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A Numerical and Theoretical Analysis of Some Spherically Symmetric Containment Vessel Problems

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A NUMERICAL AND THEORETICAL ANALYSIS OF SOME SPHERICALLY SYMMETRIC CONTAINMENT VESSEL PROBLEMS

by

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ABSTRACT

A numerical analysis of some spherically symmetric containment vessel problems is accomplished using the one-dimensional hydrodynamics code SIN. The typical problem involves a spherical steel vessel containing a detonating spherical charge of PBX-9404 at its center, with a mitigator (air or vermiculite) surrounding the charge. Two different vessels are considered — one having 17.6-cm inner radius and 0.635-cm-thick shell and the other having an 88.9-cm inner radius and a 6.35-cm-thick shell. Three different charge masses are used: 15.82 g, 8.17 kg, and 27.24 kg. In each configuration considered, the displacement of the shells and the pressure in the air at the inner wall are obtained as a function of time. The results agree well with experimental data. A simple theoretical model is also considered and gives solutions in reasonable agreement with the numerical results.

I. INTRODUCTION

The problem of the containment of explosions using spherical vessels has been investigated many times and has an extensive literature dating back many years.[1] Mathematically, the problem can be stated simply: Given a spherically symmetric vessel (usually made of steel) with an elastic shell that may be "thick" or "thin" when compared with the inside radius of the vessel, compute or determine the dynamic response of the shell when it is subjected to internal and external time-dependent pressure loads.

Cinelli[2] gave the general solution to this problem for the case when the shell deformations are small and when the external and internal pressure loads are arbitrary functions of space and time. Specialized solutions also exist for the case when the shell is thin. To this author's knowledge, no theoretical solution exists for the spherically symmetric case, where the shell deformation is large when compared to the inner radius of the vessel, whether or not the shell itself is thick or thin.

In general, the pressure loads may not be spherically symmetric, the shell may be constructed of material having elastic and plastic properties, and the vessel may be surrounded by an elastic medium.

For simplicity, we assume that the internal pressure load is spherically symmetric and that the outer surface of the shell is a free surface. The internal pressure load is produced by a detonating spherical charge at the center of the vessel, with a mitigator (air or vermiculite) surrounding the charge.

In all of the problems considered, the object of the calculations was to compute the maximum displacement of the vessel steel wall at the first excursion of the induced shock wave generated in the wall by a detonating charge of PBX-9404. Displacement of the outer wall was chosen for illustrative purposes because results were essentially the same for any point in the shell. Numerical calculations were done using the one-dimensional hydrodynamic code SIN.[3,4]

Three containment vessel (CV) configurations were considered for calculation. They were the CV-1 and CV-2 experiments, where the mitigator was air, and the CV-3 experiment, where the mitigator was vermiculite. The three calculations involved two different vessels — the V-1 and V-2. The V-1 vessel had an inner radius of 17.6 cm and a shell thickness of 0.635 cm, whereas the V-2 vessel had an inner radius of 88.9 cm and shell thickness of 6.35 cm. The mass of the explosive charge was different for the three configurations: the CV-1 charge mass was 15.82 g, the CV-2 charge mass was 8.17 kg, and the CV-3 charge mass was 27.24 kg. Figure 1 is a schematic (not to scale) of the typical CV configuration, and Fig. 2 shows the computational model used in SIN.[3,4]

The detonator for the charges was modeled identically for all three experiments and is shown in Fig. 3. The PBX-9404 explosive ($\rho_0 = 1.844$ g/cm^3) was burned using CJ volume burn technique with a burn specific volume of 0.4054 cm^3/g and a detonation velocity of 0.88 cm/μs, and was initiated with "hot spot" PETN.[4]

The same steel parameters were used for all calculations: $Y_0 = 4.137 \times 10^{-3}$ Mbar, $\mu = 0.79982$ Mbar, $\sigma = 0.29$, $E = 2.0685$ Mbar, and $\rho_0 = 7.822$ g/cm^3.

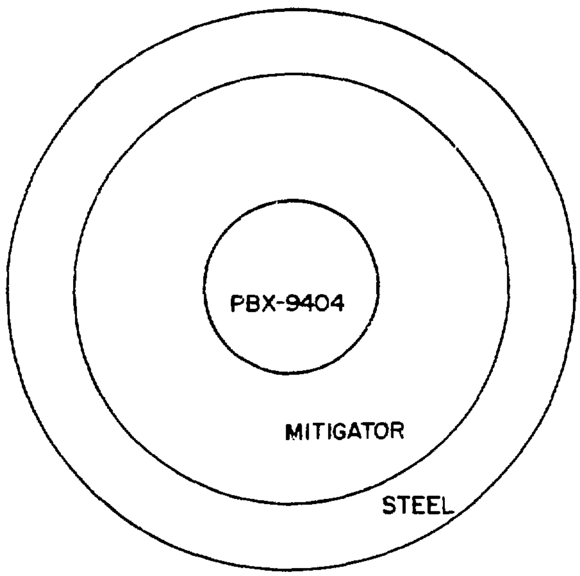

Fig. 1.
Schematic of the confinement vessel.

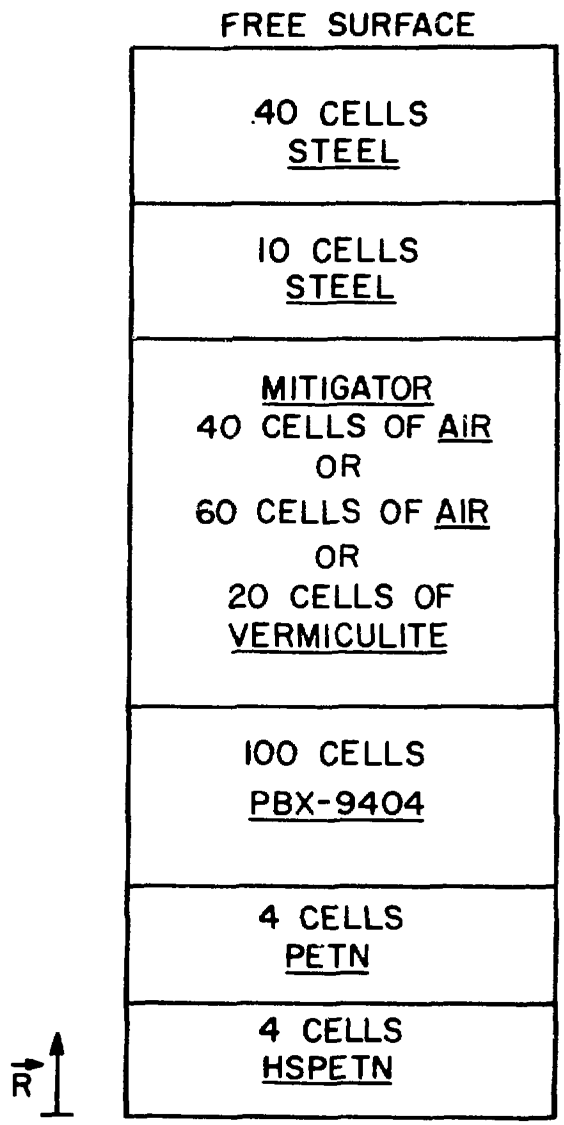

Fig. 2.
Schematic of the numerical model.

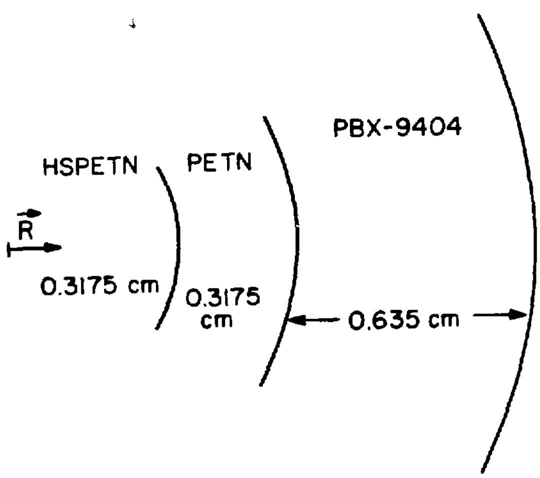

Fig. 3.
Schematic of the detonator.

Boundary conditions were the same for all computations — namely, the vessel surface was assumed to be a free surface. Note also that for all calculations, distance is measured in centimeters, velocity in centimeters per microsecond, specific volume in cubic centimeters per gram, energy in megabars per cubic centimeters per gram, pressure in megabars, temperature in kelvins, and heat capacity in calories per grams kelvin.

In Secs. II, III, and IV we discuss the numerical modeling and results for CV-1, CV-2, and CV-3, respectively, and compare them with experimental results.[5] In Sec. V we discuss the application of a simple theoretical model,[6] which assumes thin shells and small deformations to the CV-1, CV-2, and CV-3 experiments. Appendixes A and B give, respectively, the equation of state used and the equation-of-state parameters for the various explosives and materials.

II. NUMERICAL MODELING AND RESULTS FOR CV-1

In the CV-1 experiment using the V-1 vessel, the SIN[3] hydrodynamic calculations were made for a 1.27-cm-radius ball of PBX-9404 (0.635 cm of PBX-9404 divided into 100 cells) and a PETN initiator (0.635 cm of PETN divided into 8 cells), 16.33 cm of ambient air (pressure of 0.81×10^{-6} Mbar) composed of 40 cells, 1.5875×10^{-2} cm of steel composed of 10 cells, and 0.619125 cm of steel divided into 40 cells.

The calculated maximum displacement was 6.86×10^{-3} cm at a time of 82.4 μs from detonation (Fig. 4). We compared this with the experimental value of $(6.68 \pm 0.66) \times 10^{-3}$ cm. Figures 5 and 6 show the velocity-vs-time and specific volume-vs-radius profiles, respectively, at late times.

III. NUMERICAL MODELING AND RESULTS FOR CV-2

In this case, the V-2 vessel was used. We have a 10.187-cm-radius ball of PBX-9404 (9.522 cm of PBX-9404 divided into 100 cells) and a PETN initiator (0.635 cm of PETN divided into 8 cells), 78.713 cm of ambient air composed of 60 cells, 0.15875 cm of steel composed of 10 cells, and 6.19125 cm of steel divided into 40 cells.

In Fig. 7 we see that the calculated maximum displacement was 5.70×10^{-2} cm at a time of 406 μs from detonation. This compares with the experimental value of $(5.47 \pm 0.67) \times 10^{-2}$ cm. Figures 8 and 9 give the velocity-vs-time and specific volume-vs-radius profiles.

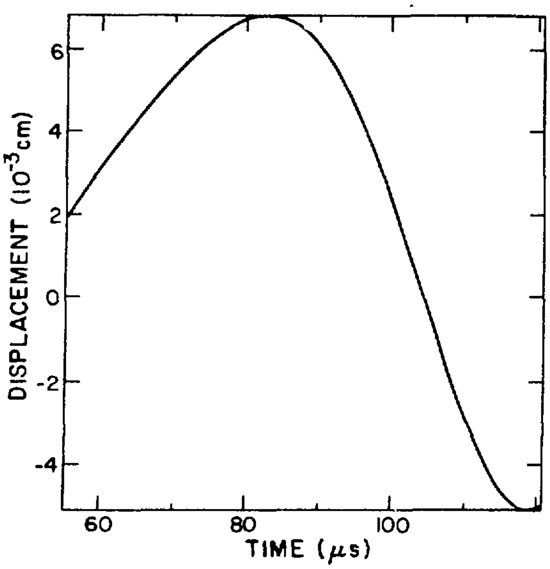

Fig. 4.
Displacement vs time for CV-1.

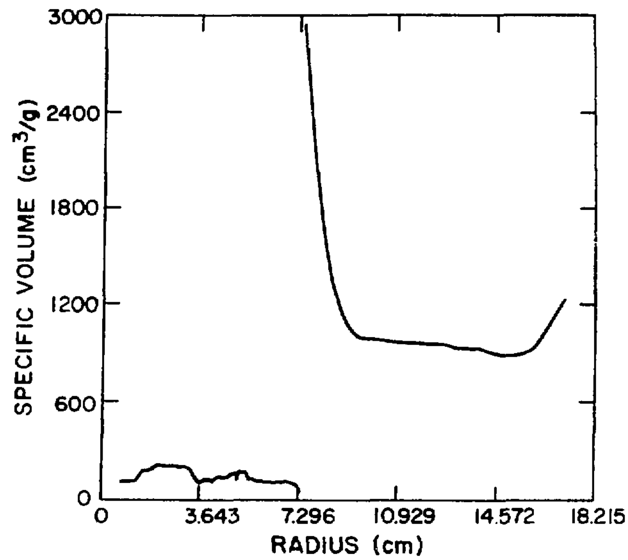

Fig. 6.
Specific volume vs radius for CV-2.

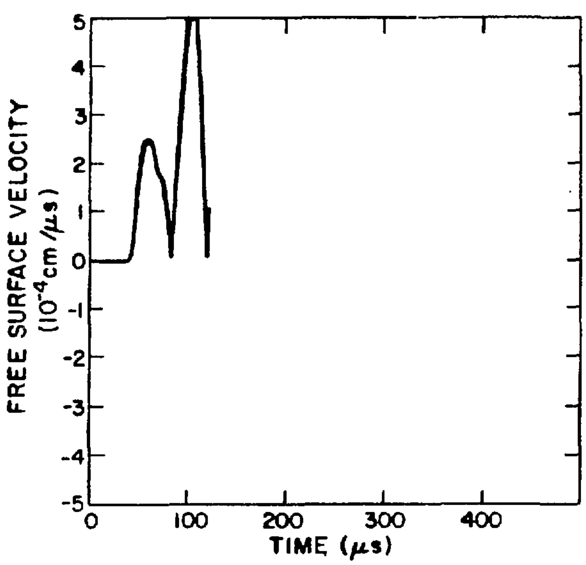

Fig. 5.
Free surface velocity vs time for CV-1.

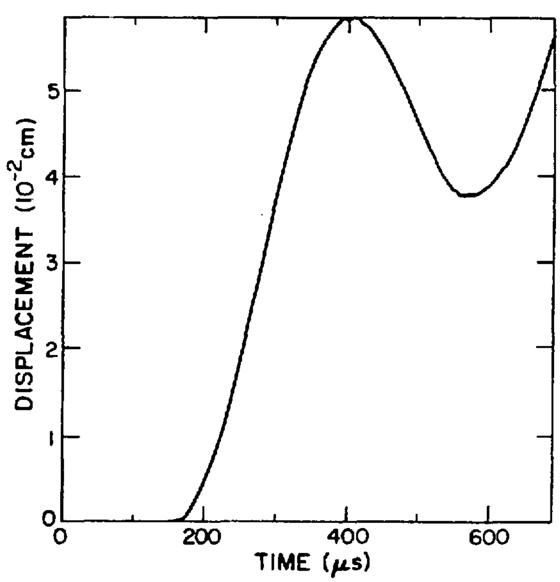

Fig. 7.
Displacement vs time for CV-2

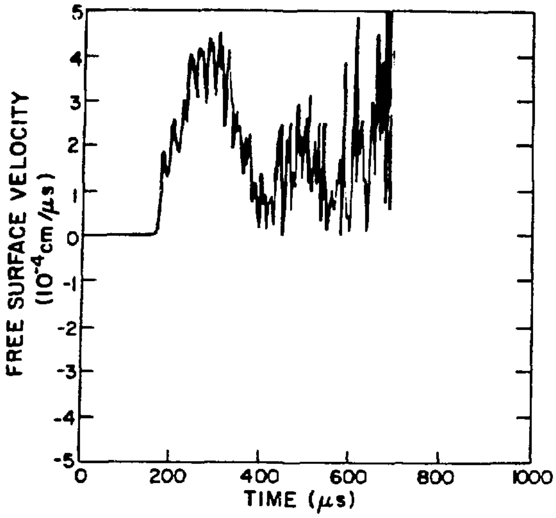

Fig. 8.
Free surface velocity vs time for CV-2.

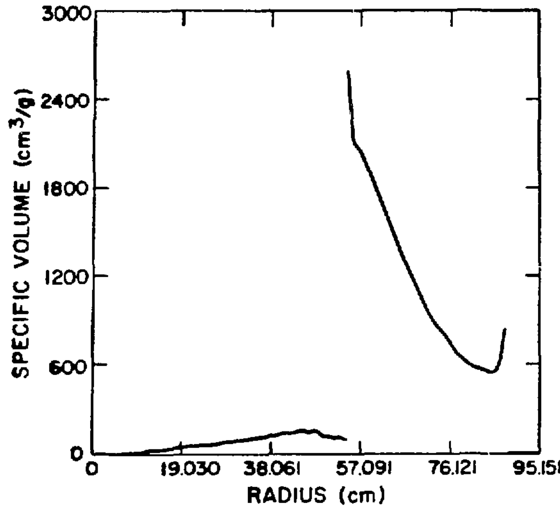

Fig. 9.
Specific volume vs radius for CV-2.

IV. NUMERICAL MODELING AND RESULTS FOR CV-3

Here we consider the V-2 vessel, where we have a 15.221-cm-radius ball of PBX-9404 (14.586 cm of PBX-9404 divided into 100 cells) and a PETN initiator (0.635 cm of PETN divided into 8 cells), 73.679 cm of vermiculite foam comprising 20 cells, 0.15875 cm of steel composed of 10 cells, and 6.19125 cm of steel divided into 40 cells.

The numerical solution of this problem was much harder than for the problems discussed in Secs. II and III because of the intrinsic, calculational difficulty of describing a foam. In fact, we decided to employ the usual $U_S = C + SU_P$ linear relation between the shock velocity U_S and the particle velocity U_P and to investigate the problem in terms of the parameters C and S (HOM equation of state).[3,4] A third parameter — the Grüneisen gamma, γ — was required because the Mie-Grüneisen equation of state was used to relate the pressure to the internal energy and specific volume.[3,4] Thus, the CV-3 calculation became a three-parameter problem for a given initial density of the vermiculite foam.

We found that the calculations were insensitive to variations in γ for $\gamma \leqslant 0.01$, so a final value of $\gamma = 0.01$ was used. Variations in S in the range $1.00 \leqslant S \leqslant 1.05$ also caused little change in calculated results. Having set $\gamma = 0.01$ and $S = 1.05$, a value of $C \cong 0.001$ cm/μs caused overall agreement with experiment. We then noted that the calculations were sensitive to the precise value of ρ_0 used for the vermiculite. In fact, an increase of 20% in ρ_0 from 0.10 to 0.12 g/cm^3 causes a corresponding decrease of 20% in the calculated maximum displacement from 3.22×10^{-1} cm to 2.55×10^{-1} cm. The experimental value of the maximum displacement is $(2.18 \pm 0.21) \times 10^{-1}$ cm. If this type of sensitivity to ρ_0 remains true, then one would expect that $\rho_0 \cong 0.128$ g/cm^3 would yield a computed value of the maximum displacement to within one standard deviation of the experimental value. Thus, the accurate determination of ρ_0 — particularly after it is packed in the vessel — is critical for comparing experimental and calculated results. The very low value of $C \cong 0.001$ cm/µs is perhaps reasonable when considering the assumption made in the calculation that a linear fit of U_S to U_P with constant C and S can be made throughout the entire problem. Even so, there is a factor of approximately 100 from the minimum to maximum density of the vermiculite when it undergoes compression and expansion between the time of detonation and the time at maximum displacement on first excursion of the induced shock wave in the steel. Thus U_S as a function of U_P for vermiculite must be determined experimentally at a higher confidence level than exists at present.

Figures 10-20 illustrate a number of radius, velocity, and specific volume profiles computed using SIN and the HOM equation of state[3,4] with $\rho_0 = 0.10$ g/cm^3, $\rho_0 = 0.12$ g/cm^3, and a range of values for γ, C, and S.

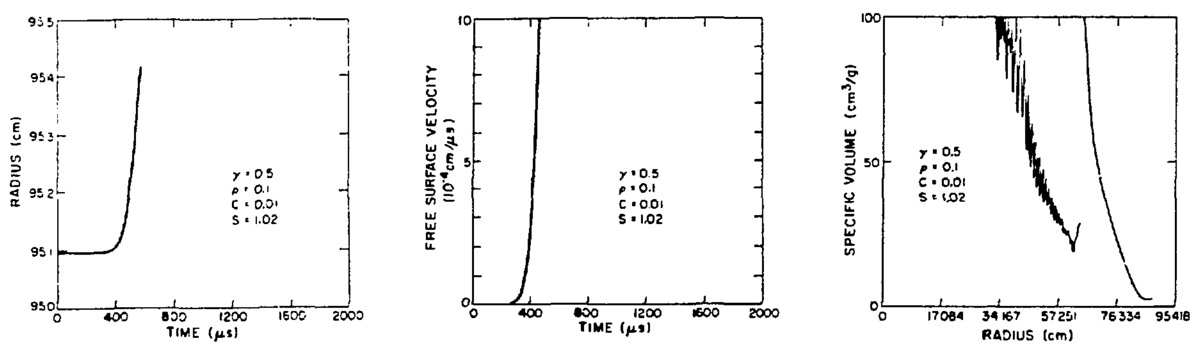

Fig. 10.
Radius vs time, free surface velocity vs time, and specific volume vs radius for CV-3.

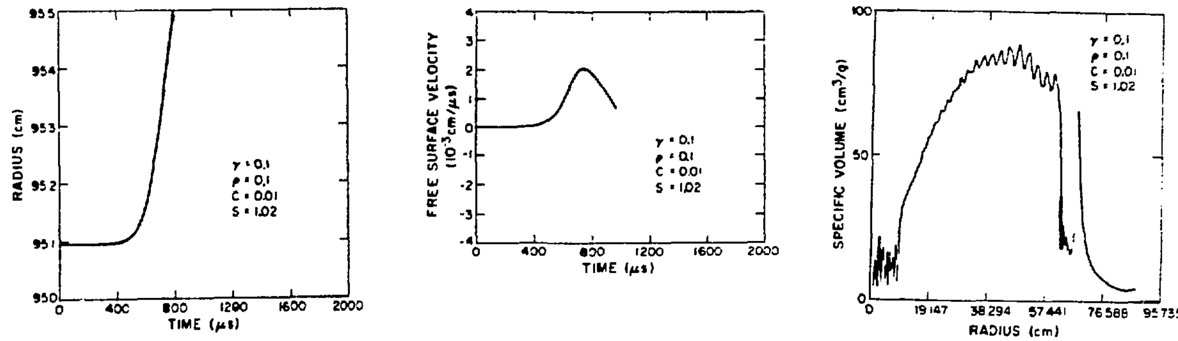

Fig. 11.
Radius vs time, free surface velocity vs time, and specific volume vs radius for CV-3.

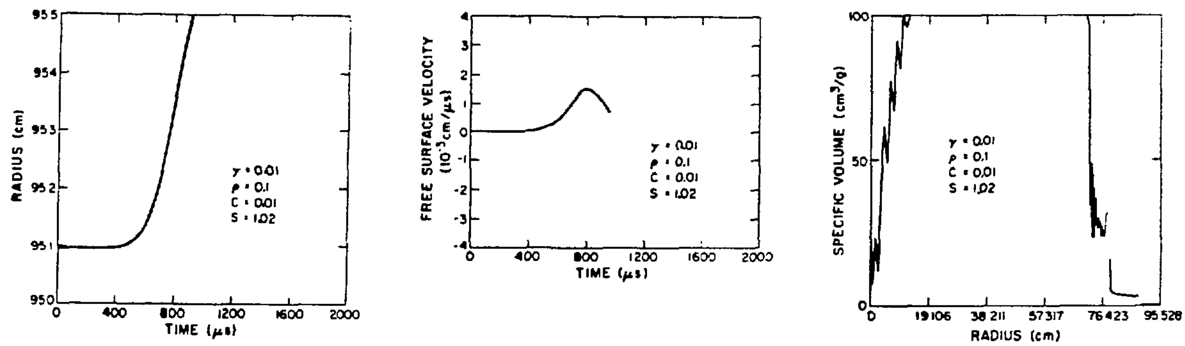

Fig. 12.
Radius vs time, free surface velocity vs time, and specific volume vs radius for CV-3.

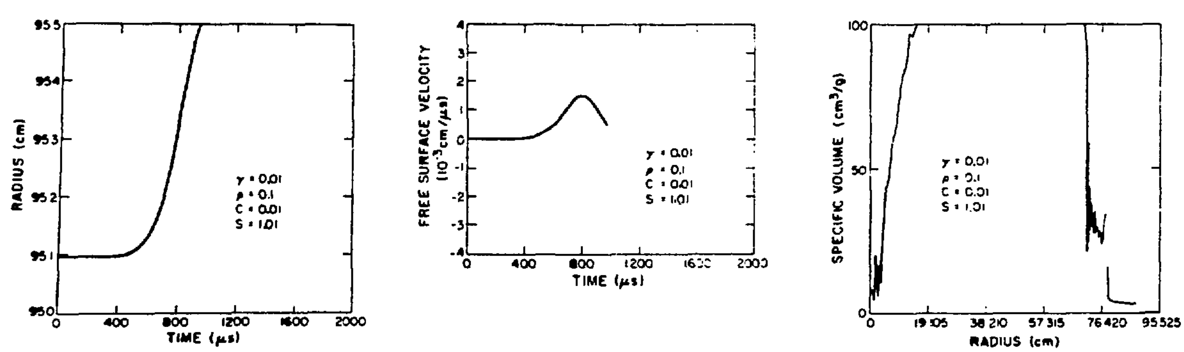

Fig. 13.
Radius vs time, free surface velocity vs time, and specific volume vs radius for CV-3.

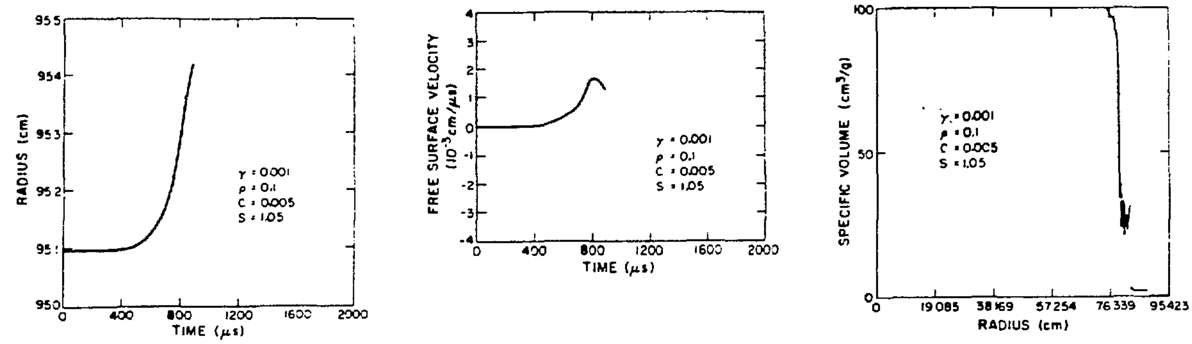

Fig. 14.
Radius vs time, free surface velocity vs time, and specific volume vs radius for CV-3.

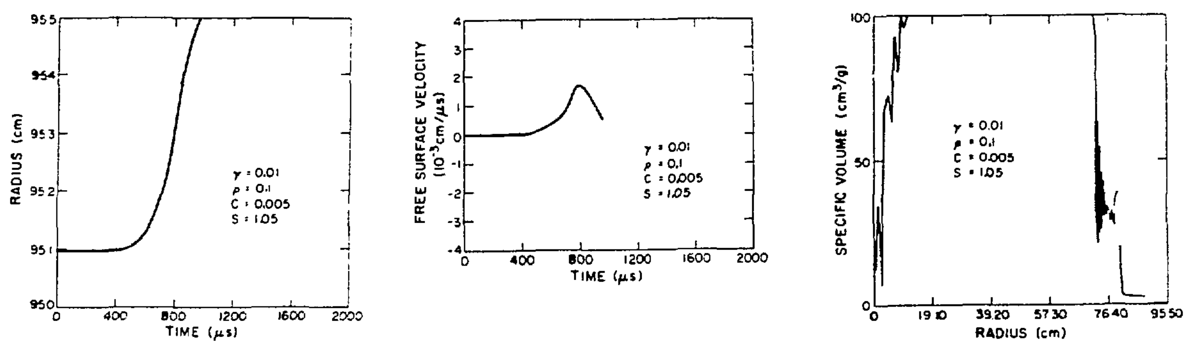

Fig. 15.
Radius vs time, free surface velocity vs time, and specific volume vs radius for CV-3.

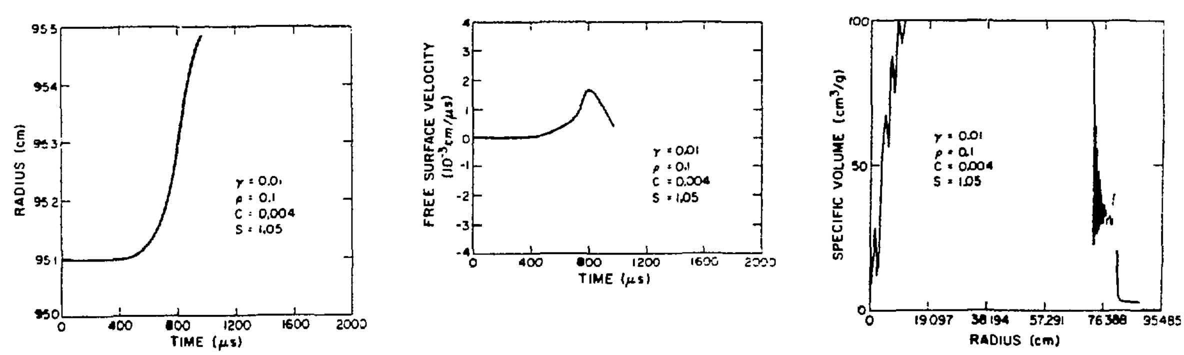

Fig. 16.
Radius vs time, free surface velocity vs time, and specific volume vs radius for CV-3.

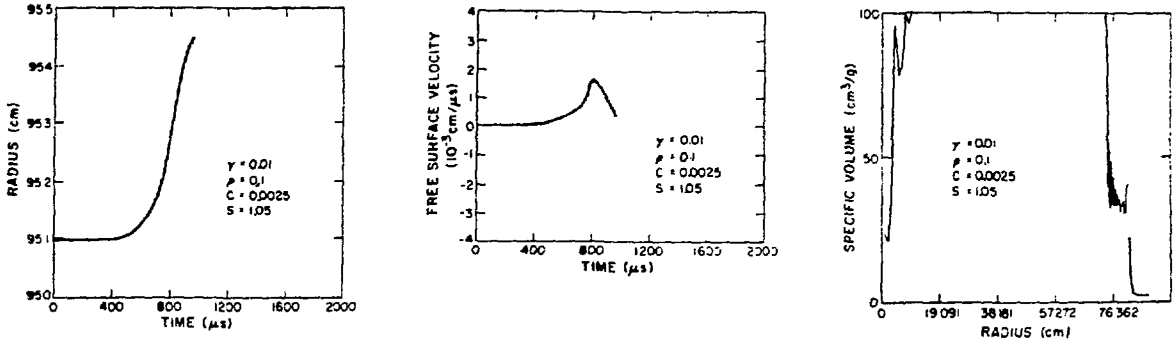

Fig. 17.
Radius vs time, free surface velocity vs time, and specific volume vs radius for CV-3.

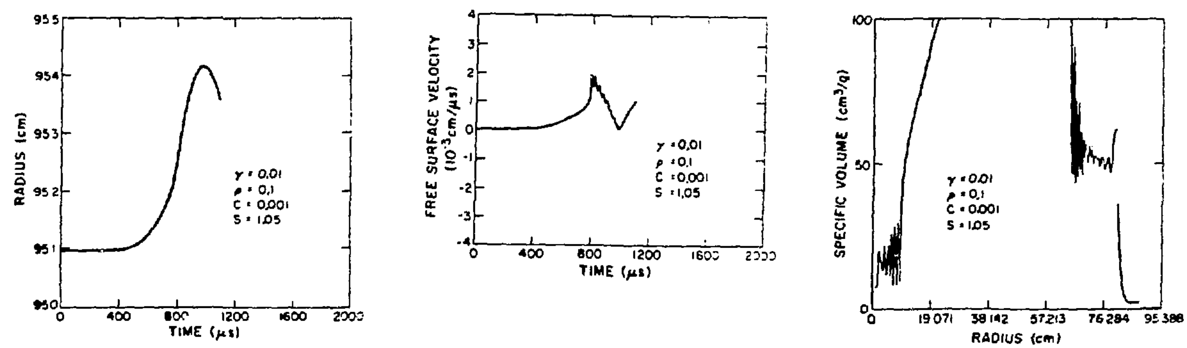

Fig. 18.
Radius vs time, free surface velocity vs time, and specific volume vs radius for CV-3.

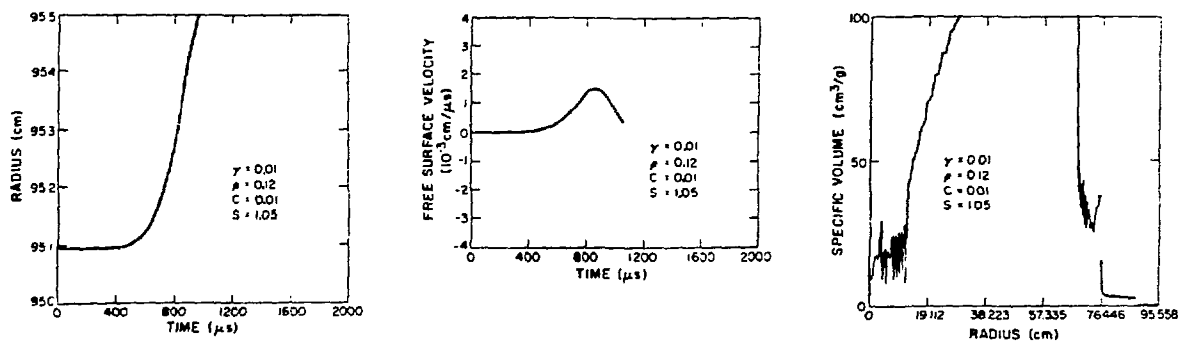

Fig. 19.
Radius vs time, free surface velocity vs time, and specific volume vs radius for CV-3.

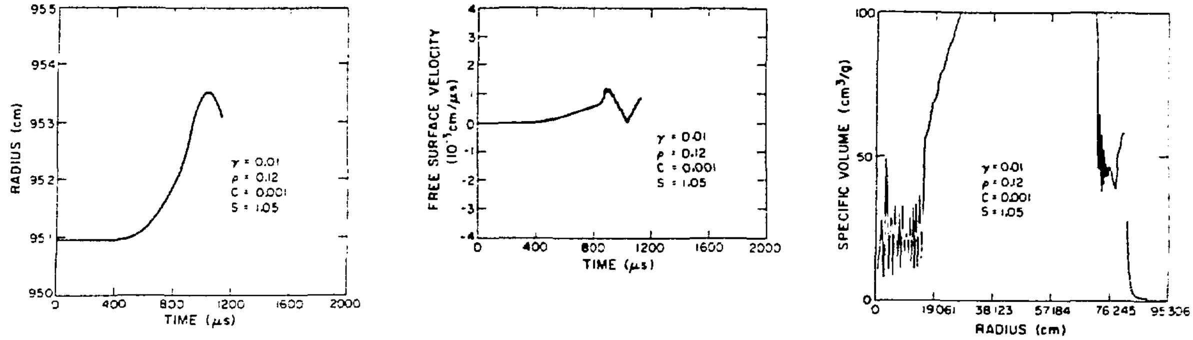

Fig. 20.
Radius vs time, free surface velocity vs time, and specific volume vs radius for CV-3.

V. THEORETICAL CONSIDERATIONS

Good theoretical estimates of the maximum displacement (denoted here by U_{max}) can be simply made if the pressure is given as a function of time at the inner wall of the vessel. An exact treatment[2] exists for spherically symmetric charge and vessel if the shell deformation is small. However, even in this case, the tacit assumption is made that the pressure loads are known functions of space and time, which can never be strictly true since the pressure at the inner wall in the mitigator [denoted by P(t)] depends somewhat on the interaction with the wall. Practically, when there is a great disparity in density, as is the case when steel and air or vermiculite border each other, the effect is slight. In the case where deformations are not small (when compared to a typical dimension of the vessel), no solution seems to exist because of the intractability of solving partial differential equations with moving boundary conditions (i.e., in Lagrangian coordinates).

We present here simple estimates of U_{max} using a theoretical model[6] that assumes P(t) is a square pulse with height P_0 and width $t_1 - t_0$, where P_0, t_1, and t_0 are determined from the calculated or experimental data (t_1, t_0 determine the ending and beginning times of the square pulse). Furthermore, we assumed that the deformations are very small so that the shell is, in fact, a thin shell. These approximations prove to be good ones for the CV-1, CV-2, and CV-3 cases because U_{max}/shell thickness was about 10% for CV-1, 1% for CV-2, and 4% for CV-3.

In particular, we use the model of Duffey and Johnson[6] and others, where the radial equation of motion (dots denote differentiation with respect to time) of a thin elastic spherical shell is given by

$$\rho_S h\ddot{U}(t) + \frac{2Eh}{R^2(1 - \sigma)} U(t) = P(t) \quad , \tag{1}$$

where ρ_S = density of steel shell = 7.822 g/cm^3; h = shell thickness; U = radial displacement, measured positively outward; and t = time, as measured from the time of detonation.

Choosing $P(t) = P_0\theta(t - t_0)\theta(t - t_1)$, we find that

$$\ddot{U}(t) + \omega^2 U(t) = \alpha\theta(t - t_0)\theta(t - t_1) \quad , \tag{2}$$

where

$$\omega^2 = \frac{2E}{\rho_S R^2(1 - \sigma)} \quad \text{and} \quad \alpha = \frac{P_0}{\rho_S h} \quad .$$

The initial conditions are

$$U(t < t_0) = \dot{U}(t < t_0) = \ddot{U}(t < t_0) = 0 \quad ,$$

$$U(t_0) = 0 \quad , \tag{3}$$

and

$$\dot{U}(t_0) = \alpha t_0 \quad .$$

The solution for $t < t_1$ is given by

$$U(t) = \left(\frac{\alpha}{\omega^2}\right)\left\{1 - \sqrt{1 + \omega^2 t_0^2} \cos\,[\omega(t - t_0) + \psi]\right\} \quad , \tag{4}$$

where

$$\psi \equiv \cos^{-1}\left\{\left(1 + \omega^2 t_0^2\right)^{-1/2}\right\} \quad .$$

The maximum displacement U_{max} is given by

$$U_{max} = \left(\frac{\alpha}{\omega^2}\right)\left(1 + \sqrt{1 + \omega^2 t_0^2}\right) = U(t_{max}) \quad , \tag{5}$$

where

$$t_{max} = \frac{\Pi - \psi}{\omega} + t_0 \quad .$$

From Figs. 21, 22, and 23, we see that the impulse $I = \int_{t_0}^{t_1} P(t)dt$ can be calculated for the CV-1, CV-2, and CV-3 cases. From $I = P_0(t - t_0)$, we can determine P_0 and thus α. In fact, $I_{CV-1} \cong 2.5 \times 10^{-3}$ Mbar-μs with $t_0 = 41.5$ μs, $t_1 = 120$ μs; $I_{CV-2} \cong 5.89 \times 10^{-2}$ Mbar-μs with $t_0 = 155$ μs, $t_1 = 691$ μs; and $I_{CV-3} \cong 6.5 \times 10^{-2}$ Mbar-μs with $t_0 = 773$ μs and $t_1 = 1140$ μs.

We find that in the CV-1 case, $U_{max} \cong 8.7 \times 10^{-3}$ cm at $t_{max} \cong 83$ μs, in the CV-2 case, $U_{max} \cong 6.6 \times 10^{-2}$ cm at $t_{max} \cong 377$ μs; and in the CV-3 case, $U_{max} \cong 3.2 \times 10^{-1}$ at $t_{max} \cong 948$ μs.

The errors in the theoretical results for U_{max} range from 15% to 27%. Note that almost all of the error comes from the ambiguity in determining t_0 and t_1 such that the actual pressure load resembles a square pulse as much as possible.

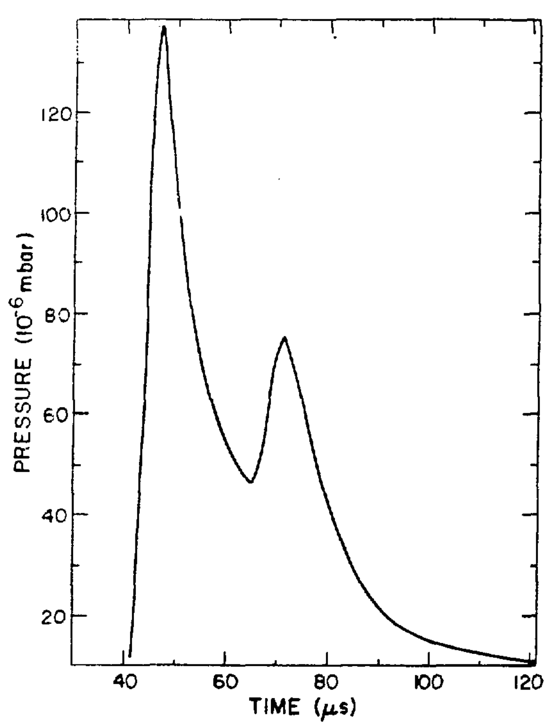

Fig. 21.
Calculated pressure vs time at the air-steel interface for CV-1.

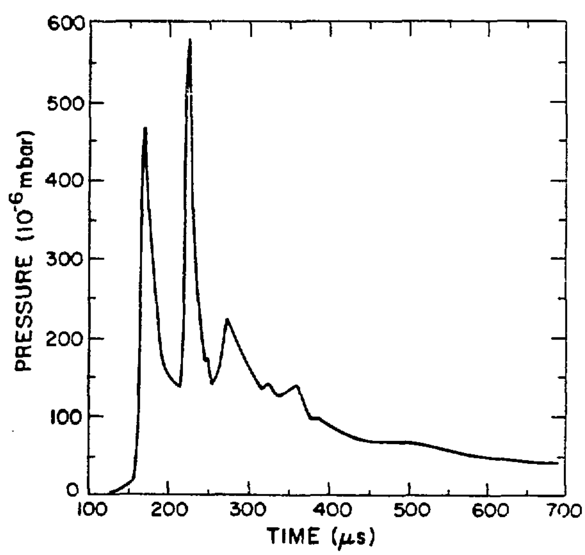

Fig. 22.
Calculated pressure vs time at the air-steel interface for CV-2.

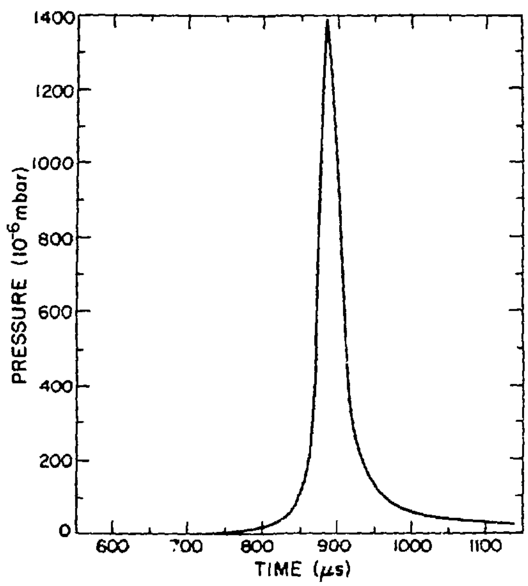

Fig. 23.
Calculated pressure vs time at the vermiculite-steel interface for CV-3.

It is possible to do much better theoretically if the differential equation is integrated numerically with the pressure load, or integrated analytically with the pressure load represented by an analytical fit.

VI. CONCLUSIONS

We have found that with the SIN[3] one-dimensional hydrodynamic code we can numerically calculate the displacement of a spherical shell when subjected to internal pressure loading caused by the blast wave generated by a spherical detonating charge and propagated by a mitigator, such as air or vermiculite. The results are in excellent agreement with experiment.[5] We also found that even a simple theoretical model can yield reasonable estimates for the displacement.

ACKNOWLEDGMENTS

I thank James N. Johnson for many useful and illuminating discussions concerning the theoretical aspects of this work.

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APPENDIX A

EQUATION OF STATE

The HOM equation of state is used to solve for pressure P and temperature T in a cell, with specific volume V and specific internal energy I as input. The shock velocity U_S and the particle velocity U_P are related by

$$U_S = C + SU_P \quad .$$

The equations for a solid are

$$P_H = C^2(V_0 - V)/[V_0 - S(V_0 - V)]^2 + P_0$$

$$X = \ln V$$

$$\ln T_H = F + GX + HX^2 + IX^3 + JX^4$$

$$I_H = (1/2)(P_H + P_0)(V_0 - V)$$

$$P = (\gamma/V)(I - I_H) + P_H$$

$$T = (I - I_H)(23\ 890)/C_V + T_H$$

The equations for a gas are

$$X = \ell n\ V$$

$$Y = \ell n\ P_i$$

$$Y = A + BX + CX^2 + DX^3 + EX^4$$

$$\ell n\ I_i = K + LY + MY^2 + NY^3 + OY^4$$

$$I_i = I_i - Z$$

$$\ell n\ T_i = Q + RX + SX^2 + TX^3 + UX^4$$

$$-1/\beta = R + 2SX + 3TX^2 + 4UX^3$$

$$P = [1/(\beta V)](I - I_i) + P_i$$

$$T = (I - I_i)(23\ 890)/C_V' + T_i$$

APPENDIX B

EQUATION-OF-STATE CONSTANTS

HOT SPOT PETN

C	2.33000000000E-01	J	-7.03513328034E+00
S	1.84200000000E+00	γ	7.70000000000E-01
F	-1.13774340704E+00	C_V	2.60000000000E-01
G	-3.43223247054E+01	V_0	5.64971751412E-01
H	-6.11668345590E+01	α	5.00000000000E-05
I	-4.26099439006E+01		
A	-3.47737732103E+00	O	3.12989398035E-05
B	-2.47418234015E+00	Q	7.51031200685E+00
C	2.57527846749E-01	R	-4.80832718599E-01
D	-5.07804204106E-03	S	5.09397444908E-02
E	-3.79647309692E-03	T	3.35500372609E-02
K	-1.60847428108E+00	U	-1.03061080438E-02
L	4.87607433920E-01	C_V'	5.00000000000E-01
M	5.50773585908E-02	Z	1.00000000000E-01
N	-2.67315879716E-03		

PETN

C	2.33000000000E-01	J	-5.36251579151E+01
S	1.84200000000E+00	γ	7.70000000000E-01
F	-7.66189781324E+00	C_V	2.60000000000E-01
G	-7.95847702476E+01	V_0	6.45161290000E-01
H	-1.74863616490E+02	α	5.00000000000E-05
I	-1.65120245643E+02		
A	-3.10639868833E+00	O	5.15057824089E-05
B	-2.25218297065E+00	Q	8.10009012302E+00
C	1.93865645401E-01	R	-3.67433055630E-01
D	-1.06761114309E-02	S	-1.38196579791E-03
E	-5.71317097698E-05	T	8.14028829459E-03
K	-1.43880401718E+00	U	-7.34294504930E-04
L	4.17630232758E-01	C_V'	5.00000000000E-01
M	4.43146793248E-02	Z	1.00000000000E-01
N	2.43302842995E-03		

PBX-9404

C	2.42300000000E-01	J	-2.21893825727E+01
S	1.88300000000E+00	γ	6.74700000000E-01
F	-9.04187222042E+00	C_V	4.00000000000E-01
G	-7.13185252435E+01	V_0	5.42299349000E-01
H	-1.25204979360E+02	α	5.00000000000E-05
I	-9.20424177603E+01		
A	-2.88303447687E+00	O	5.31474988838E-05
B	-2.25910150671E+00	Q	9.24707528084E+00
C	2.09836811364E-01	R	-4.89536325865E-01
D	-1.62402872478E-02	S	6.12169699021E-02
E	4.14247701072E-04	T	-3.22067926443E-03
K	-1.27244575845E+00	U	-5.13495324073E-06
L	4.27159472916E-01	C_V'	5.00000000000E-01
M	4.61539702874E-02	Z	1.00000000000E-01
N	2.54544398316E-03		

AIR

A	-4.59256514634E+00	O	-3.43883754010E-06
B	-9.16844491252E-01	Q	9.14112194252E+00
C	-2.12887045546E-01	R	1.00994190807E-01
D	5.41467029547E-02	S	-2.18376867054E-01
E	-4.66515725006E-03	T	5.49014249677E-02
K	-1.61815078888E+00	U	-4.70352490744E-03
L	8.59669028575E-02	C_V'	5.00000000000E-01
M	1.66889390906E-03	Z	1.00000000000E-01
N	-1.27025922472E-04		

VERMICULITE

C	5.40000000000E-01	J	0.
S	1.40000000000E+00	γ	1.00000000000E-02
F	5.70378247500E+00	C_V	1.00000000000E-01
G	0.	V_0	3.70370370400E-01
H	0.	α	1.00000000000E-05
I	0.		

STEEL

C	4.53000000000E-01	J	-1.66391615983E+02
S	1.51000000000E+00	γ	2.02000000000E+00
F	-3.82382587453E+03	C_V	1.07000000000E-01
G	-7.03211954024E+03	V_0	1.27844541000E-01
H	-4.82670213894E+03	α	1.17000000000E-05
I	-1.46678402118E+03		