspace{2cm} Output
V(6) \( T^B \) \hspace{2cm} Output
V(7) \( I^A \) \hspace{2cm} Output
V(8) \( I^B \) \hspace{2cm} Output
V(9) \( V^A \) \hspace{2cm} Output
V(10) \( V^B \) \hspace{2cm} 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.

The Method

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 \( V^S_0 \), otherwise we use \( 0.99 V^S_0 \). We have the following relationships.

(a) \[ V = X (V^S) + (1 - X) (V^G) \]
and

(b) \[ P = P^S = P^G \] \hspace{1cm} (A-13)

Knowing \( V^S \) and \( V^G \), we calculate \( I^S_H \) from Eq. (2) and \( I^G_i \) from Eq. (5).

(c) \[ I^S = X (I^S_H) + (1 - X) (I^G_i) \]

(d) \[ I^S = X (I^S_H) + (1 - X) (I^G_i) \]

(e) \[ I^S = I^S_H + (I - I^H) \left( X(I^S_H) / I^S \right) \]
and

(f) \[ I^G = I^G_i + (I - I^i) \left( (I - X) (I^G_i / I^G) \right) \]

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

\[ \frac{Y_s^S}{V^S} (I^S - I^S_H) + P^S_H - \frac{1}{\beta V^G} (I^G - I^G_i) - P^G_i \]
\[ = 0. \] \hspace{1cm} (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.

\[
\begin{align*}
V(1) & \quad V \quad \text{Input} \\
V(2) & \quad I \quad \text{Input} \\
V(3) & \quad X \quad \text{Input} \\
V(4) & \quad P \quad \text{Output} \\
V(5) & \quad T^S \quad \text{Output} \\
V(6) & \quad T^G \quad \text{Output} \\
V(7) & \quad IS \quad \text{Output} \\
V(8) & \quad I^G \quad \text{Output} \\
V(9) & \quad VS \quad \text{Output} \\
V(10) & \quad VG \quad \text{Output}
\end{align*}
\]

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.

\[
V^A = \frac{V}{X + \frac{V^B}{V^A} (1 - X)}
\]

We have the following relationships.
(a) \( V = X (V^A) + (1 - X) V^B \)
and
(b) \( P = P^A = P^B \).

Knowing \( V^A \) and \( V^B \), we calculate \( I^A_i \) and \( I^B_i \) using Eq. (5).

(c) \( I' = X (I^A_i) + (1 - X) (I^B_i) \)
(d) \( I'^n = X (|I^A_i|) + (1 - X) (|I^B_i|) \)
(e) \( I^A_i = I^A_i + (I - I') \left( X(|I^A_i|)/I'^n \right) \)
and
(f) \( I^B_i = I^B_i + (I - I') \left( (1 - X) (|I^B_i|)/I'^n \right) \).

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

\[
\frac{1}{\beta^A V^A} (I^A - I^A_i) + P^A_i - \frac{1}{\beta^B V^B} (I^B - I^B_i) = 0.
\]

(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.

\[
\begin{align*}
V(1) & \quad V \quad \text{Input} \\
V(2) & \quad I \quad \text{Input} \\
V(3) & \quad X \quad \text{Input} \\
V(4) & \quad P \quad \text{Output} \\
V(5) & \quad T^A \quad \text{Output} \\
V(6) & \quad T^B \quad \text{Output} \\
V(7) & \quad I^A \quad \text{Output} \\
V(8) & \quad I^B \quad \text{Output} \\
V(9) & \quad V^A \quad \text{Output} \\
V(10) & \quad V^B \quad \text{Output}
\end{align*}
\]

INP = 0 for normal exit
= -5 for iteration error.

V. HOM2SG

HOM2SG is used for mixtures of an un decomposed explosive, detonation products, and a non-reactive 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 unde decomposed explosive \( V^{(1)} \), the volume of the detonation products \( V^{(2)} \), and the volume of the non reactive component \( V^{(3)} \), we guess a volume for \( V^{(2)} \) of 0.9 of \( V^{(1)} \) 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) \( P = P^{(1)} = P^{(2)} = P^{(3)} \), \hspace{1cm} (A-17)
(b) \( T^{(1)} = T^{(2)} \), \hspace{1cm} (A-18)
(c) \( V^{(1+2)} = W(V^{(1)}) + (1-W) V^{(2)} \), \hspace{1cm} (A-19)
(d) \( V = X(V^{(3)}) + (1-X)(V^{(1+2)}) \), \hspace{1cm} (A-20)
(e) \( I^{(1+2)} = W(I^{(1)}) + (1-W)(I^{(2)}) \), \hspace{1cm} (A-21)
(f) \( I^{(1+2)} = W(H^{(1)}) + (1-W)(H^{(2)}) \), \hspace{1cm} (A-22)
(g) \( I^{(1+2)} = X(H^{(3)}) + (1-X)(I^{(1+2)}) \), \hspace{1cm} (A-23)
(h) \( I^{(3)} = I^{(3)} + (1-I^{(3)}) \) \hspace{1cm} (A-24)
(i) \( I^{(1+2)} = (I^{(1+2)}) + (1-I^{(1+2)}) \) \hspace{1cm} (A-25)
and
(j) \( I = I^{(3)} - I^{(1+2)} + I^{(1+2)} + I^{(3)} \)

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

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

From Eq. 2,

(l) \[ P^{(3)} = P^{(3)} + \frac{V^{(3)}}{V^{(1)}} \left[ I^{(1+2)} - I^{(3)} \right] \] \hspace{1cm} (A-26)

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

(m) \[ f_{1} = P = P^{(3)} + \frac{V^{(3)}}{V^{(1)}} \left[ I^{(1+2)} - I^{(3)} \right] \] \hspace{1cm} (A-27)

From Eq. (7),

(n) \[ P^{(2)} = P^{(2)} + \frac{1}{\beta V^{(2)}} \left[ I^{(1+2)} - I^{(2)} \right] \] \hspace{1cm} (A-28)

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

\[ f_{2} = P = \left[ I - \frac{V^{(3)}}{V^{(1)}} + \frac{V^{(1)} P^{(1)} w}{V^{(3)}} \right] \] \hspace{1cm} (A-29)

From Eq. (7),

\[ T^{(1)} = T^{(1)} + \frac{I^{(1+2)} - I^{(1)}}{I^{(2)}} \] \hspace{1cm} (A-30)

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

\[ f_{3} = P = \left[ \frac{T^{(2)} - T^{(1)}}{I^{(2)}} + \frac{P^{(1)} V^{(1)}}{C_{V}^{(1)}} - \frac{P^{(2)} \beta V^{(2)}}{C_{V}^{(2)}} \right] \] \hspace{1cm} (A-31)

To keep \( I_{1} \) positive, the energy base for all the components is raised by \( Z \) for the iteration procedure.

Taking

\[ F = f_{1} - f_{3} = 0 \]
\[ G = f_{2} - f_{3} = 0 \]

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

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

\[
\frac{\partial V}{\partial t} = -\frac{\partial (P+Q)}{\partial Z}
\]

\[
\frac{\partial V^n_{i,j}}{\partial t} = V^n_{i,j} - \frac{\delta t}{\rho_{i,j}} \frac{\partial}{\partial Z} \left[ \left( P + q_{i,j}^n \right)_{l+\frac{1}{2}} - \left( P + q_{i,j}^n \right)_{l-\frac{1}{2}} \right]
\]

\[
P^n_{i,j} = \frac{\left( P^n_{i,j} + P^n_{i,j+1} \right)}{2} = \frac{\left( P^n_{i,j} + P^3 \right)}{2}
\]

\[
P^n_{i,j-\frac{1}{2}} = \frac{\left( P^n_{i,j} + P^1 \right)}{2}
\]

\[
\frac{\partial V^n_{i,j}}{\partial t} = V^n_{i,j} - \frac{\delta t}{\rho_{i,j}} \frac{\partial}{\partial Z} \left[ \frac{P^3 - P^1}{2} + Q^3_{i,j} - Q^1_{i,j} \right]
\]
\[
\frac{\partial U}{\partial t} = - \frac{\partial (P+q)}{\partial R}
\]

\[
\tilde{U}^n_{i,j} = U^n_{i,j} - \frac{\delta t}{\rho^n_{i,j}} \left\{ \frac{1}{2V^n_i} \left[ S^n_{1+i,0} (P^n_{i+1,j} - P^n_{i,j}) - S^n_{1-i,0} (P^n_{i-1,j} - P^n_{i,j}) \right] + \frac{1}{\delta R} \left[ q^n_{i+1,0,j} - q^n_{i-1,0,j} \right] \right\}
\]

\[
S^n_{1+i,0} = 2\pi (i-1) \delta R \delta Z
\]

\[
V^n_i = 2\pi (i-1) \delta R \delta Z
\]

\[
\tilde{U}^n_{i,j} = U^n_{i,j} - \frac{\delta t}{\rho^n_{i,j}} \left\{ \frac{1}{2V^n_i} \left[ \left( i-1 \right) (P^n_{i+1,j} - P^n_{i,j}) - \left( i-1 \right) (P^n_{i-1,j} - P^n_{i,j}) \right] + q^n_{i+1,0,j} - q^n_{i-1,0,j} \right\}
\]

II. DERIVATION OF ENERGY EQUATION

\[
\rho \left( \frac{\partial M}{\partial t} + U \frac{\partial M}{\partial R} + V \frac{\partial M}{\partial Z} \right) = -P \left( \frac{\partial U}{\partial R} + \frac{\partial V}{\partial Z} + \frac{U}{R} \right)
\]

\[
\rho \left( \frac{\partial M}{\partial t} + U \frac{\partial M}{\partial R} + V \frac{\partial M}{\partial Z} \right) = -P \left( \frac{1}{R} \frac{\partial UR}{\partial R} + \frac{\partial V}{\partial Z} \right)
\]

eliminating the transport terms

\[
\frac{\partial M}{\partial t} = -P \frac{\partial UR}{\partial R} - P \frac{\partial V}{\partial Z}
\]

Add on viscosity to P.

\[
\frac{\partial M}{\partial t} = -\frac{(P+q)}{R} \frac{\partial UR}{\partial R} - (P+q) \frac{\partial V}{\partial Z}
\]

\[
\frac{\partial M}{\partial t} = -P \frac{\partial UR}{\partial R} - q \frac{\partial UR}{\partial R} - P \frac{\partial V}{\partial Z} - q \frac{\partial V}{\partial Z}
\]

\[
\frac{\partial M}{\partial t} = -P \frac{\partial UR}{\partial R} - \frac{1}{R} \frac{\partial UR}{\partial R} + U \frac{\partial M}{\partial R} - P \frac{\partial V}{\partial Z} - q \frac{\partial V}{\partial Z} + V \frac{\partial M}{\partial Z}
\]

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

\[
\gamma^n_{i,j} = \left( U^n_{i,j} - \frac{\delta t}{\rho^n_{i,j}} \right) \left\{ \left( P^n_{i,j} \right) \left( S^n_{1+i,0} + S^n_{1-i,0} \right) + \frac{1}{\delta R} \left( q^n_{i+1,0,j} + q^n_{i-1,0,j} \right) \right\}
\]

\[
\left( S^n_{1+i,0} + S^n_{1-i,0} \right) = \left( U^n_{i+1,j} + U^n_{i-1,j} \right)
\]

\[
\left( q^n_{i+1,0,j} + q^n_{i-1,0,j} \right) = \left( q^n_{i+1,0,j} + q^n_{i-1,0,j} \right)
\]

\[
\left[ \tilde{V}^n_{i,j+k} \left( P^n_{i,j+k} + q^n_{i,j+k} \right) - \tilde{V}^n_{i,j-k} \left( P^n_{i,j-k} + q^n_{i,j-k} \right) \right]
\]
\[
\begin{align*}
\bar{U}_{i,j}^n &= \frac{1}{2} \left( U_{i,j}^n + \bar{U}_{i,j}^n + U_{i+1,j}^n + \bar{U}_{i+1,j}^n \right) \\
\bar{V}_{i,j}^n &= \frac{1}{2} \left( V_{i,j}^n + \bar{V}_{i,j}^n + V_{i,j+1}^n + \bar{V}_{i,j+1}^n \right) \\
\bar{U}_{i,j}^n &= \frac{1}{2} \left( U_{i,j}^n + \bar{U}_{i,j}^n \right) \\
\bar{V}_{i,j}^n &= \frac{1}{2} \left( V_{i,j}^n + \bar{V}_{i,j}^n \right) \\
\bar{V}_{i,j}^n &= \frac{1}{2} \left( i, j \right) = \left\{ \begin{array}{l}
\bar{V}_{i,j}^n \left( U_{i,j}^n + \bar{U}_{i,j}^n \right) \\
\bar{V}_{i,j}^n \left( V_{i,j}^n + \bar{V}_{i,j}^n \right) \\
\bar{V}_{i,j}^n \left( T_3 + \bar{U}_{i,j}^n \right) + \bar{V}_{i,j}^n \left( T_3 - \bar{U}_{i,j}^n \right) \\
\bar{V}_{i,j}^n \left( V_{i,j}^n + \bar{V}_{i,j}^n \right)
\end{array} \right.
\end{align*}
\]

where

\[
\begin{align*}
S^r_{i,j} &= 2\pi \left( i - \frac{1}{2} \right) \delta R \delta Z \\
V^r_{i,j} &= 2\pi \left( i - \frac{1}{2} \right) \delta R^2 \delta Z \\
S^Z_{i,j} &= 2\pi \left( i - \frac{1}{2} \right) \delta R^2 \\
U_1 &= \left( U_{i-1,j}^n + \bar{U}_{i-1,j}^n \right) \\
U_2 &= \left( U_{i+1,j}^n + \bar{U}_{i+1,j}^n \right) \\
V_1 &= \left( V_{i,j-1}^n + \bar{V}_{i,j-1}^n \right) \\
V_2 &= \left( V_{i,j+1}^n + \bar{V}_{i,j+1}^n \right) \\
T_3 &= \left( U_{i,j}^n + \bar{U}_{i,j}^n \right) \\
T_1 &= \left( \bar{V}_{i,j}^n \right) \\
\bar{V}_{i,j}^n &= \left( i, j \right) = \left\{ \begin{array}{l}
\bar{V}_{i,j}^n \left( T_3 + U_2 - (i - 1) (T_3 - U_1) \right) + \frac{Q^4_{i,j}}{2(2i-1)\delta R} \left[ (i + \frac{1}{2}) U_2 - (i - \frac{1}{2}) T_3 \right] \\
\bar{V}_{i,j}^n \left( V_2 - V_1 \right) + \frac{1}{2\delta Z} \left[ E_{i,j} (V_2 - V_1) + Q^4_{i,j} \right] \left( V_2 - T_1 \right) + Q^4_{i,j} \left( T_1 - V_1 \right) \end{array} \right.
\end{align*}
\]
III. DERIVATION OF MASS MOVEMENT EQUATION

The O'Rourke method for velocity weighting is derived below. The mass to move across a surface element between a and b where $d = b - a$; thus, $d = \bar{u}\Delta t$ where $\bar{u}$ is the weighted velocity at $d$. Using the first two terms of the Taylor series at a distance $-d$ from $b$, we expand

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

$$\bar{u} = \frac{u_{i-1,j} + u_{i,j}}{2} + \left( \frac{\partial}{\partial R} \left( u_{i-1,j} - u_{i,j} \right) \right) \cdot$$

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

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

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

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

$$= 2\pi R (i - \frac{d}{2}) \Delta Z$$

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

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

The volume of cell i-1, j is

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

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

I.

\[ DM = \frac{\text{Mass Moved}}{\text{Unit Volume}} = \frac{n^R (2i - 1) \Delta Z \bar{\rho}_{i-1,j} \bar{u}_{i,\Delta t}}{n(2i - 1) \Delta R^2 \Delta Z}. \]

\[ DM = \frac{(2i - \delta)}{(2i - 1)} \bar{\rho}_{i-1,j} \left( \frac{\bar{u}_{\Delta t}}{\Delta R^2} \right) \]

\[ = \bar{\rho}_{i-1,j} \left( \frac{2i - \delta}{2i - 1} \right) \bar{\rho}_{i-1,j} \eta_{i-1,j} \Delta \]

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.
RH@O(K)  Initial density, used only for skipping tests.
ACTE(K)  Activation energy.
FREQ(K)  Frequency factor.
MTYPE(K)  3HGAS for a gas, 4HSOLID 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.

Equation-of-state parameters for the solid.
Equation-of-state parameters for the detonation products.
Initial density, used only for skipping tests.
Activation energy.
Frequency factor.

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 HPIST@N).
B2  Boundary 2 (default value = 4HAXIS).
B3  Boundary 3 (default value = 9HCÔNTINUUM).
B4  Boundary 4 (default value = 9HCÔNTINUUM).

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

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>NR</td>
<td>Number of rectangles.</td>
</tr>
<tr>
<td>RW(M)</td>
<td>Width of the M th interval.</td>
</tr>
<tr>
<td>ZW(N)</td>
<td>Width of the N th interval.</td>
</tr>
<tr>
<td>IR(M)</td>
<td>Number of cells in the M th interval.</td>
</tr>
<tr>
<td>JZ(N)</td>
<td>Number of cells in the N th interval.</td>
</tr>
<tr>
<td>DELR(M)</td>
<td>Cell width in the M th interval (currently the same for all intervals).</td>
</tr>
<tr>
<td>DELZ(N)</td>
<td>Cell width in the N th interval (currently the same for all intervals).</td>
</tr>
</tbody>
</table>

For the L th rectangle:

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>KMAT(L)</td>
<td>Material K for the rectangle.</td>
</tr>
<tr>
<td>RHØ(L)</td>
<td>Initial cell density.</td>
</tr>
<tr>
<td>PO(L)</td>
<td>Initial cell pressure.</td>
</tr>
<tr>
<td>TO(L)</td>
<td>Initial cell temperature.</td>
</tr>
<tr>
<td>UO(L)</td>
<td>Initial cell velocity in the U direction.</td>
</tr>
<tr>
<td>VO(L)</td>
<td>Initial cell velocity in the V direction.</td>
</tr>
</tbody>
</table>
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.
RH@OC(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.

PCGS Starting print cycle (default value = 1).
PCIS Print cycle increment (default value = 50).
PCES 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

ISÓPLÔT(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 =
64 = W mass fraction.

To get more than one plot per frame, values are added together for ISÓPLÔT(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.
NPLÔTS 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.
If . T., positions of mixed cells are plotted with an asterisk.

ZDE 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

\[
\begin{align*}
\text{ICON(L)} &\quad \text{Contains IXZ indices that define cross sections parallel to the Z axis.} \\
\text{JCON(L)} &\quad \text{Contains JXR indices that define cross sections parallel to the R axis.} \\
\text{PTYPE(M)} &\quad \text{Determines which cell quantity is plotted.} \\
\text{KPLOTS} &\quad \text{Number of one-dimensional plots. This variable is set by the preprocessor; however, if it is modified here by being set equal to zero, all one-dimensional plots will be eliminated from the output.}
\end{align*}
\]

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

\[
\begin{align*}
\text{IXL} &\quad \text{Grid left coordinate (default value = 120).} \\
\text{IXR} &\quad \text{Grid right coordinate (default value = 980).} \\
\text{IYT} &\quad \text{Grid top coordinate (default value = 50).} \\
\text{IYB} &\quad \text{Grid bottom coordinate (default value = 910).}
\end{align*}
\]

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.

\[
\begin{align*}
\text{DEBUG(L)} &\quad \text{For the logical variables L = 1 through 5, phases 1 through 5 are debugged. Flags 6 and 7 produce dump information for the mixed-cell and dump routine.} \\
\text{DBS} &\quad \text{Cycle control starting the debug dump.} \\
\text{DBI} &\quad \text{Cycle increment for dumping.} \\
\text{DBE} &\quad \text{Terminating cycle for dumping.}
\end{align*}
\]

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

\[
\begin{align*}
\text{IGS} &\quad \text{Starting radial or I index.} \\
\text{IGE} &\quad \text{Ending radial or I index.} \\
\text{JGS} &\quad \text{Starting Z or J index.} \\
\text{JGE} &\quad \text{Ending Z or J index.}
\end{align*}
\]

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."

\[
\begin{align*}
\text{DCYCLE} &\quad \text{Initially zero. Set to the problem cycle for picking up dumps.} \\
\text{COMMENT} &\quad \text{Up to 70 Hollerith characters that go to the printer and express file.} \\
\text{TAPE} &\quad \text{Up to 10 Hollerith characters for a dump tape label.} \\
\text{DTI} &\quad \text{Dump time increment (default value = 300 sec).} \\
\text{SECS} &\quad \text{Tolerance that allows time for the last dump before}
\end{align*}
\]
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. NAMELIS T 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  NJZ
KCIR   IĆØN  IGS  KMH
PCS    JĆØN  NCYLI M  NT CY
PCI    PTYPE  IGE  KCIR
PCE    VCNT  JGS  NĆØNL
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
RHΦØ  VO  GMAX  EAPP
ACTE  WO  GMIN  .WAPP
FREQ  IO  GDELT A  VAPP
RHØ   DELR  DTI  MAPP
IOC   DELZ  SECS  MNWT

MINGRHØ WOC  RHØOC  ZO
FREPR  ZW  RO  RAD
TFCT  DTI

LOGICAL

IHE  SLAB
IREACT  NTRFCE
DEBUG  DICE

HOLLERITH

ID  B1
NAME  B2
COMMENT  B3
TAPE  B4

MTYPE

VI. STORAGE REQUIREMENTS

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.

REFERENCES


