28
9-27-76

61-379

UCRL-50028-76-2

H-DIVISION QUARTERLY REPORT

April through June 1976

MASTER

Prepared for U.S. Energy Research & Development
Administration under contract No. W-7405-Eng-48

NOTICE

"This report was prepared as an account of work sponsored by the United States Government. Neither the United States nor the United States Energy Research & Development Administration, nor any of their employees, nor any of their contractors, subcontractors, or their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness or usefulness of any information, apparatus, product or process disclosed, or represents that its use would not infringe privately-owned rights."

Printed in the United States of America
Available from
National Technical Information Service
U.S. Department of Commerce
5285 Port Royal Road
Springfield, VA 22161
Price: Printed Copy \$; Microfiche \$2.25

<u>Page Range</u>	<u>Domestic Price</u>	<u>Page Range</u>	<u>Domestic Price</u>
001-025	\$ 3.50	326-350	10.00
026-050	4.00	351-375	10.50
051-075	4.50	376-400	10.75
076-100	5.00	401-425	11.00
101-125	5.25	426-450	11.75
126-150	5.50	451-475	12.00
151-175	6.00	476-500	12.50
176-200	7.50	501-525	12.75
201-225	7.75	526-550	13.00
226-250	8.00	551-575	13.50
251-275	9.00	576-600	13.75
276-300	9.25	601-up	*
301-325	9.75		

*Add \$2.50 for each additional 100 page increment from 601 to 1,000 pages:
add \$4.50 for each additional 100 page increment over 1,000 pages.

LAWRENCE LIVERMORE LABORATORY
University of California Livermore, California 94550

UCRL-500028-76-2

H-DIVISION QUARTERLY REPORT
April through June 1976

MS. date: July 14, 1976

NOTICE
This report was prepared as an account of work sponsored by the United States Government. Neither the United States nor the United States Energy Research and Development Administration, nor any of their employees, nor any of their contractors, subcontractors, or any person making any legal warranty, accepts or implies or assumes any liability or responsibility for the accuracy, completeness, or usefulness of any information appearing in this report. It is the policy of the United States Government to make available as soon as possible the results of research and development performed by the United States Government.

Preface

This quarterly report has a dual purpose: to acquaint the reader with the overall goals of each of the five groups comprising H-Division of the Physics Department; and to supply a concise statement of the status of the projects under way in each group. References and experimental details are kept to a minimum. Readers who desire additional information are encouraged to contact the individual(s) associated with each project.

H-Division quarterly reports prior to January 1975 have been numbered UCID-16457-74-2, 3, and 4. Beginning with the quarter for January through March 1975, the quarterly reports are series-numbered starting with UCRL-500028-75-1, where 75 is the year and 1 is the quarter of that year.

Contents

I.	Theoretical EOS Group (<i>R. Ascher, Group Leader</i>)	1
	Single-Band Electron Excitation Model (<i>R. Grover and</i> <i>A. McWhirer</i>)	1
	A New EOS of SiO_2 (<i>R. Ascher</i>)	3
	Melting of Magnesium at High Dynamic Pressures (<i>R. Grover and J. Terjes</i>)	7
	EOS Representations (<i>C. E. Jenson</i>)	9
	EOS of Aluminum (<i>G. E. McWhirer</i>)	12
II.	Code Development Group (<i>C. L. Edwards, Group Leader</i>)	14
	The CHAMP Hydrodynamics Package (<i>C. L. Edwards,</i> <i>J. B. Hickman, G. L. Brown, and J. Nichols</i>)	14
	LASER-KO Code (<i>C. L. Edwards and J. L. Grantham</i>)	14
	Availability of More Versatile Zoning in the 2D-HEMP-Code (<i>C. L. Edwards</i>)	16
	HEMPDST: A Version of HEMP with Sliding on J-Lines, K-Lines, and Triangles (<i>J. Grantham</i>)	17
	A Mesh Generator for Cylinders (<i>E. A. Bird</i>)	18
III.	Experimental Physics Group (<i>C. W. Shaner, Group Leader</i>)	20
	Effectiveness of Alumina Armor Plate Against High Velocity Projectiles (<i>B. L. Ford</i>)	20
	Hugoniot Measurements on Aluminum (<i>A. J. Mitchell</i> and <i>A. W. Johnson</i>)	22
	Properties of Materials at High Pressure (<i>W. H. Gust</i>)	22
	BRL Vehicular Armor Program (<i>C. E. Goodner</i>)	23
IV.	Solid Mechanics Group (<i>D. M. Morris, Group Leader</i>)	25
	Fundamental Study of Crack Initiation and Propagation (<i>D. M. Morris, M. L. Wilkins, M. E. Prado, B. Morin,</i> <i>W. H. Hoover, D. F. Quinones, and Y. M. Chen</i>)	25
	The Thermal Yield of the Shallow Burst Munitions (<i>M. Kamagata</i>)	27
	Studies in Fracture Mechanics (<i>W. G. Hoover</i>)	28

V.	Fluid Mechanics Group (<i>M. Ross, Group Leader</i>)	33
	Rainout: Development of Low-Speed Turbulence Generator	
	(<i>A. C. Buckingham</i>)	33
	A Reynolds-Number-Dependent Scheme for the Solution	
	of "Diabolic" Equations (<i>B. R. Bowman and</i>	
	<i>L. A. Truong</i>)	36
References		44

H-DIVISION QUARTERLY REPORT

April through June 1976

I. Theoretical EOS Group

(R. Grover, Group Leader)

The Theoretical EOS Group has two primary tasks: the development of theoretical techniques for the description of material properties under extreme conditions and the construction of equation-of-state (EOS) tables for specific LLL materials applications.

SINGLE-BAND ELECTRON EXCITATION MODEL

(R. Grover and A. McMahan)

• A simple analytic representation of the thermal properties of a partially filled electron band is given for use in equation-of-state models.

In constructing a thermal EOS for metals from a fundamental band-structure calculation (e.g., augmented-plane-wave)¹ or a phenomenological Grüneisen model (GRAY code),² we found it useful to model the thermal excitations of electrons as those of an idealized Fermi gas. In the Grüneisen model, this is usually a simple open-ended, free-electron gas having an energy density-of-states, $D(\epsilon)$ proportional to $\epsilon^{1/2}$,

which is unbounded at high energies. However, for those materials whose electronic structure is characterized by a band gap, this form is inappropriate. For example, the Hugoniot for solid iodine appears to be affected significantly by the 5p- to 5d-band gap.¹ We found in the iodine work that the electronic density of states could be very well modeled by

$$D_1(\epsilon) \propto [(\epsilon - \epsilon_a)(\epsilon_b - \epsilon)]^{1/2} \quad (1)$$

for the lower partially filled band (ϵ_a and ϵ_b are the band edges); to which was added $D_2(\epsilon) \propto [\epsilon - \epsilon_c]^{1/2}$ for the excited states above the band gap (ϵ_b to ϵ_c), which constitute the free-electron continuum. In these calculations, the thermodynamic properties of the electron excitations are calculated by integrals of Fermi distribution functions over this density-of-states.

Such a simple electron model would appear also to have a number of useful advantages in phenomenological Grüneisen models used to fit experimental data at high pressure and temperature.

● A limited instead of unbounded behavior of the electronic specific heat at high temperature for those materials where the band gap is extremely large.

● A smoothly vanishing electronic specific heat at low density if the band width decreases with expansion.

● A more realistic representation of the actual band structure of many metals such as the transition metals having narrow, dense bands.

To simplify the use of this model in EOS calculations, we have made a simple analytic fit to the thermodynamic functions of the single-band model, Eq. (1), and about 1% accuracy. It is straightforward to add the corresponding expressions for the free-electron continuum above the band gap, when desired. We shall not do so here. Here we report fits to accurate numerical calculations of the thermal energy for the one-band model, from which all thermodynamic functions may be calculated.

Consider a band of electron energies centered at $\epsilon = 0$ width w having σ states per atom. Then the electron energy E and chemical potential μ at temperature T are determined from the number of electrons per atom N by

$$N = \frac{2\sigma}{\pi} \int_{-1}^{+1} \frac{(1-x^2)^{1/2} dx}{e^{\beta w(X-X_\mu)/2} + 1},$$

$$E = \frac{\sigma w}{\pi} \int_{-1}^{+1} \frac{(1-x^2)^{1/2} x dx}{e^{\beta w(X-X_\mu)/2} + 1}, \quad (2)$$

where

$$X = \frac{2\epsilon}{w}, \quad X_\mu = \frac{2\mu}{w}, \quad \beta = (k_B T)^{-1}.$$

As $T \rightarrow 0$, $X_\mu \rightarrow X_f = 2 \frac{\epsilon_f}{w}$ in terms of the "Fermi energy," ϵ_f , and

$$N = \frac{\sigma}{2} + \frac{1}{\pi} \times \left[\sin^{-1} X_f + X_f (1 - X_f^2)^{1/2} \right],$$

$$E_0 = -\frac{\sigma w}{3\pi} (1 - X_f^2)^{3/2}. \quad (3)$$

Figure 1 shows the electron thermal energy $E_{th} \equiv E(T) - E_0$ calculated from Eqs. (2) and (3) as a function of $\tau \equiv k_B T/w$ for various occupancy

Fig. 1. Exact numerical calculations of the scaled electron thermal energy vs scaled temperature. Curves are approximated by Eq. (4).

fractions $\nu = n/0$. The curves are symmetric about $\nu = 0.5$ because of particle-hole symmetry.

We found that curves for E_{th}/ω can be approximated for all values of ν by the following function

$$\frac{E_{th}}{\omega} = \frac{A\tau^2}{1 + B\tau^2} + De^{-C/\tau} (e^{-C/\tau} - 1), \quad (4)$$

where the first term is determined solely by the low and high temperature limits of Eqs. (2) and (3)

$$A = \frac{2\pi}{3} \left(1 - X_F^2\right)^{1/2}$$

$$B = 2\pi^2 / \left(1 - X_F^2\right)$$

$$\begin{aligned} X_F(\nu) &= -1 + \sqrt{2} (1 - \pi/4) \nu^{1/2} \\ &+ (\pi - 2) \nu \text{ for } \nu \leq 1/2 \\ &= 1 - 2\sqrt{2} (1 - \pi/4) (1 - \nu)^{1/2} \\ &- (\pi - 2)(1 - \nu) \text{ for } \nu \geq 1/2. \end{aligned}$$

The second term of Eq. (4) is relatively small and produces a good fit of corrections to the limiting values at high and intermediate temperatures with

$$C \approx (0.3 + 0.6 \nu) \ln 2;$$

$$D \approx 0.069 \nu (1 - \nu).$$

The remaining thermodynamic functions can be obtained by differentiation or integration of Eq. (4). For instance, the thermal Helmholtz free energy F_{th} is given by

$$\begin{aligned} \ln \frac{F_{th}}{\sigma} &= - \int_0^\infty \frac{E}{\omega} d\omega \\ &= - \frac{A}{B^{1/2}} \tan^{-1} B^{1/2} \tau \\ &- \frac{D}{2C} e^{-C/\tau} (e^{-C/\tau} - 2) \end{aligned}$$

Since the thermal energy depends (for fixed ν) on the volume through $k_B T/\omega$ only, the electron thermal pressure P_e is determined by the dependence of ω on the atomic volume V_a .

$$P_e = \gamma_e E_{th}/V_a,$$

$$\gamma_e \equiv - \frac{d \ln \omega}{d \ln V_a}.$$

A NEW EOS OF SiO_2

(F. Ree)

• Theoretical EOS of SiO_2 applicable to several LLL programs was developed. The range considered here covers from $1.5 \cdot 10^{-6} \text{ mg/m}^3$ to 150 Mg/m^3 in density and from room temperature to 25 keV.

At present, there is no physically reliable EOS expression for SiO_2 in the LLL EOS library. A common

practice to date has been to use either a perfect-gas ionization equilibrium model (as in MEG) or an expression suitable for an entirely different material (as in LASNEX) with possible use of arbitrary pressure and energy multipliers, thereby, ignoring possible pitfalls associated with such over-simplified models. The EOS of soil in MEG, for example, produces an unphysical shock front whose strength decreases with increasing compression.³ A theoretically realistic EOS is difficult because of the physical complexity of SiO_2 as evidenced by the many crystal polymorphs observed in solid SiO_2 . Nevertheless, because SiO_2 is one of the most commonly occurring materials in nature and because it plays an important role in several LLL programs, a serious effort to improve the EOS is justified.

To this end, we have developed a new tabular EOS of SiO_2 for use with MEG. The range considered here is from $1.5 \cdot 10^{-6}$ to 150 Mg/m^3 in density and from 0.025 eV to 25 keV in temperature. This range covers nearly all possible applications of the EOS, such as a study on ground response caused by underground nuclear explosion and a simulation of a silica-glass microcapsule containing D-T gas in the LLL laser-fusion program.

Since the density-temperature region described above is very large,

one single theoretical model cannot describe the entire region. As was done previously for polystyrene and water, our approach was to use several theoretical models describing different physical behaviors at different ranges of temperature and density. The five different EOS codes used for this purpose are TIGER, GRAY, OCCIPITAL, TFCMIX and MASTER.

- TIGER for low density, ρ , (≤ 2.2 to 2.6 Mg/m^3) and low T ($\leq 1 \text{ eV}$) to describe a chemical equilibrium state of the reacting mixtures composed of gaseous species (O , O_2 , Si , Si_2 , Si_3 , SiO , SiO_2) and condensed species (liquid and solid Si , SiO_2).
- GRAY for low T ($\leq 1 \text{ eV}$) and medium ρ (between normal density 2.65 Mg/m^3 of quartz at standard state and about twice the normal density) to describe liquid and solid (quartz and stishovite) phases of un-ionized SiO_2 .
- OCCIPITAL for low ρ (≤ 0.1 to 0.8 Mg/m^3) and high T ($\geq 1 \text{ eV}$) to describe ionization equilibrium.
- TFCMIX for high ρ (≥ 0.5 to 0.7 Mg/m^3) and high T ($\geq 40 \text{ eV}$) to describe the Thomas-Fermi model.
- MASTER for temperature below 40 eV to modify the physics behind TFCMIX at low temperatures.

Figure 2 shows the pressure isotherms to 25 keV resulting from the present work. A large liquid-vapor coexistence region can be seen clearly. In the density interval

Fig. 2. Pressure isotherms of SiO_2 from 0.01 eV to 25 keV.

between 2 and 5 Mg/m^3 , liquid-solid and solid-solid phase changes occur. These features are incorporated in the present work, but they are too fine a structure to be able to discern from the plot. The vapor-solid coexistence region, which lies below 0.18 eV, is not shown in the plot,

since the vapor pressure is exceedingly small (for example, $6.1 \cdot 10^{-17}$ TPa at $T = 0.13$ eV). Since the vapor pressure is small even for a relatively hot gas (for example, $7.2 \cdot 10^{-6}$ TPa at $T = 0.35$ eV) and since it is only a function of temperature and does not

depend on density (i.e., between 0.01 and 2.157 Mg/m³ in the above example), even a tiny amount of gaseous impurities can affect the pressure enormously at densities, where the precipitation of liquid SiO₂ causes the total amount of the gaseous components (O, O₂, Si, Si₂, Si₃, SiO, SiO₂) to fall below that of the impurities. As a result, a high-density flat portion of a pressure isotherm for a contaminated system in the first-order vapor-liquid (or vapor-solid) transition region is destroyed and replaced by the partial pressure of the impurities. This point should be kept in mind when the theoretical EOS is to be applied in an actual experimental situation, since elimination of various impurities is impossible in practice.

Figure 3 shows the Hugoniot pressure vs density obtained from the present work. The calculated result

is compared with experimental points obtained by Wackerle⁴ and by Trunin, *et al.*⁵ The agreement is good to 5 Mg/m³ in density (or to 0.1 TPa in pressure), but the theoretical Hugoniot becomes slightly softer than the experimental data beyond this range. A likely source for the observed discrepancies lies in the MASTER-corrected TFCMIX region. It is known⁶ that the calculated second-order quantum corrections in TFCMIX are thermodynamically inconsistent in the low temperature region (≤ 10 eV) and that this in turn produces a softer Hugoniot. A small flat portion of the experimental Hugoniot near $\rho = 4.5$ Mg/m³ is associated with the quartz-stishovite phase transition. In the GRAY code, the isotherms belonging to this portion are assumed to be smooth and continuous with relatively small positive slopes.

One of the most troublesome areas encountered during the course of the present work was a lack of an efficient scheme to fill "holes" in

Fig. 3. SiO₂ Hugoniot pressure vs density. Experimental points are from Refs. 4 and 5. An irregular appearance of the theoretical Hugoniot is because of the tabular EOS form (rather than an analytic form) used in this calculation.

the density-temperature region where the above mentioned theoretical models are not applicable. One such case occurs in a region bounded by density between 2.2 and 2.65 Mg/m³ and temperature below 1 eV. This region separates the GRAY- and the TIGER-generated EOS data. In this region the pressure increases by several decades, as clearly seen in Fig. 1. The next most difficult "hole"-region occurs in the density between 5 and 6.5 Mg/m³ separating the GRAY and the MASTER EOS data. The difficulty occurs here because the MASTER-generated isotherms (as described previously) are too soft, and reliable information regarding the Grüneisen γ and the specific heat at constant volume, which are needed in GRAY, are not available. Improvements in the TFCMIX and GRAY models are under development, which should help resolve the interpolation difficulties encountered in the present work.

MELTING OF MAGNESIUM AT HIGH DYNAMIC PRESSURES

(R. Grover and P. Urtiew*)

● Temperature measurements on shock-compressed magnesium are interpreted to support the Lindemann melting law at high pressures.

* P. Urtiew is in the Chemistry Department.

Extensive experimentation was carried out several years ago by P. Urtiew, then in S-Division (now H-Division), to measure the temperature of shock-compressed materials by radiation techniques. The black-body temperature deduced from the measured spectral intensities were, however, considerably higher than reasonable theoretical estimates. An explanation of this data eventually came from taking account of the reshocking of the radiating layers of the sample material in the small gap between the sample and the anvil that supports the shock wave pressure. We have previously described a calculational study of the reshocking effect at interfaces, especially in the presence of a melting transition.^{7,8} In this study we concluded that the observed temperatures lie on the high pressure melting line over a wide pressure range *below* the normal melting pressure on the Hugoniot.

In the present work,⁹ this explanation has been applied to the extensive amount of temperature data taken on samples of a Mg alloy (AZ-31B) in the pressure range 35 to 50 GPa. The measured melting data has been compared with a number of theoretical and experimental laws in Fig. 4. A standard Simon law prediction, as well as the Kraut, Kennedy (KK) law, are seen to disagree seriously with the present data.

Fig. 4. Comparison of various predicted melting lines (see text) with experimental data.

The remaining curves are examples of Lindemann law predictions with different assumptions about the high density behavior of the Grüneisen coefficient $\gamma_G(\rho)$. According to the Lindemann law, the melting temperature, T_m , varies with the density according to

$$\frac{d \ln T_m}{d \ln \rho} = \gamma_G \equiv v \frac{\partial P}{\partial E} v.$$

The assumed $\gamma_G(\rho)$ are from Slate (SL), Dugdale-MacDonald (DM), and free-volume (FV) theories. These theories

lead to the same differential equation for $\gamma_G(V)$ in terms of the zero-degree isotherm $P_0(V)$

$$\gamma_G = \frac{\tau - 2}{3} - \frac{1}{2} \frac{d \ln [d(P_0 V^{2\tau/3})/d \ln V]}{d \ln V} \quad (5)$$

with different values of τ (0, 1, and 2 respectively). Note that SL and DM are closest to our data, but that a satisfactory fit to both the dynamic data and hydrostatic melting temperature data requires an intermediate γ corresponding to a τ of about 0.5.

Such nonintegral values of τ can be justified by the argument of Vashchenko and Zubarev.¹⁰ Shock velocity data for Mg together with this value of τ in Eq. (5) predicts a value of γ_G at normal conditions of 1.65, in reasonable agreement with the experimental value of about 1.6. This theory predicts that the principal Hugoniot will pass into the two-phase liquid-solid region at about 57 GPa, as shown also in Fig. 4.

These experiments thus lend support to the Lindemann melting law at high pressures that is often used in EOS models (e.g., GRAY). They furthermore suggest that other manifestations of melting along the Hugoniot be examined in the vicinity of 57 GPa.

EOS REPRESENTATIONS

(R. J. Olness)

● We have examined a number of thermodynamic variable sets to identify possible choices that might prove better suited to EOS representations in hydro and hydro/transport codes than those in current use. A scheme based on internal energy as a function of density and entropy, $E(\rho, S)$, offers several advantages. We describe its use briefly to illustrate various procedures and to point out certain current problems. A more detailed report on this subject has been issued separately.¹¹

Most weapon codes in current use employ one of two basic EOS representations:

1) Direct functional representations of $P(\rho, E)$ for pure hydro^{*} applications, and

2) $P(\rho, T)$, $E(\rho, T)$ tabulations for hydro/transport applications.

Several problems can be identified as follows:

- a. Detailed behavior of almost any material is generally difficult, if not impossible, to fit with a single $P(\rho, E)$ form over the entire range of interest.
- b. The change from ρ, E variables to ρ, T variables on linking a pure hydro problem to a hydro/transport code often produces serious anomalies caused by inequivalence of the EOS representations.
- c. The weak thermal dependence of P and E in the low- T region is difficult to characterize adequately. This feature contributes to problem b above and also to the thermodynamic inconsistency that is frequently found in low- T , high- ρ regions.
- d. The use of ρ, T variables in hydro/transport codes is inefficient in treating the pure hydro processes that generally occur in most problems. (T

*For purposes of this report, 1) and 2) are distinguished by the absence of significant radiation field effects in pure hydro calculations.

must be calculated at every cycle for no purpose beyond its use as an independent variable of the EOS representation.)

E(ρ, S) Representation

Several aspects of the problems listed above suggest adoption of the thermodynamic potential E (internal energy) as a function of density (ρ) and entropy (S) as the basic EOS representation for use in both applications: pure hydro and hydro/transport. The typical different-equation scheme permits more or less direct calculation (on a zone-by-zone basis) of the time-advanced values of both independent variables; ρ from the time-dependent geometry (a fundamental objective of most calculations) and S through its relation to known entropy-increasing processes. The latter include, for example, shock heating, radiation transport effects, and heating due to energy sources:

$$dS = \frac{dE + PdV}{T}$$

$$= - \frac{Q_{dV} + (\text{radiation transportation, sources})}{T}$$

The pressure (P), which enters the dynamical equations, is one of two conjugate variables in the $E(\rho, S)$ system.*

$$P = P(\rho, S) = - \left(\frac{\partial E}{\partial V} \right)_S$$

$$\text{and } T = T(\rho, S) = \left(\frac{\partial E}{\partial S} \right)_\rho$$

With direct advance (in time) of ρ and S , the pure hydro cycle is complete; $\rho' \rightarrow \rho + d\rho$, $S' \rightarrow S + dS$, and $P' = P(\rho', S')$ or $-(\partial E / \partial V)_S$ depending on the representation. A value of T can be calculated if desired, but is not necessary in the pure hydro problem.

With finite radiation field effects, it is necessary to separate the matter (M) and radiation field (R) contributions to S at each cycle. dS is given schematically above and $S' = S + dS$, but the components S'_m and S'_R whose sum makes by S' are unknown. [The EOS representation describes only the matter, $E_m(\rho, S_m)$. Although some simplification might occur if the radiation field were included, various complications would also appear, particularly in the treatment of nonequilibrium problems.] The separation $S = S_m + S_R$ can be carried out in two ways:

1) Since dE is directly calculable (it occurs in dS) we have $E' = E + dE$ and can solve the following equation for S_m (omitting primes):

$$E = E_m(\rho, S_m) + E_R(\rho, S - S_m).$$

We know ρ, E , and S , whereas E_m and E_R are known functions of the indicated variables. $S_R = S - S_m$ and

* $V = 1/\rho$.

we can proceed with the next time step, obtaining a value of T if desired from

$$S_R = \frac{16}{3} \frac{\sigma}{c} \frac{T^3}{\rho} \text{ or } T = \left(\frac{\partial E_m}{\partial S_m} \right)_\rho.$$

2) As an alternative, we can solve for T (which implies complete knowledge of the equilibrium radiation field) by calculating dT as follows:

$$dT = \left(\frac{\partial T}{\partial S} \right)_\rho dS + \left(\frac{\partial T}{\partial \rho} \right)_S d\rho,$$

$$T' = T + dT.$$

A variant of this approach is used in some current T-based codes.

The derivatives in 2) include both matter and radiation. We note further that the second method requires an adequate characterization of the second derivative

$$\left(\frac{\partial T}{\partial S_m} \right)_\rho = \left(\frac{\partial^2 E_m}{\partial S_m^2} \right)_\rho.$$

If we choose instead to represent the conjugate variables $P(\rho, S)$ and $T(\rho, S)$, problems of thermodynamic consistency arise through the identity

$$\left(\frac{\partial T}{\partial \rho} \right)_S = \frac{1}{\rho^2} \left(\frac{\partial P}{\partial S} \right)_\rho.$$

If the numerical representation problem can be overcome, tabulation

of the single quantity $E(\rho, S)$ seems clearly preferable. The elimination of T as an independent variable in favor of S is likely to resolve the weak thermal dependence problem directly. There seems to be no equivalent problem associated with S.

While we think in terms of tabulation for the broad range of parameter space encountered in the complete spectrum of calculations, the desirability of direct functional representations (e.g., ratio-of-polynomial forms) will undoubtedly persist. There is reason to believe that $E(\rho, S)$ may prove better suited to this application¹² than $P(\rho, E)$.

Other Variables

Space considerations prohibit a similarly detailed discussion of other thermodynamic variable choices. The major defects in the present $E(\rho, T)$, $P(\rho, T)$ system have been indicated above. Some remarks concerning the use of a hybrid set $P(\rho, E)$, and $E(\rho, T)$, are included in Ref. 11. Many of the same disadvantages presently associated with the use of T as an independent variable would persist on switching to the Helmholtz free energy $F(V, T)$. The use of F to derive and tabulate the conjugate variables P and S leads to thermodynamic consistency problems arising through the identity

$$\left(\frac{\partial S}{\partial V}\right)_T = \left(\frac{\partial P}{\partial T}\right)_V.$$

The thermodynamic potentials $G(P,T)$ and $H(P,S)$ are both handicapped by the absence of ρ as an independent variable. The density is a fundamental parameter in hydro calculations and schemes which circumvent its direct use seem likely to become rather complicated.

Conclusions

The possible use of $E(\rho,S)$ as the basis for EOS representations seems to merit further investigation. It is well-suited to pure hydro calculations, likely to resolve a number of current problems associated with weak temperature dependences and is probably no worse than equivalent, in the hydro/transport regime, to temperature-based schemes. The systematic use of entropy as a guide in design/calculation procedures could lead to significant benefits. Simultaneous use of the same $E(\rho,S)$ representation in hydro and hydro/transport codes would resolve link problems stemming from the use of different representations.

EOS OF ALUMINUM

(A. K. McMahan)

• The Hugoniot and zero-K isotherm have been calculated for aluminum using electron band theory. The

agreement with shock data is quite good at high pressures, above about 20 GPa. Below this pressure, the agreement is less good because of a calculated bulk sound speed that is 4% too small. This is nevertheless a rather successful determination of the sound speed from first-principles theory.

A first-principles calculation of the bulk properties of metallic solids must be based on electron band theory. We have previously outlined a program of such EOS calculations for metals using the self-consistent, augmented-plane-wave (APW) code for the zero-K isotherm; supplemented by model calculations for the thermal effects.¹³ These techniques have proved quite successful in calculating the Hugoniot of metallic iodine.¹⁴ Here we report similar calculations for aluminum.

The zero-K isotherm was calculated for aluminum using the APW code, taking the Hedin-Lundqvist¹⁵ exchange-correlation potential. The electronic thermal contributions were computed using a free electron model in which the density-dependent effective mass was determined from the APW density of states. The electronic thermal contributions were found to be almost totally negligible over the range of pressures investigated. Thermal contributions from the nuclear vibrations were computed using a Grüneisen model, with the value of γ at each density determined from the

APW zero-K isotherm by means of the Dugdale-MacDonald expression.

Our results for the Hugoniot are presented in Fig. 5 (solid curve) in the form of a shock velocity (U_s) vs particle velocity (U_p) plot. Temperatures along the Hugoniot are indicated by the arrows. The error bars indicate the sensitivity of these results to uncertainties in the Grüneisen- γ 's. The Slater-Landau and free-volume expressions for γ result in values about 10% larger and smaller respectively than those we have used.

The dashed line in Fig. 5 gives the experimental results for 2024-Al.¹⁶ An extrapolation of this line beyond the range of the data (dotted line) is given to show the

curvature in the U_s - U_p curve predicted by our calculations. Note, though, that we have not included corrections for liquid disorder. Our results are in close agreement with the data above $U_p = 1$ km/s (about 20 GPa). The deviation at lower particle velocities is caused by a calculated sound speed from the zero-K APW results that is 4% too small. It is to be emphasized that the U_s - U_p curve is sensitive to the derivative of the pressure at low compressions, yet only on the value of the pressure itself at higher compressions. Larger errors are therefore expected for small particle velocities. In fact, however, 4% agreement for the sound velocity as calculated from first-principles theory is quite good.

Fig. 5. Shock velocity (U_s) vs particle velocity (U_p) for aluminum Hugoniot. Calculated results are given by the solid line, with temperatures along the Hugoniot indicated by arrows. The dashed line gives the LASL experimental results for 2024-Al (Ref. 16), and are extrapolated beyond the region of the data as the dotted line.

II. Code Development Group

(L. L. Edwards, Group Leader)

THE CHAMP HYDRODYNAMICS PACKAGE

(L. L. Edwards, R. Hickman,
J. Hobson, and T. Michels)

- The controller and alter phases of the CHAMP package have been completed, as well as additions to the main code and the running of numerous problem calculations for both B and H Divisions. Work was also started on a single-grid CHAMP code in addition to consulting sessions on the incorporation of second-order-accurate Eulerian differencing in the CHAMP framework.

The controller for the CHAMP package is in final stage of debug, and the testing of the production mode remains. A preliminary version of a Lagrange alter program using the existing routines for HEMP written by A. Leibee was completed. Capabilities include point altering and some rezone/dezone facilities. Further coding will be done as the need arises for more general alter capabilities. Other work on the CHAMP package included:

- The storage optimization of some temporary crossing-point boundary arrays that reduced SCM storage by 15,000 octal words while increasing code capability.
- The CHAMP Eulerian routines and the serial HEMP code and generator were modified and recompiled to

provide a nontemperature diffusion version of the code.

- The design of a linking package for CHAMP has begun.

Reformulation of the Eulerian overlay in CHAMP to produce a single-grid version of the code has been started. Redesign of this part of CHAMP has only recently started and will involve altering the Eulerian difference equations. Also, we consulted with other members of the group in an effort to put second-order-accurate Eulerian differencing into CHAMP. Essentially, this involves replacing the Eulerian overlay in the main CHAMP code with a version of TEULER fitted to run in the CHAMP environment.

The debug of the CHAMP system has been aided by running and assisting H. Vantine of B-Division with parametric weapons design calculations. Also, the CHAMP code has been used to continue to investigate various phases of the Nuclear Regulatory Commission (NRC) downcomer simulation.

LASER-KO CODE

(R. B. Hickman and
P. V. Grantham)

- The coupling of LASNEX laser physics with KO hydrodynamics has

been essentially completed. The LASER-KO code has applications in an energy density regime that requires strength of materials.

B. Harrach of T-Division presented to us the requirement for a program that would model laser deposition in opaque materials in a regime of energy density for which material strength is important. Although the initial experiment on laser initiation of high explosive can be analyzed with the aid of a one-dimensional code, it is anticipated that eventually two-dimensional effects will be important. To meet these needs a program embodying the equations of motion from KO¹⁷ and the laser deposition and non-equilibrium energy coupling and diffusion from LASNEX¹⁸ was conceived. The extension to two-space dimensions would logically demand the melding of HEMP with a modification of the non-equilibrium diffusion and laser overlay.

The development of the LASER-KO code has been divided into three phases: 1) the removal of the existing EOS and internal energy advance from KO, 2) the elimination of particle diffusion, non-Maxwellian electrons and non-Planckian photons, as well as two-dimensional diffusion and laser deposition from the non-hydrodynamic sections of LASNEX, and

3) the construction of a translator to convey information between the KO and laser overlays. A fourth phase, the introduction of the H-Division bilinear-log EOS library and interpolation routine has not been completed. All the coding is done and is in debug.

The use of KO as a basis for integrating the equations of motions offers the opportunity to calculate the material response to laser-initiated shocks in metals, plastics, and high explosives. The void-opening capability will permit laser-induced spall to be observed. To retain the ability to model these phenomena, the KO equations were altered only to move the internal energy update to the laser physics overlay using the KO-calculated work done by artificial viscosity and deviatoric stresses.

The laser physics section begins with the deposition of energy from a laser source whose power vs time history is user-selected. Deposition may be made in metal or plasma with reflection from either when the critical electron density for the laser is reached. All absorbed laser energy is deposited to the electrons. The electron temperature is coupled to both the ion and radiation temperatures, and all three temperatures are separately diffused. Work terms for the pressure associated with each

of the temperature fields serve to modify the temperatures, whereas the energy terms calculated in KO are used only in the advance of the ion temperature. To calculate the laser absorption as well as the temperature-coupling coefficients, a partial ionization calculation is performed to determine in each zone the population of each ionic species, which in turn, allows the specification of the requisite average ionization parameters. Although the initial pass at the laser overlay follows faithfully the LASNEX logic to facilitate the debug process, future modification to improve energy conservation properties is envisioned.

The basis for a two-dimensional code might be either HEMP or HEMPMHD with the addition of the principal new physics represented by a laser-ray-tracing algorithm. This presumably would be closely based on the existing LASNEX laser subroutine. The existence of slide lines in HEMP, while adding to the versatility of the code, poses problems for two-dimensional diffusion that may be attacked either along the lines of the current HEMPMHD (the form of coupling used in CHAMP) or by a replacement of the alternating-direction-implicit approach by some other inversion scheme.

AVAILABILITY OF MORE VERSATILE ZONING IN THE 2D-HEMP CODE

(P. P. Weidhaas)

- Logic has been added to HEMP to introduce fine zoning in a subregion of the HEMP grid and to let the zoning become progressively coarser further away from that region. This option is applied to the study of crack-propagation by making the zoning in the vicinity of the crack-tip fine as compared to the rest of the grid.

The mass term used in HEMP's "tied sliding" has been modified (using the Z-factor) to pick up the correct mass when zoning changes occur across a slide line (as in Fig. 6). Two new point-types (5 and 6) have been introduced: type-6 points are "tied" (slave point coincides with master point), whereas type-5 points are subject to two restraining conditions:

- They must stay on the connecting line segment between two neighboring type-6 points.
- They must maintain a constant distance-ratio (a/b) for all time (see Fig. 6).

This logic and the point-types apply to both types of slide lines (upright and inverted) used in HEMP. The only restriction is that the coarser zoning should be on the master side of the slide line.

Fig. 6. Portion of HEMP grid showing type-5 and type-6 slide points, where b is the master zonal spacing and a is the slave zonal spacing.

HEMPDST: A VERSION OF HEMP WITH
SLIDING ON J-LINES, K-LINES,
AND TRIANGLES

(P. Grantham)

- The code is completed and has been applied to several problems.

Studies by M. Kamegai and M. Wilkins of surface disturbances from underground explosions require the use of HEMP on triangulated zones with complicated material interfaces. (See Fig. 7.) To service this requirement and to provide a general analytic tool for future work, a version of HEMP has been written that contains all the previous slide-line logic from two codes by A. Liebee.

The new code HEMPDST features:

- Sliding along arbitrary intersecting J-lines and K-lines.
- Triangular zones with sliding along a zone edge.
- Closing and opening voids along intersecting slide lines.
- Automatic generation of calculational grids using both triangular and quadrilateral zones.

The graphics capability consists of a version of the HEMP graphics package by A. Liebee and modified by J. A. Levatin.

In addition to the application to underground explosion, the code has been successfully applied by M. Van Thiel to the design of a

Fig. 7. Sample calculation grid using triangulated slide lines.

shaped-charge component. (See Figs. 8, 9, and 10.) Also, a B-Division design has been generated and run.

Current code work includes addition of contour plotting capability and incorporating the bilinear logarithmic interpolation scheme (by R. Olness) for the EOS models.

An input manual¹⁹ with completed examples is available from H-Division offices.

Fig. 8. Materials for shaped-charge component.

Fig. 9. Initial calculation grids for shaped-charge component.

A MESH GENERATOR FOR CYLINDERS

(B. J. Bird)

- A mesh generator was written for a right-circular cylinder with a circular hole cut in the side.

CYLCUT, a three-dimensional mesh generator, was written for use in conjunction with HEMP3D. It generates a mesh for a right-circular cylinder with a circular hole cut in its side. By assuming a symmetry plane, the mesh for only one-half of the cylinder needs to be generated. An example is shown in Fig. 11. A close-up of the circular cut is shown in Fig. 12. The output file from CYLCUT is called CYLMESH and can be used as the grid file input to GEN3D, the restart file generator for HEMP3D. CYLCUT is available on the Photostore under .074275:CYLCUT. It runs only on the CDC 7600 and is executed by typing

CYLCUT / t v

Fig. 10. Calculational grid for shaped-charge component after void closure at 2.7 μ s.

Fig. 11. Computer plot of right circular cylinder with circular cut-out.

The program then lists the input data required and the order in which it must be given. If you already know the data and its order, it may be included in the execute line. After the input data has been given, CYLCUT prints the J,K

Fig. 12. Computer plot of circular cut-out.

node point information defining the circular cutout in the form of region definition cards that are inputs to GEN3D

Documentation and complete user instructions for CYLCUT will be written during the next quarter.

III. Experimental Physics Group

(J. W. Shaner, Group Leader)

The Experimental Physics Group conducts investigations of the properties of materials at extreme conditions of pressure and temperature and develops new techniques in performing these investigations. In addition, studies are carried out on the response of materials to a wide range of dynamic pressures and temperatures. These activities provide information for both theoretical equation-of-state and simulation efforts.

A major effort in the experimental group this quarter has been a study and engineering redesign of the post-shot dilution system of the two-stage gun. A valve leak or malfunction resulted in air mixing with H_2 pump gas in the catch tank. The subsequent H_2 burn damaged the catch tank door. After repairing the door, experiments proceeded using N_2 and He for pump gas. At the same time, a N_2 system was designed to dilute the H_2 below the flammability limit within seconds after a shot. This system should be functional in the next quarter.

EFFECTIVENESS OF ALUMINA ARMOR PLATE AGAINST HIGH VELOCITY PROJECTILES

(B. L. Hord)

• We determined the thickness of alumina armor plate that will stop a

10-g steel projectile traveling at 2.1 km/s and 3.0 km/s.

Studies have shown that sintered alumina can be an effective armor against projectiles with velocities of 1 km/s and less. The alumina thickness required to stop 10-g steel projectiles was roughly linear with projectile velocity.²⁰ The present study was undertaken for the Air Force to determine the stopping thickness of alumina armor plate for 10-g steel projectiles with velocities of 2 and 3 km/s.

A 10-g steel slug was imbedded in a polycarbonate sabot to form the projectile that would be accelerated in the LLL two-stage gas gun. The slug was about 13 mm diameter by 10 mm long, a different aspect ratio from the 30-caliber slug used in the previous lower velocity studies. The polycarbonate sabot was required to be stripped from the steel slug prior to the impact test.

The stripping of the polycarbonate sabot traveling at 3 km/s was accomplished by allowing the 29 mm diameter projectile to impact around the edge of a 19-mm hole in a 6-mm-thick steel plate.²¹ The slug was slightly distorted from the resulting shock wave, but the sabot was removed quite

adequately. Two intermediate baffles were set between the stripper and armor plate to intercept most of the shrapnel; the first at 215 mm from the stripper, the second about 300 mm further down range. The armor was centered about 40 mm past the second baffle.

The stripper had to be modified for the 2-km/s projectile. The hole in the steel plate was reamed out to a conical section, and the front section of the sabot was machined to match (see Fig. 13). This configuration stripped the sabot adequately, but the trajectory of the steel slug was affected to such an extent that it was about one diameter off center at the second baffle plate prior to impacting the armor. To correct this, the armor was moved in closer to the stripper and one baffle was removed. The single baffle was placed about 190 mm from the stripper with the armor about 40 mm further down range.

The effectiveness of the alumina as an armor against the high velocity steel slug was determined by observing if the 6-mm aluminum back-up plate glued to the alumina was penetrated or not. (See Fig. 14 for results of tests.) Each test sample was made of 152-mm-diam alumina to reduce the possibility of edge effects. The results are presented in Table 1.

These results do not extrapolate from the low velocity data. They

Fig. 13. Schematic of sabot stripping scheme.

Fig. 14. Ballistic limit of aluminum-backed alumina armor plate.

Table 1. Results of 10-g steel slug impacting alumina plate.

Projectile velocity (km/s)	Armor thickness (mm)	Back-up plate condition
2.26	28.6	Penetrated
2.10	38.1	Not penetrated
3.01	38.1	Penetrated
2.95	50.8	Not penetrated

indicate the alumina thickness on the 6-mm back-up plate must be 50 to 60% greater than the thickness obtained by extrapolation of the low velocity data.

HUGONIOT MEASUREMENTS ON ALUMINUM

(A. C. Mitchell and J. W. Shaner)

• In continuation of Hugoniot measurements on pure aluminum, we have measured the Hugoniot between 80 to 180 GPa. We found an anomalous region between 130 to 150 GPa, which is believed to be the onset of the aluminum liquid phase. Above 150 GPa, aluminum is probably in the liquid phase.

Aluminum and aluminum alloys such as 2024 and 921-T are commonly used as standard material for impedance-matching experiments. To develop a more accurate high-pressure standard for EOS experiments and to avoid the difficulties of using alloys, we chose to measure the Hugoniot of pure aluminum.

Preceding our work, Isbell, *et al.*,²² found anomalies occurring for 2024 aluminum in the pressure range between 100 to 150 GPa, which is indicated by their large data scatter. Since this anomalous region occurs at the upper end of the two-stage light-gas gun range, it was not clear whether this scatter was because of a change in physical properties or in increasing inaccuracy in the data.

To check this region, we conducted 18 experiments on pure aluminum. For these experiments the uncertainty in the projectile velocity was less than 0.3%, which introduces a maximum error of 0.5% in the aluminum particle velocity determination. The maximum error in the aluminum shock velocity was 1% at 180 GPa. For all experiments below this pressure, the shock-velocity measurement error is about 0.5%. With this high precision, the transformation region between 130 to 150 GPa is quite distinct. This work is now being completed and will appear in a Laboratory report.

PROPERTIES OF MATERIALS AT HIGH PRESSURE

(W. H. Gust)

• Equation-of-state experiments are continuing on materials of interest to LLL. High pressure Hugoniot data for UO_2 are reported.

The Laboratory two-stage, light-gas gun has been used to determine

Hugoniot parameters for uranium dioxide (UO_2) from 200 to 330 GPa using tantalum projectiles.²³ The material was of very high purity; initial density was 19.35 Mg/m^3 , or more than 95% of theoretical density.

A linear relation between shock and particle velocities was found; no anomalies were observed. The data can be described by $U_s = 5.62 + 1.30 (U_p - 2.0) \text{ km/s}$ for $U_p > 2.0 \text{ km/s}$.

Only a fair fit to unpublished low-pressure data from the Los Alamos Scientific Laboratory was obtained. The LASL data can be described by $U_s = 3.6 + 0.9 U_p$ for $0 < U_p < 2.0 \text{ km/s}$, followed by a kink of steep slope for $2.0 < U_p < 2.5 \text{ km/s}$ that does not fair into our curve very well. Some low pressure experiments will be done in order to clarify the plot in the region of the discontinuity.

BRL VEHICULAR ARMOR PROGRAM

(J. K. Scudder)

o Work continues on a BRL-funded project to study the significance of structural design and intrinsic material properties on the defeat of long-rod penetrators. Results show that significant armor weight savings are possible through careful design. One-tenth scale tests will be repeated at one-quarter scale to test geometric scaling sensitivity.

H-Division has, for the past year, been conducting a combined computa-

tional and experimental vehicular armor program for the Ballistic Research Laboratory in Aberdeen, Maryland. Through scale model laboratory experiments and HEMP code simulations, we have investigated many aspects of the attack of high-velocity long-rod penetrators on heavy military vehicle armor. For example, the frontal configuration of U.S. made medium and heavy tanks involves ramp structures that force a horizontally attacking projectile to impact with about 30° grazing incidence. The significance of this "oblique" impact in terms of armor weight effectiveness has been studied in detail with HEMP and with 1/10th scale projectiles.

In addition to structural properties, we have studied the role of the intrinsic material properties (strength, toughness, density, etc.) of armor for defeating the long-rod penetrator.

Our investigations this quarter demonstrated the weight-saving available by a careful selection of material and armor geometry. Weight differentials of a factor of 2 to 4 over the conventional steel plate have been observed in the laboratory.

The next phase of this program will test the sensitivity of the armor's performance to overall geometric scale. Some of the most promising armor designs established

at 1/10th scale will be retested at 1/4 scale. If the favorable trends persist, full scale tests will be

conducted. *These larger scale tests* will be made at the BRL facilities in Maryland.

IV. Solid Mechanics Group

(D. M. Norris, Group Leader)

This group is responsible for calculations in the general area of solid mechanics. Work currently underway includes determination of surface environment from shallow-buried nuclear weapons and of crack initiation and propagation in nuclear pressure vessels. Code development associated directly with this work includes modifications of finite-difference and finite-element computer programs and the companion service software.

FUNDAMENTAL STUDY OF CRACK INITIATION AND PROPAGATION

(D. M. Norris, M. L. Wilkins, M. E. Prado, B. Moran, W. H. Hoover, D. F. Quinones, and Y. M. Chen)

● The goal is to characterize the ductile fracture and arrest in a large heavy section steel technology (HSST) pressure vessel when the fracture is initiated by a surface flaw in a weld. The method of characterization differs from conventional approaches in that it uses macroscopic physics models of damage accumulation and growth in computer simulations (using HEMP and HEMP3D) of quasi-static and dynamic experimental tests on A508 and A533 steels, weld material, and welded steel. A variety of test geometries will be used to exercise the model for different loading conditions, and the adjustable constants of the model will be established by a set of experiments. The calibrated models

and necessary coordinate generation routines will be included in the EPRI two- and three-dimensional codes to transfer the technology to the pressure vessel industry. The work is funded by the Electric Power Research Institute (EPRI).

Work on this research started March 18, 1976, which is the basis date for the quarterly work schedule of the proposal.²⁴ The calculational goals for this period are EOS programming in HEMP3D and Charpy-V notch simulation on HEMP2D. The experimental goals are material procurement, mechanical properties specimen preparation, and mechanical properties tests.

The experimental goals are complete. The A533B Class 1 archival steel mechanical properties are in general agreement with the combustion-engineering data reported in Ref. 25. Charpy V-notch data at -20, 50, and 212°F in both rolling and transverse directions agree with the C-E transverse (lower, $C_v = 100$ ft-lb) data. Tensile testing and metallurgy indicate a planar region of slag inclusions parallel to the cut-out surface.

Work is still proceeding on the calculational goals. A HEMP2D

Fig. 15. Charpy-V-notch HEMP calculation at 60 μ s.

Fig. 16. Contours of hydrostatic tension at 56 μ s. Maximum tension is ahead of the crack.

Charpy V-notch calculation has been debugged and is now at 60 μ s (see Fig. 15) and running well. Figures 16, 17, and 18 are contours of hydrostatic tension, effective plastic strain, and internal energy at 56 μ s. Large strains are developed at the notch root with associated high internal energy and corresponding temperature rise. The hydrostatic tension field ahead of the notch is the mechanism for crack initiation and growth. Similar 3D calculations are underway to evaluate the plane strain assumption inherent in the above 2D calculations.

The major problem faced by the program is the dependence of the damage criteria on zone size. Five zone studies with extrapolation and J-integral techniques are being conducted to resolve this problem. The

Fig. 17. Effective plastic strain contours at 56 μ s. Large strains develop at the notch root.

Cycle = 9345
HEMP CHARPY-H Time = 5.600E+01

Fig. 18. Internal energy (HEMP code units where 1.E-4 corresponds to a temperature rise in steel of 2.9°C)

fine zoning has proved to be very costly in computer time both for the 3D and 2D calculations.

A second simulation used to calibrate the computer damage model is the uniaxial tension test. The onset of necking instability is shown in Fig. 19, with contours of effective plastic strain in Fig. 20.

THE THERMAL YIELD OF THE SHALLOW BURST MUNITIONS

(M. Kamegai)

- The thermal yield of the shallow burst munitions (SBM) was examined.

Fig. 19. Tensile specimen necking before failure.

Fig. 20. Effective plastic strain contours of 0.2, 0.4, and 0.6 prior to failure.

Computation was done on CEL for a 1-kt source at three depths of burial, 0.5, 1.5, and 3.0 m. Based on the measured thermal yield of the atmospheric explosions, the relative thermal yield of SBM is less than 5% for these DOB's.

An investigation of the thermal radiation from the shallow burst munitions was conducted for the Defense Nuclear Agency. Computation was carried out on CEL for a 1-kt source at three depths of burial, 0.5, 1.5 and 3 m. Each problem was calculated for more than 10 ms.

These shallow explosions quickly communicate with the ground surface, and the source preferentially moves upward resulting in a "mushroom effect" of the debris in the atmosphere. The airblast appears as if it originated from a virtual center of explosions located at about 20 m above the ground surface. The "mushroom effect" leaves a hot gas at the top and cold materials in the lower region of the debris. Thus,

the thermal radiation mainly comes from the upper region of the debris. Figure 21 shows a vertical temperature profile at the center of the debris.

The minimum temperature for the thermal radiation was arbitrarily chosen to be 0.25 eV (3000 K). Thus, the debris materials at temperatures greater than 0.25 eV was examined. The energy density of the radiating source (the materials at temperatures greater than 0.25 eV) is plotted in Figs. 22, 23, and 24 for the three DOB's.

The relative thermal yield has been measured for a number of atmospheric explosions. The relative thermal yield vs the yield to mass ratio (the

energy density) is plotted in Fig. 25. Based on the measured thermal yield (Fig. 25), the computed results shown in Figs. 18, 19, and 20 give the following upper limits on the thermal yields of a 1-kt source for the three DOB's.

DOB (m)	Relative thermal yield (%)
0.5	4
1.5	3 - 4
3.0	1.5

STUDIES IN FRACTURE MECHANICS

(W. G. Hoover)

• Molecular-dynamical calculations reveal a well-defined zero-temperature value of the stress intensity at crack

Fig. 21. Vertical temperature profile at the center of the airborne debris; $t = 3.6$ ms, DOB = 1.5 m.

Fig. 22. Energy density of the radiating source; yield = 1 kt, DOB = 0.5 m.

Fig. 23. Energy density of the radiating source; yield = 1 kt, DOB = 1.5 m.

Fig. 24. Energy density of the radiating source; yield = 1 kt, DOB = 3.0 m.

Fig. 25. Relative thermal yield vs yield to mass ratio for low-yield devices.

arrest lying about 8% below the stress intensity at crack initiation. Calculations characterizing the static properties of dislocations are under way.

Previous work with Bill Ashurst (Sandia Laboratories, Livermore) has established the threshold velocity of crack propagation in a two-dimensional triangular-lattice crystal with nearest-neighbor forces. The stress required to make a starter crack propagate is proportional to the critical stress-intensity factor, K_{Ic} . We have recently generalized the earlier calculations in two ways. By using long-strip systems with strain and stress varying linearly along the strip, we found that cracks propagate into regions with insufficient stress intensity to initiate cracks. Thus, less stress is required to propagate a crack than to initiate an otherwise identical crack. The difference, for the simple triangular-lattice material we have investigating, is about 8% for several values of the stress gradient along the strip. We are also undertaking calculations to determine the temperature

effect on crack growth and crack healing so as to develop an Eyring-Arrhenius picture of thermal crack propagation in parallel with our study of small-crystal nonequilibrium thermodynamics.

Some new calculations with Nathan Hoover (Livermore High School) have been carried out on the structure of dislocations in the two-dimensional triangular lattice. Previous research has shown that two different dislocation structures occur in this crystal, but the relative importance of these types in propagation and the relative energy are both unknown. By using viscous damping in parallel with Hookean nearest-neighbor springs, we find that the energy and volume of an N-particle crystal with a dislocation both exceed the corresponding values for a perfect N-particle crystal by the amounts shown in Table 2. The energy data are fitted by the expression

$$\Delta\phi = kd^2(0.022972 \ln N$$

$$+ 0.0055 - 0.0711/L^2)$$

where k is the force-constant, d the interparticle spacing, and L the edge

Table 2. Energy and volume changes for N-particle crystal containing a dislocation.

N+	8	21	40	65	96	133
$\Delta\phi/kd^2$	0.03491	0.06786	0.08593	0.09858	0.10838	0.11639
$\Delta v/d^2$	0.07528	0.06831	0.13703	0.17904	0.10863

length, related to N by $N = 3L^2 - 2L$. An equilibrium dislocation configuration is shown in Fig. 26.

Future work is being directed toward finite-temperature crack propagation and zero-temperature dislocation propagation.

Fig. 26. Minimum energy structure of a two-dimensional triangular-lattice crystal with stress-free boundaries and nearest-neighbor Hookean-spring interactions.

V. Fluid Mechanics Group

(M. Ross, Group Leader)

This group is responsible for the modeling and simulation of fluid flow phenomena.

In this quarterly, A. Buckingham reviews the theoretical support in turbulent fluid mechanics we are providing the D-Division Rainout project. Although this is a new project for us, it has been made possible by virtue of our continued interest in developing the second-order-accurate Eulerian code TEULER with turbulent modeling.

B. Bowman and L. Truong summarize their completed solution of "diabolic" equations. This study originated from a need to efficiently compute flows in which transitions are made from laminar to turbulent by using either implicit or explicit techniques in the appropriate regime.

RAINOUT: DEVELOPMENT OF LOW-SPEED TURBULENCE GENERATOR

(A. C. Buckingham)

● We are providing theoretical-calculational support in turbulent fluid mechanics for a D-Division experimental program in rainout. There is a need for LLL to predict fallout from a nuclear event in a rainy atmosphere. We have completed a preliminary theoretical study leading to a swirl generator design for low-speed multiphase turbulence experiments.

Under development at LLL is an experimental facility that will test the enhancement of attachment rate of aerosol particles to water droplets when turbulence is present. We plan future experiments to examine the effects of both electrical and plasma field properties on the attachment rate with concomitant turbulent field effects. In addition, the effects of droplet phase change on the turbulent flow field and attachment mechanism are to be examined.

The basic experimental difficulty initially encountered is that of *generating and maintaining* turbulence in a low-speed (low Reynolds number) flow environment. Figure 27 shows the flow geometry in two conceptual wind tunnel droplet cloud configurations. The upper sketch illustrates use of multiple turbulent grid screens with turbulent counter-flow jet mixing to retard the axial velocity. The lower sketch illustrates our current design, a plugged nozzle with a rotating plug to induce a high-speed swirl component of velocity and transition to turbulence. The aerosol flow indicated by the arrows is moving vertically upward in the experiment. The droplets are generated in injection capillary tubes that are vibrationally excited with an acoustic

Fig. 27. Sketches of initial test configurations.

wave. They are then injected into a test chamber section at the top. Droplet size is controlled by the frequency of excitation, the injector pressure, and capillary injector diameter. The aerosol flow speed along the vertical axis must be low enough (10 to 40 mm/s) so that it closely matches the free gravity fall velocity of the small (40- μ m mean diameter) water droplets in the test section. In this way, a usefully long residence time (order of seconds) is provided for droplet-aerosol interaction in the test chamber so that attachment rates can be determined within a reasonable statistical error band.

The slow velocity, however, is a severe restriction in that the associated Reynolds number is intolerably low for generating turbulence. Furthermore, the turbulence, once generated, cannot be maintained in the absence of high shearing or large velocity gradients. Another associated problem is the size scale of the turbulent fluctuation. The fluctuating cell or blob of fluid clearly must be of the order of the droplet size or droplet-to-droplet separation distance in order to affect the aerosol droplet encounter dynamics. Figure 28 shows the results of some preliminary calculations for a 10% turbulence intensity (rms fluctuational energy ratioed to mean

flow kinetic energy) for an assumed mean axial flow speed of 0.4×4.4 mm/s. The calculated spectral dissipation rate (energy density per unit time) is shown on the ordinate to vary inversely as the log of the fluctuational wave length. For a wave length scale variation of about 1 mm down to the desired droplet size range (10 μ m), the dissipation rate is seen to increase about 4 orders of magnitude. Consequently even if produced, the fine scale turbulence of primary interest is

Fig. 28. Turbulence grid spectral dissipation rate in direction of flow vs spectral length scale.

dissipated too rapidly unless a shearing field is provided.

The lower sketch in Fig. 22 shows the initial configuration for the first phase experiments. A swirling component of flow is introduced by spinning up the conical plug, whose surface is roughened with a randomly distributed fine scale roughness (mean roughness height of about 1/2 mm). The calculated swirl velocities are high enough to produce a developing wall turbulent boundary layer with structure in the scale range of interest. Moreover, the swirling component is theoretically uncoupled from the axial component and persists throughout the test section. Hence, the turbulence field being generated is strongly coupled to the swirling component and thereby is anisotropic, affecting the diffusional mixing in the radial and azimuthal directions.

Later test configurations will be designed to minimize this anisotropy. We are exploring use of sound waves to help enhance the turbulence fine scale intensity while maintaining isotropy and homogeneity. The modeling and computational procedures are simultaneously being improved so that we can properly support the following aspects of the program:

- Characterize the frequency-dependent turbulent structure of the experiment.

- Theoretically relate the experiment to the physical situation in cloud physics.

- Set up spectral procedures for automatic reduction and analysis of the measured turbulence structure.

- Develop a predictive computational tool for assistance in developing new experiments that simulate the actual physical process. This tool will be a refined three-dimensional version of the current 2D TEULER code with two-equation closure turbulence model and a fast Fourier transform procedure to explicitly simulate grid scale spectral effects.

A separate interim LLL technical report is currently being prepared that describes the theoretical model and the numerical procedures in detail.

A REYNOLDS-NUMBER-DEPENDENT SCHEME FOR THE SOLUTION OF "DIABOLIC" EQUATIONS

(B. R. Bowman and L. A. Truong)

o A numerical procedure for solving "diabolic" equations (conservation equations containing positive source terms) is presented. The solution scheme is forward differenced in time and centrally differenced in space. Every term except the time derivative is expressed as a convex combination of the present and the advanced time step. The selection of the convex combination is determined by analyzing the magnitude of the coefficients of a linear one-dimensional model equation

$$\frac{\partial \phi}{\partial t} + U \frac{\partial \phi}{\partial x} = A\phi + D \frac{\partial^2 \phi}{\partial x^2}$$

together with the spatial and temporal step sizes. Typical examples of numerical solutions to this equation are compared for different convex combinations. These results indicate that the judicious choice of the combination may avoid some of the difficulties encountered when using purely implicit or purely explicit schemes.

In the course of this study, a computer-automated method of analysis is developed with particular application to reacting flows, mixed-phase flows, and some aspects of turbulence modeling.

Introduction

This study was begun to find methods of solving numerically the systems of equations that are coupled by source or sink terms. Examples of physical equations including source terms are: 1) The conservation equations governing multiphase flow in nuclear reactor pressure suppression systems where the source terms appear as coupling terms representing condensation and vaporization rates of the working fluid (steam/water).^{26,27} 2) The turbulence model equations in a time-dependent system contain turbulence production terms.²⁸

The mathematical form of these equations is parabolic; however, there are natural flow regimes in which the convective derivative becomes large and the system behaves as if hyperbolic. Implicit solution schemes

devised for parabolic equations do not work very well for hyperbolic equations. As a result, flow regimes where this problem occurs can cause a great deal of difficulty in obtaining a solution. The presence of a positive source term in the equations can further complicate matters and cause the solution to grow exponentially. This, combined with numerical dispersion is described by Chin,²⁹ can make the solution scheme appear to be unstable.

Solutions of these equations are often carried out explicitly, and the time-step associated with the criteria for stability can be unrealistically small for many real problems. Many flow conditions are such that a more rapid solution procedure (larger problem time-step) could be used.

This report discusses the development of a solution scheme for flows in which numerical stability is weakly dependent on the cell Reynolds number but strongly dependent on the magnitude of the source term.

The Model Equation

The one-dimensional model equation is considered

$$\frac{\partial \phi}{\partial t} + \frac{\partial (U_i \phi)}{\partial x_i} = A\phi + \frac{\partial}{\partial x_i} \left(\frac{\partial \phi}{\partial x_i} \right), \quad (6)$$

where the symbol D is a diffusion coefficient, ϕ is the dependent variable of interest, U the convective velocity, and A is a constant source term coefficient.

Solution Procedure

The one-dimensional form of the model equation, Eq. (6), is linearized by assuming U and D to be constant and the finite-difference form is written as a convex combination of the explicit and implicit (time-advanced) terms as

$$\frac{\phi_i^{n+1} - \phi_i^n}{\Delta t} + (1 - F) U \delta \phi_i^{n+1} + F U \delta \phi_i^n = (1 - F) A \phi_i^{n+1} + F A \phi_i^n + D(1 - F) \delta^2 \phi_i^{n+1} + D F \delta^2 \phi_i^n, \quad 0 \leq F \leq 1, \quad (7)$$

where the operators δ and δ^2 are central difference operators defined as

$$\delta \phi = (\phi_{i+1} - \phi_{i-1}) / 2\Delta x \quad (8)$$

$$\delta^2 \phi = (\phi_{i+1} - 2\phi_i + \phi_{i-1}) / (\Delta x)^2. \quad (9)$$

In Eq. (7), superscript n refers to the time-step and subscript i refers to a spatial location with Δt and Δx defined as the time and spatial step sizes.

A functional form for the quantity F is sought so that a natural selection of an all-implicit $F = 0$,

all-explicit $F = 1$, or a mixed scheme is made automatically. The determination of F is based on a numerical stability argument. To avoid small time steps required for explicit solutions, it is desirable to use an implicit scheme whenever possible. However, for certain combinations of the cell Reynolds number, Δt and the source term coefficient A , the coefficient matrix of an all-implicit solution scheme is nearly singular and results in a numerical instability (and possibly problems of convergence). Therefore, F must be selected as close to zero as possible still avoiding the region of numerical instability.

To our knowledge, no smooth automatic transition method exists for changing F from 0 to 1 during a calculation. This present work emphasizes a formalization and extension of earlier ideas on mixed schemes with a goal of developing an automated procedure for the transition.

To determine the function F , it is convenient to define

$$G = 1 - F,$$

then expand Eq. (7) using Eqs. (8) and (9)

$$G \left[\frac{U \Delta x}{2D} - 1 \right] \phi_{i+1}^{n+1} + \left[\frac{\Delta x^2}{D \Delta t} + G \left(2 - \frac{A \Delta x^2}{D} \right) \right] \phi_i^{n+1}$$

$$\begin{aligned}
& + G \left[-\frac{U\Delta x}{2D} - 1 \right] \phi_{i-1}^n \\
& = F \left[-\frac{U\Delta x}{2D} + 1 \right] \phi_{i+1}^n \\
& + \left[\frac{\Delta x^2}{D\Delta t} + F \left(\frac{A\Delta x^2}{D} - 2 \right) \right] \phi_i^n \\
& + F \left[\frac{U\Delta x}{2D} + 1 \right] \phi_{i-1}^n. \quad (10)
\end{aligned}$$

The quantity $\frac{U\Delta x}{D}$ is the cell Reynolds number,

$$\text{Re}_{\text{cell}} = \frac{U\Delta x}{D} \quad (11)$$

which Chin²⁹ suggests must be less than 2 to prevent numerical dispersion for the linear case and less than $\sqrt{3}$ for the nonlinear case.

The eigenvalues of Eq. (10) are

$$\begin{aligned}
\lambda_i &= 1 + G\Delta t \\
&\times \left[\frac{2D}{\Delta x^2} \left(1 + \sqrt{1 - \alpha^2} \cos \frac{i\pi}{I+1} \right) - A \right], \quad (12)
\end{aligned}$$

$$\text{where } \alpha = \left(\frac{\text{Re}}{2} \right)_{\text{cell}}.$$

The function G is defined to avoid the numerical instability by examining the eigenvalues λ_i . When any of the λ_i are close to zero the system is unstable. To insure a well conditioned matrix, the λ_i may be moved away from zero by adjusting the value of G .

For real λ_i we must consider the three cases:

- i. All of the λ_i are positive.
- ii. Some λ_i are negative and some positive.
- iii. All of the λ_i are negative.

Case i. If the smallest eigenvalue λ_1 is far from zero, then G may be set to 1. If a λ_i is close to zero, reducing G will move all of the λ_i to the right so that the smallest eigenvalue λ_1 is sufficiently greater than some small value, δ .

Case ii. This may be treated exactly as the second part of case i b. reducing G until all λ_i are positive and $\lambda_1 > \delta$.

Case iii. If all λ_i are far to the left, then setting $G = 1$ will insure that all λ_i remain removed from 0. When the largest λ_i is close to zero, reducing G will again move the λ_i to the right until $\lambda_1 > \delta$.

For all situations except that where $\lambda_1 < 0$, the procedure is to choose G such that the smallest eigenvalue λ_1 remains positive. To keep λ_1 away from zero, some small value δ is chosen such that

$$\lambda_1 > \delta. \quad (13)$$

To determine G we replace $\cos \frac{i\pi}{I+1}$ in Eq. (12) with -1 and write Eq. (13) as

$$\begin{aligned}
& G \left[\frac{A\Delta x^2}{D} + 2\sqrt{1 - \alpha^2} - 2 \right] \\
& \leq \frac{\Delta x^2}{D\Delta t} - \delta. \quad (14)
\end{aligned}$$

G lies in the interval

$$0 \leq G \leq 1$$

so that as long as $(\Delta x^2/D\Delta t) > \delta$ and

$$\frac{A\Delta x^2}{D} + 2\sqrt{1 - \alpha^2} - 2 \leq \frac{\Delta x^2}{D\Delta t} - \delta,$$

we set $G = 1$. When $G \leq \delta$ we set $G = 0$, and for the case where $\lambda_1 \ll 0$, we again set $G = 1$. The magnitude of δ was arbitrarily set to be

$$\delta = 0.1 \frac{\Delta x^2}{D\Delta t}.$$

When none of the above cases are true, then G is calculated from

$$G = \frac{\frac{\Delta x^2}{D\Delta t} - \delta}{\frac{A\Delta x^2}{D} + 2\sqrt{1 - \alpha^2} - 2}.$$

Another point that needs to be discussed here is the case when we purposely violate Chin's²⁹ dispersion criterion so that

$$\alpha > 1.$$

For this case, the eigenvalues of Eq. (10) are complex and of the form

$$\lambda_j = \lambda + j\gamma_j,$$

where $j = \sqrt{-1}$.

Here the λ_1 are displaced on a vertical line with the value of the real intercept λ ; hence if λ is sufficiently far from zero, then the absolute value $|\lambda_1| > 0$ and the coefficient matrix is well conditioned. For this case, the selection of G is based on one of the inequalities

$$G\Delta t \left[A - \frac{2D}{\Delta x^2} \right] \ll 1$$

or

$$G\Delta t \left[A - \frac{2D}{\Delta x^2} \right] \gg 1.$$

In cases represented here, the largest possible value of G is sought for which the solution scheme remains stable (i.e., $\lambda_1 = 0$). Care must be taken when the system approaches the all-explicit case $G = 0$. Here the time-step selected for computation must be adjusted so that it does not exceed the explicit stability criterion given by

$$\frac{D\Delta t}{\Delta x^2} \leq 1/2.$$

Results

Results for the one-dimensional model equation are shown for several cases. The results given are not all-inclusive, but serve to exemplify the ideas developed in the preceding section.

The first three figures are included to show the effect of violating Chin's²⁹ numerical dispersion criterion. Numerical dispersion is present in all three cases, independent of the solution scheme, and appears as a bounded oscillation in the solution. Figure 29a is a single time frame from a stable explicit calculation. Figure 29b is the same calculation run in an all implicit mode, and Fig. 29c is again the same calculation using the method described in the previous section. Figure 29d is the mixed-mode calculation with a reduced spatial step size so that the cell Reynolds number is less than 2, and the numerical dispersion is eliminated. The values of the coefficients used in Eq. (10) and the spatial and time-step sizes are indicated on the figures.

To demonstrate the strong effect of the source term in determining the value of G in Eq. (10), a set of variables was chosen for the source term coefficient: ($A = 58$) and the time-step ($\Delta t = 0.2$), which would be unstable is used in an all-implicit calculation. These two values were determined by setting Eq. (14) equal to 0, $G = 1$, and adjusting the product $A\Delta t$ for a representative set of the variables $\Delta x = 0.05$, $D = 0.05$, and $U = 5$. The results of the all-implicit calculation are shown in Fig. 30a for the fifth time cycle

and are clearly unstable. The results of implementing a mixed-mode calculation are given in Fig. 30b. The computation automatically selects a value of $G = 0.99$, which is stable, but displays some numerical dispersion because of the relatively large cell Reynolds number of 25.

To get better resolution of the solution behavior, another series of calculations similar to those shown in Figs. 31a and b were carried with a smaller time-step $\Delta t = 0.01$. The explicit calculation in Fig. 31a was unstable; however, it could be made stable by reducing the time-step Δt to 5×10^{-4} . Both the implicit and the mixed-mode calculations were identical and are shown in Figs. 31b and c. In the automatic-selection-mode case, G was chosen to be 1. The curves for implicit solutions do not reveal a smearing of the solution apparent when the actual numbers used to generate the plots are closely inspected. This smearing is typical of the global nature of the implicit method and may have an adverse effect in problems involving shock and discontinuity propagation in supersonic flow.

Conclusions

We have demonstrated that the presence of a positive source term in a linear one-dimensional equation, incorporating the features of most

Fig. 29. Examples showing numerical dispersion independent of solution scheme:
a) explicit, b) implicit, c) automatic selection mode $G = 1$,
d) implicit with dispersion removed.

conservation equations, may prevent a stable solution using an all implicit technique. We also have shown that a stable explicit solution to this same equation may require a time-step so small that the cost of

the calculation becomes uneconomical. The proper convex combination of implicit and explicit terms in the solution scheme may relieve both of these difficulties. If large time-steps are required and this convex

Fig. 30. Effect of a large source term on stability at a lower time-step:
 a) implicit, b) automatic
 $G = 0.99$.

Fig. 31. Comparison of time-step requirements for stable explicit and implicit solution:
 a) unstable explicit,
 b) stable implicit,
 c) stable automatic $G = 1$.

combination of implicit/explicit terms meets stability requirements, then it may be possible to automatically adjust the mixed-mode method to achieve an acceptable and economic

level of accuracy. This work represents only the initial phase of a much more extensive effort to investigate all aspects of convex combination solution schemes.

References

1. A. K. McMahan, B. L. Hord, and M. Ross, *An Experimental and Theoretical Study on Metallic Iodine*, Lawrence Livermore Laboratory, Rept. UCRL-78234 (1976).
2. R. Grover, "Liquid Metal Equation-of-State Based on Scaling," *J. Chem. Phys.* 55, 3435 (1971).
3. M. Kamegai, "Surface Disturbance From Deep Underground Explosions," in *H-Division Quarterly Report, October through December, 1975*, Lawrence Livermore Laboratory, Rept. UCRL-50028-75-4 (1975).
4. J. Wackerle, *J. Appl. Phys.* 33, 922 (1962).
5. R. F. Trunin, G. V. Simakov, M. A. Podurets, B. N. Moiseyev, and L. V. Popov, *Izv. Acad. Sci. USSR Phys. Solid Earth*, 1, 13 (1971).
6. H. C. Graboske, R. Grover, and K. W. Johnson, "Theoretical Hugoniot for High Z Metals," in *H-Division Quarterly Report, October through December, 1975*, Lawrence Livermore Laboratory, Rept. UCRL-50028-75-4 (1975).
7. R. Grover and P. A. Urtiew, "Thermal Relaxation at Interfaces Following Shock Compression," *J. App. Phys.* 45, 146 (1974).
8. P. A. Urtiew and R. Grover, "Temperature Deposition Caused by Shock Interactions with Material Interfaces," *J. App. Phys.* 45, 140 (1974).
9. P. A. Urtiew and R. Grover, *The Melting Temperature of Magnesium under Shock Loading*, Lawrence Livermore Laboratory, Rept. UCRL-78365 (to be published).
10. Y. Ya. Vaschenko and N. Zubarev, *Sov. Phys. Solid State* 5, 653 (1963).
11. R. J. Olness, *EOS Representations*, internal document HTN-264 (1976). Readers outside the Laboratory who desire further information on LLL internal documents should address their inquiries to the Technical Information Department, Lawrence Livermore Laboratory, Livermore, CA 94550.
12. Private communication from R. Grover (1976).
13. A. K. McMahan and M. Ross, *High Temperature Electron Band Calculations*, Lawrence Livermore Laboratory, Rept. UCRL-78233 (1976).
14. A. K. McMahan, B. L. Hord, and M. Ross, *An Experimental and Theoretical Study on Metallic Iodine*, Lawrence Livermore Laboratory, Rept. UCRL-78234 (1976).
15. L. Hedin and B. I. Lundqvist, *J. Phys.* C4, 2064 (1971).

16. R. G. McQueen, S. P. Marsh, J. W. Taylor, J. N. Fritz, and W. J. Carter in *High Velocity Impact Phenomena*, R. Kinslow, Ed. (Academic Press, New York, 1970), Ch. VII.
17. M. L. Wilkins, *Calculation of Elastic-Plastic Flow*, Lawrence Livermore Laboratory, Rept. UCRL-7322, Rev. I (1969).
18. A. Edwards, N. Ferriter, J. A. Fleck, Jr., and A. M. Winslow, *A Theoretical Description of the Interaction of a Pulsed Laser and a Target in an Air Environment*, Lawrence Livermore Laboratory, Rept. UCRL-51489 (1973).
19. P. Grant and A. Leibe, *Problem Generation for Interacting and Triangular Slides*, internal document HTN-265 (1976).
20. M. L. Wilkins, C. F. Cline, and C. A. Henidel, *Light Armor*, Lawrence Livermore Laboratory, Rept. UCRL-71817 (1969).
21. L. B. Hord in *H-Division Quarterly Progress Report January through March 1976*, Lawrence Livermore Laboratory, Rept. UCRL-50028-76-1 (1976).
22. W. M. Isbell, F. H. Shipman, and A. H. Jones, *Hugoniot Equation of State Measurements for Eleven Materials to Five Megabars*, Materials and Structures Lab., Manufacturing Development, G. M. Corp., G. M. Technical Center, Warren, Michigan, Rept. MSL-68-13 (1968).
23. J. J. Folkins and W. H. Gust, "Hugoniot Parameters for Tantalum from 2.3 to 4.2 Megabars," *Bull. Am. Phys. Soc.* 20(12), 1514 (1975).
24. M. L. Wilkins, D. M. Norris, and M. E. Prado, *Fundamental Study of Crack Initiation and Propagation*, Lawrence Livermore Laboratory, LLL Proposal 125 (1975), p. 32.
25. *Fracture Toughness of Ferritic Materials in Light Water Nuclear Reactor Vessels*, Electric Power Research Institute, Palo Alto, CA, Rept. EPRI 232-2 (December 1975).
26. W. C. Rivard and M. D. Torrey, *Numerical Calculation of Flashing from Long Pipes Using a Two Field Model*, Los Alamos Scientific Laboratory, Rept. LA-6104-MS (1975).
27. C. W. Hirt and N. C. Romero, *Application of a Drift Flux Model to Flashing in Straight Pipes*, Los Alamos Scientific Laboratory, Rept. LA-6005-MS (1975).
28. D. C. Wilcox and I. E. Alber, "A Turbulence Model for High Speed Flows," in *Proc. of the 1972 Heat Transfer and Fluid Mechanics Institute*, 23rd Meeting at San Fernando Valley State Coll., Northridge, CA, June 14-16, 1972 (Stanford Univ. Press, 1972) p. 231.

29. R. C. Y. Chin, "Dispersion and Gibbs Phenomena Associated with Difference Approximations to Initial Boundary Value Problems for Hyperbolic Equations," *J. Comp. Phys.* 18 (3) 233 (1975).