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DEWFALL VALIDATION EXPERIMENT DESIGNS

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RECEIVED

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OSTI

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I. INTRODUCTION

The analysis models being developed for the large vessel project emphasize the processes which the vessel wall undergoes after the initial release of energy. To validate these models a set of intermediate scale experiments is proposed which allows measurement of the various processes of interest. An earlier SEA report¹ proposed six conceptual designs, ranging from add-ons to NTS events to simple laboratory scale steam/ice experiments. We have focused the present effort on laboratory or intermediate scale tests that could be conducted in local or LANL facilities. The emphasis is on viable near term tests that do not require the development of untested diagnostic techniques, and provide the highest confidence in the measurables significant to the validation effort.

II. SIGNIFICANT PROCESSES OF THE DEWFALL MODEL

The details of the DEWFALL model have been described elsewhere^{1,2}. Processes of the model which need to be treated in the validation exercise include:

1. Vaporization and recondensation of the vessel wall material due to energy transfer from the source.
2. Melt and refreeze of vessel wall material.
3. Condensation and solidification of the source material.

Major uncertainties of the actual large vessel process, which may or may not be treated by DEWFALL, were described in the prior report but will be repeated here because of their importance:

1. For a given wall or liner material, how thick of a melt layer will be formed?
2. How much of the wall or liner material will be vaporized?

3. At what rate will the metallic vapor recondense, and will all of the recondensation take place at the walls?
4. What happens to the liquid layer on the walls? How much pooling at the bottom of the vessel is likely to occur?
5. Will other constituents of the vapor (like air and HE products) cause it to act substantially different than a pure metallic vapor?
6. Are the process rates conduction limited? Convection? Radiation?

The energy and geometric scaling parameters of the large vessel process are shown in Table

1. Observations from recent DEWFALL calculations are provided in Reference 2.

The primary measurables of interest in the experiments are intended to coincide with the DEWFALL model outputs:

1. Pressure history in the vessel.
2. Temperature history and distribution in the vessel volume.
3. Temperature history and distribution in the vessel wall.
4. Phase history of the vessel wall material (how much of it liquifies, vaporizes, recondenses, resolidifies).

The time scale of interest in the experiments includes the period when vaporization and liquifying occurs, out to recondensation / solidification and complete pressure decay. We are not interested in the very early processes associated with initial energy deposition in the open vessel volume.

Table 1. Large vessel test parameters.

Total Energy (J)			4.2×10^{11}
Mass (g):	Source plus air at	60 torr	1.3×10^6
		10 torr	4.7×10^4
		No air	2.3×10^4
Geometry:	Vessel radius (m)		14.9
	Vessel internal surface area (m ²)		2.8×10^3
	Vessel volume (m ³)		1.4×10^4
	Vessel volume/surface area	5.0	
E/M:	Energy/Mass (J/g)	60 torr	3.2×10^5
		10 torr	8.9×10^6
		No air	1.8×10^7
E/A:	Energy/Vessel Volume (J/m ³)		3.0×10^7
E/A:	Energy/Area (J/m ²)		1.5×10^8
M/V:	Mass/Volume (g/m ³)	60 torr	93
		10 torr	3.4
		No Air	1.6
Materials:	Source	Aluminum, Beryllium, HE	
	Liner	Aluminum or Steel	
	Wall	Steel	

III. EXPERIMENT DESCRIPTIONS

While the energy and geometric scaling parameters of Table 1 are tangible objectives, they are not the only relevant considerations in designing a validation test. An effective validation test requires the following:

1. The major processes of the "real" situation are present: melt, vaporization, condensation, solidification.
2. Materials and major processes are appropriately modeled by the code.

With this in mind, we reduced the set of potential experiments described in Reference 1 to three relatively simple test configurations:

Vaporized metal experiment

This test would be conducted in a facility such as the Los Alamos Pegasus facility, which consists of a 1.5 MJoule capacitor bank regularly used in exploding foil experiments. The configuration of the test is shown in Figure 1. The metal slug to be vaporized is nested in an insulating material, sandwiched between an electrode and the spherical chamber (which acts as the other electrode). When the slug is vaporized by the electric current discharge, it jets into the evacuated spherical void as a plasma/metal gas. Pressure and temperature measurements in the vessel wall record the response to the energy deposition. The assembly would be sectioned after the test to measure the amount of material lost to evaporation and observe melting trends. Metallographic tests could infer the melt depth by the changes brought about in the crystal structure. Its scale precludes a great deal of material loss (see the experiment analysis section at the end of this section), and there are large uncertainties in how long the assembly can act as a sealed pressure vessel (the insulator is most likely to fail) and how effeciently the metal slug will be vaporized. It is also probable that some of the slug will be projected as solid material into the opposite wall of the vessel and erode the surface.

Hydrogen/oxygen combustion in an ice lined vessel

This test departs dramatically from the use of representative materials in the experiments, but does represent the appropriate processes. A spherical void is cast in an ice block, contained in a pressure vessel (Figure 2). The void is filled with a stoichiometric mixture of hydrogen and oxygen and ignited. Temperature sensors in the void and ice record their respective histories, and the sensors cast into the ice will detect the melting of the wall material. Pressure sensors record both the relatively fast combustion pressure and the more relevant pressure decay due to condensation or refreezing of the water. This test allows tailoring of the energy density (by changing the mass of initial combustible gas in the void) and the phase change processes are sufficiently slow to be recorded without exotic diagnostics.

Saturated steam injected into an ice lined vessel

This test would use the same test vessel as the combustion experiment, except that the initial energy and mass deposition would occur by injecting steam into the void (Figure 3). Without getting into extreme pressures and temperatures, this test would tend to be of lower energy density than the combustion test but may be more controllable (and more straightforward from a safety standpoint). Diagnostics are identical to the combustion test.

Analysis of the experiment designs

This analysis determines the maximum amount of material that could be melted and vaporized with a given experiment design, to judge how "measurable" the test would be. To predict the maximum amount of wall material that could be melted (given a vapor filling the vessel of the same material as the wall) we use that fraction of the initial vessel internal energy available at and above the fusion temperature:

$$E_{\text{tot}} = \text{total energy available inside vessel}$$

H = latent heat of phase change

T = temperature

C_p = specific heat of material

M = maximum mass of material vaporized or melted

E_{fusion} = energy available to melt wall material

$$= E_{\text{tot}} \times (H_{\text{vaporization}} + C_p(T_{\text{end}} - T_{\text{fusion}})) / (H_{\text{fusion}} + H_{\text{vaporization}} + C_p(T_{\text{end}} - T_{\text{initial}}))$$

The maximum mass of wall material melted is then:

$$M_{\text{fusion}} = E_{\text{fusion}} / (H_{\text{fusion}} + C_p(T_{\text{fusion}} - T_{\text{initial}}))$$

Solve for material thickness given M_{fusion} and vessel initial inside diameter.

A similar equation is used to solve for the maximum amount of material vaporized:

$$E_{\text{vaporization}} = E_{\text{tot}} \times (C_p(T_{\text{end}} - T_{\text{vap}})) / (H_{\text{fusion}} + H_{\text{vaporization}} + C_p(T_{\text{end}} - T_{\text{initial}}))$$

$$M_{\text{vaporized}} = E_{\text{vaporization}} / (H_{\text{vaporization}} - H_{\text{fusion}} + C_p(T_{\text{vaporization}} - T_{\text{initial}}))$$

Solve for wall thickness vaporized given initial geometry of vessel and M_{vaporized}.

These equations were applied to the experiments using material properties in Table 2.

Table 2. Material properties.

Material	H _{fusion}	H _{vap.}	T _{fusion}	T _{vap.}	C _p	Density
Iron	83 c/g	1515 c/g	1535C	2750C	.108 c/g-C	7.87 g/cc
Aluminum	95	2517	699	2327	.213	1.7
Water	80	540	0	100	1	1

The results are summarized in Table 3 below.

Table 3. Validation experiment summary.

<u>Experiment</u>	<u>Energy Source</u>	<u>Vessel Radius</u>	<u>Maximum Thickness</u>	
			<u>Melted</u>	<u>Vaporized</u>
Vaporized metal	1.5 MJ (3.6E6 c)	10 cm.	0.4 cm	0.03 cm (Al)
			0.15	0.015 (Fe)
H2/O2 Combustion	4 atmospheres (initially)	30	0.7	0.07
Saturated steam	80 atm., 300C (initially)	30	0.2	0.02

IV. SUMMARY

Three experiments are proposed as tests to validate the DEWFALL model. A methodology was developed to analyze the maximum thickness of material melted and vaporized with given experimental configurations and initial energies. This is a very brief record of the techniques and test designs that could be used for validation of the model.

REFERENCES

1. Lowry, W.E., and Keller, C.E., "Experiments to Simulate the Large Vessel Test Processes", SEA Topical Report No. 88-22, July 26, 1988.
2. Walsh, B. and Ruiz, N.K., "Energy Transfer in a Containment Vessel", Fifth Symposium on Containment of Underground Nuclear Explosions, Sept. 1989.

Figure 1. Vaporized Metal Experiment (Pegasus facility)

Figure 2. Hydrogen/oxygen combustion experiment.

Figure 3. Saturated Steam in Ice Vessel

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DEWFALL REFERENCE CALCULATIONS

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Reference DEWFALL Calculations

ABSTRACT

Two reference calculations are the first applications of DEWFALL, software that predicts energy transfer by thermal conduction and radiative diffusion when a gas is hot enough to vaporize its container. The objectives are to test the software and to explain the calculated phenomena.

Analysis of the predictions reveals no serious problems in the software. Calculations of early-time wave propagation appears to be unnecessary.

The time scale for cooling of the interior is sensitive to the optical properties of the vaporized inner surface.

DEWFALL
Reference Calculations

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DEWFALL
Reference Calculations

1.0 INTRODUCTION

1.1 SCOPE

This report documents the results of reference DEWFALL calculations performed by Science and Engineering Associates, Inc. (SEA) for Los Alamos National Laboratory (LANL). It is the sole deliverable item for Task 1 of Subcontract 9-X69-9088Y.

1.2 APPLICABLE DOCUMENTS

9-X69-9088Y-1	Subcontract between the Regents of the University of California (Los Alamos National Laboratory) and Science and Engineering Associates, Inc. for "Research in Thermal Model Code Development and Model Verification Experiment Design and Support," 27 January 1989
SC-RR-71-0713	Sandia Laboratories Report, "Improvements in the Chart D Radiation-Hydrodynamic Code II: A revised Program," S.L. Thompson and H.S. Lauson, Albuquerque, February, 1972.
SC-RR-71-0714	Sandia Laboratories Report, "Improvements in the Chart D Radiation-Hydrodynamic Code III: Revised Analytic Equations of State," S.L. Thompson and H.S. Lauson, Albuquerque, March 1972.
SEASF-TR-89-001	SEA Santa Fe Topical Report, "DEWFALL X.0 (Unverified Prototype) Draft User Manual," Bob Walsh, Nancy Ruiz, and Paul Mattingly, 1 June 1989.

1.3 BACKGROUND

DEWFALL is a tool for studying the confinement of material that may be hotter than the vaporization temperature of its container. This software

predicts radial energy transfer in an idealized spherical vessel for one or more seconds after introduction of the hot material.

The reference calculations were the first application of DEWFALL. They had a succession of objectives, as follows:

- (1) verification that DEWFALL provides the required output in an appropriate format,
- (2) detection of errors in the software or algorithm that lead to physically unreasonable results,
- (3) evaluation of alternative models, and
- (4) prediction of energy transfer for the reference configurations, with explanations of the calculated phenomena and any anomalies present.

The first three objectives were successfully met, culminating with publication of the DEWFALL X.0 Draft User Manual. This report explains the calculated phenomena.

LANL funded DEWFALL development to predict the effect of the large heat source from a nuclear burst in a lined vessel on the pressure and temperature profile and anticipated phase changes in the vessel liner and wall. For the first reference calculation, LANL generated initial conditions with Chart D. The Chart D output described a 29-meter diameter steel sphere with an inner lining of aluminum, one millisecond after introduction of a 418 GJ (100-ton) heat source.

We completed the DEWFALL program as planned, including incorporation of the Chart D analytic equation of state package (ANEOS) described in SC-RR-71 0714, and began the first reference calculation. Because the planned DEWFALL model had not included radiative energy transfer, the temperature profile in the vaporized aluminum steepened until the gradients were clearly unrealistic.

We therefore extended the model and computer program to simulate radiative energy transfer. The DEWFALL X.0 User Manual documents the resulting software.

With radiative transfer included in the model, DEWFALL can make credible energy transfer predictions that start with the introduction of the heat

source. Because DEWFALL does not model wave propagation, such predictions would omit the heating of the wall by shock waves, but shock heating typically represents only a small portion of the original heat source. Therefore SEA prepared a second reference calculation using a simple initial heat source and no liner.

We discuss the simpler calculation (#2) first, in Section 2. Then the original reference calculation is presented in Section 3.

1.4 SUMMARY

Detailed review of the calculations revealed no serious problems with DEWFALL. However, the integration grid and material properties could be improved in the input files.

Comparing the two predictions, it appears that the simple initial conditions are adequate. This should be verified with a direct test.

The blow-off from the wall forms an opaque barrier that controls heat transfer. With the ANEOS material models, the wall materials are opaque above 1 eV. There is a marked transition when the vapor cools enough to become transparent; the time required for this to occur characterizes the time scale.

Without a liner, the interior became transparent at about 0.6 seconds; the aluminum liner delayed this effect to 1.6 seconds. The time scale is sensitive to the optical properties of the metal vapor, and the ANEOS opacity model may not be valid at the important temperatures.

2.0 IONIZED AIR IN STEEL CONTAINER

(Reference Calculation #2)

2.1 INPUT

2.1.1 Initial Conditions

Figure 2.1 portrays a sphere of high-temperature air surrounded by room temperature air, all enclosed in a steel container. The 0.25-m-thick wall of reference-density, room-temperature steel has an outer radius of 14.34 m. The air density is uniform at 77.5 g/m^3 , corresponding to a pressure of 6.67 KPa (50 Torr) at room temperature. The hot air contains 418 GJ of excess heat.

The DEWFALL input data in Figure 2.2 models this configuration with 72 mass elements, 9 in the air and 63 in the steel. The steel partitioning matches the 63 zones in a comparison calculation that is being performed with the Chart D program. The air elements have equal mass, approximately matching the nearest wall element. All of the excess energy is in the innermost air element, which extends to a radius of 6.77 m.

2.1.2 Material Properties

The material representation for steel is a combination of several models. The solid phase is based on a reference density of 7.85 Mg/m^3 , a thermal conductivity of 108 J/m-s-K , and the following relationship between shock and material velocities, U_s and U_m , near the reference state:

$$U_s = 1.49 U_m + 4.58 \text{ km/s.}$$

Melting occurs at 1741 K (0.15 eV), requires a heat of fusion of 302 kJ/kg, and lowers the thermal conductivity to about 70 J/m-s-K . The vapor phase is a gas composed of 70% iron, 19% chromium, and 11% nickel, with a Russian model for ionization and photon cross sections that treats absorption by electron scattering and by partial and complete ionization.

Air is represented by the built-in Chart D parameters for dry air. These describe a gas composed of 78.5% atomic nitrogen, 21.1% atomic oxygen, and 0.47% helium, with the Russian ionization model for opacity. Because the ANEOS

Figure 2.1 Initial Conditions for Reference Calculation #2.

```

***** DEWFALL Input File *****
* Problem ID
$problem
* probid is the problem id - 40 characters in single quotes.
  probid = ' Ref.Calc.#2 - 100 ton, steel vessel (r=1434, d=25)',
$end
* Invariants
$invar
* nelmnt is the number of elements (integer <= 100)
nelmnt = 72,
* totvol is the total volume (cm3)
totvol = 1.235e+10,
* mass is the array of element masses (grams)
mass = 9*100876.,
  101810.,
  117080.,
  134650.,
  154840.,
  178070.,
  204780.,
  235500.,
  270820.,
  311450.,
  358160.,
  411890.,
  473670.,
  544720.,
  626430.,
  720400.,
  828460.,
  952730.,
  1095600.,
  1260000.,
  1449000.,
  1666300.,
  1916300.,
  2203700.,
  2534300.,
  2914400.,
  3351600.,
  3854300.,
  4432500.,
  5097300.,
  5861900.,
  6741200.,
  7752400.,
  8904800.,
  10508000.,
  12399000.,
  14631000.,
  17264000.,
  20372000.,
  24039000.,
  28366000.,
  33472000.,
  39497000.,
  46606000.,
  54995000.,
  64894000.,
  76575000.,
  90359000.,
  106620000.,
  125820000.,
  148460000.

```

Figure 2.2 Input for Reference Calculation #2.

```

142150000.,
149260000.,
156720000.,
164550000.,
162870000.,
195140000.,
234530000.,
281410000.,
337720000.,
405270000.,
486320000.,
583580000.,
700300000.,
* isubid is the array of element substance IDs - integer
isubid = 9*2, 63*1,
$end
* Distribution
$distrib
* eltime is the elapsed time (secs) - here the initial problem time.
eltime = 0.0,
• dteos is the max. time step because of eos discontinuities
dteos = 1.e-7,
* energy is the array of element energies (ergs)
* energy = 9*4.651467e17,
energy = 4.184258e18, 8*2.577382e14,
1.3825798e+14,
1.5899464e+14,
1.828547e+14,
2.1027272e+14,
2.4181906e+14,
2.7809124e+14,
3.19809e+14,
3.6777356e+14,
4.229491e+14,
4.8638128e+14,
5.5934662e+14,
6.4324386e+14,
7.3972976e+14,
8.5069194e+14,
9.783032e+14,
1.12504868e+15,
1.29380734e+15,
1.4879248e+15,
1.71108e+15,
1.967742e+15,
2.2628354e+15,
2.6023354e+15,
2.9926246e+15,
3.4415794e+15,
3.9577552e+15,
4.5514728e+15,
5.2341394e+15,
6.019335e+15,
6.9221334e+15,
7.9604602e+15,
9.1545496e+15,
1.05277592e+16,
1.20927184e+16,
1.4269864e+16,
1.6837842e+16,
1.9868898e+16,
2.3444512e+16,
2.7665176e+16,
3.2644962e+16,

```

Figure 2.2, continued

```

3.8521028e+16,
4.5454976e+16,
5.3636926e+16,
6.3290948e+16,
7.468321e+16,
8.8126052e+16,
1.0398885e+17,
1.22707522e+17,
1.4478996e+17,
1.7086356e+17,
2.0160868e+17,
1.930397e+17,
2.0269508e+17,
2.1282576e+17,
2.231589e+17,
2.2117746e+17,
2.6540752e+17,
3.1849174e+17,
3.8219552e+17,
4.5862376e+17,
5.5035666e+17,
6.6042256e+17,
7.9250164e+17,
9.510074e+17,
* vol is the array of element volumes (cm3)
vol = 9*1.301626e9,
12969.42675159,
14914.64968153,
17152.86624204,
19724.84076433,
22684.07643312,
26086.62420382,
30000.,
34499.36305732,
39675.15923567,
45625.47770701,
52470.06369427,
60340.12738854,
69391.08280255,
79800.,
91770.70063694,
105536.3057325,
121366.8789809,
139566.8789809,
160509.5541401,
184585.9872611,
212267.5159236,
244114.6496815,
280726.1146497,
322840.7643312,
371261.1464968,
426955.4140127,
490993.6305732,
564649.6815237,
649337.5796178,
746738.8535032,
858751.5923567,
987566.8789809,
1134369.426752,
1338598.726115,
1579490.44586,
1863821.656051,
2199235.66879,
2595159.235669

```

Figure 2.2, continued

```

3062292.993631,
3613503.184713,
4263949.044586,
5031464.968153,
5937070.063694,
7005732.484076,
8266751.592357,
9754777.070064,
11510700.63694,
13582165.6051,
16028025.47771,
18912101.91083,
18103280.25478,
19014012.73885,
19964331.21019,
20961783.43949,
20747770.70064,
24896815.28662,
29876433.12102,
35852229.29936,
43021656.05096,
51626751.59236,
61951592.35669,
74341401.27389,
89210191.0823,
$end
* Material Parameters
$matpar
* nsubst is the number of substances (integer <= 10)
nsubst = 2,
* msubid is the ordered array of possible substance IDs
msubid = 1, 2,
* Steel Air
* k0 is the 1st array of solid conductivities (erg/cm-s-eV)
k0 = 126.e9, 1.,
* k1 is the 2nd array of solid conductivities (erg/cm-s-eV-eV)
k1 = .0766e9, 1.,
* lmvol is the array of liquid molar volumes (cm3/mole)
lmvol = .08, 1.,
* molwt is the array of molecular weights
molwt = 55.85, 2.,
* sigma is the 1st array of Lennard-Jones constants (Angstroms)
sigma = 2.34, 2.,
* ek is the 2nd array of L-J constants of form e/k (eV)
ek = .299, .3,
$end
* Requests
$reqsts
$reqsts
* nreqst is the number of solution times requested (integer <=100)
nreqst = 34,
* soltim is the array of solution times requested (secs)
soltim = 0.0, .00001, .000018, .00002, .00005,
.0001, .0002, .0005,
.001, .002, .005,
.01, .02, .05,
.1, .2, .3, .4, .5,
.6, .7, .8, .9, 1.0,
1.1, 1.2, 1.3, 1.4, 1.5,
1.6, 1.7, 1.8, 1.9, 2.0,
* proflg is the array of profile flags (logical: .t. or .f.)
proflg = 34*.true.,
$end
***** end of DEWFALL input file *****
* equation of state input

```

Figure 2.2, continued

```
* for the steel vessel
aneos1 -1 'steel vessel'
aneos1 3 4 7.85 -1 0 -4.58e05 2.0 0
aneos1 1.49 0 7.3e10 0.15 0 0 0 0
aneos1 -1 0 0 0 0 0 -1 0
aneos1 26.0 -0.70
aneos1 24.0 -0.19
aneos1 28.0 -0.11
* for the air layer
aneos2 -2 'air layer' lib=1 type=2 rhug=-1 thug=-1
```

Figure 2.2, continued

model does not treat molecules, the model is inaccurate if the air is not hot enough to assure dissociation of N_2 and O_2 (overcoming dissociation energies of 9.756 and 5.080 eV, respectively).

2.1.3 Initial Pressure Equalization

Before performing heat transfer, DEWFALL adjusted the volumes of the air elements to bring them all to the same pressure, 9.51 MPa. To reach this pressure, the high-energy air expanded more than seven-fold to a density of 10.5 g/m^3 , compressing the cooler air to 390 g/m^3 to reach the configuration in Figure 2.3. The work associated with this process heated the room-temperature air to 2.2 eV and cooled the expanded element to 20.7 eV. However, over 80% of the excess heat remained within the original hot air.

2.1.4 Restarts

In the original input, the first three solution times were 0, 10 and 20 microseconds. However, DEWFALL stopped just after 18 microseconds because the splitting interval determined at 10 microseconds was no longer small enough. We restarted the calculation from 0 seconds with the solution times in Figure 2.2, including 0, 10, 18 and 20 microseconds. DEWFALL reduced the splitting interval at 18 microseconds, and the calculation continued to 20 microseconds and beyond.

DEWFALL stopped just after 1.055 seconds, because the splitting interval computed at 1.0 seconds was again too large for the current conditions. Because 144 minutes of Cray computer time had been consumed, we restarted the problem at 1.0 seconds, using the calculated energy and volume distributions to prepare a new input file. We added a solution time at 1.050 seconds, but the problem occurred again at 1.065 seconds. We restarted again from 1.0 seconds with three more solution times, 1.055, 1.060, and 1.065 seconds. The calculation reached 2 seconds of elapsed time with 26 more minutes of Cray computer time.

Figure 2.3 Initial Configuration After Pressure Equilization.

We merged output files from the two successful runs. The DEWPOST post-processor generated history and profile plots from the merged file.

2.2 CALCULATED PHENOMENA

2.2.1 Evaporization/Condensation

Figure 2.4 shows the vapor mass rising smoothly from the initial air mass of 0.9 Mg to a peak of 47 Mg at 0.65 seconds. The ratio of maximum steel vapor mass to wall area is 18 kg/m^2 ; that is, a 2.3-mm layer of steel has vaporized at 0.65 seconds.

The calculation used a material model that requires about 6.0 MJ/kg to vaporize room-temperature steel. If all of the original excess heat had been used to vaporize steel, with no superheating, it would have produced 70 Mg of steel vapor. The calculated peak is 66% of this maximum.

This is verified in Figure 2.5, which shows the distribution of the original excess heat after 0.6 seconds of heat transfer. Less than two percent of the original excess heat still remains in the air. Sixty-nine percent is in steel vapor, and most of that has been consumed in achieving vaporization; the excess vapor heat is less than three percent of the original excess heat.

For further understanding of how the energy is stored temporarily in the vaporized steel, we plotted a steel isobar in Figure 2.6. The pressure, 2.9 MPa, corresponds to the calculated uniform pressure at 0.60 seconds, and the temperature range, 0.025 to 0.65 eV, spans the calculated steel temperature at that time. The large discontinuity represents the heat of vaporization; it is the dominant feature of the isobar.

ANEOS assumes that recondensation occurs fast enough to maintain local equilibrium; there are no supersaturated states. In the calculation, the vapor mass gradually decreased, reaching 29 Mg at 2.0 seconds. Therefore the layer of recondensed "steel" must have grown to 0.8 mm. ANEOS assumes that the steel remains fully mixed; therefore it recondenses with its original concentrations.

DEWFALL (Unverified Prototype)

Ref.Calc.#2 - 100 ton steel vessel (r=1434 d=25)

Figure 2.4 Ablation History, Reference Calculation #2.

Distribution of Excess Heat After 0.6 Seconds

Figure 2.5 Distribution of Excess Heat After 0.6 Seconds.

Figure 2.6 Energy Content of Hot Steel.

However, a basic DEWFALL assumption was violated after about 1.0 seconds. DEWFALL assumes a well-defined condensation surface, with vapor inside and condensed material outside. But recondensation on the surface reduced the pressure, and the interior vapor had to expand. The expansion cooled the interior vapor below the energy required for complete vaporization. As at the surface, ANEOS assumed condensation at the maximum rate, producing two-phase mixtures away from the surface.

DEWFALL always assumes the phases are separated. Every two-phase element was assigned the thermal conductivity of the gas at its inner boundary and the appropriate liquid thermal conductivity at its outer boundary. At this temperature, heat transfer by radiation, which has less phase dependence, is much greater than thermal conduction. Nevertheless, results after 1.0 seconds are suspect.

2.2.2 Vapor Energy Removal

When the ANEOS equation of state package is given a density-temperature pair that corresponds to a two-phase state, it calculates the specific energy of each phase. However, it does not make that information available; instead, it returns the mean specific energy of the mixture. Because DEWFALL does not need phase energies, the programming and computer time necessary to recover them were saved.

On the other hand, DEWPOST needs the energy of the vapor phase of the liquid-vapor element to calculate accurately the total vapor energy history (Figure 2.7) but that would require calls to ANEOS. Instead, the current version of DEWPOST approximates the vapor specific energy by using the mean specific energy of the mixture.

Hand calculations show that the correct treatment would remove the apparent noise shown in Figure 2.7. In fact, the vapor energy decreased smoothly, reaching 170 GJ at 2.0 seconds. Of this amount, 4 GJ was the room-temperature energy of the vaporized material and the remaining 166 GJ was 40% of the initial excess heat. Sixty percent of the excess heat had transferred into condensed material in 2.0 seconds.

Ref.Calc.#2 - 100 ton steel vessel (r=1434 d=25)

Figure 2.7 Energy Containment, Reference Calculation #2.

2.2.3 Pressure History

Before 1 ms, the pressure history (Figure 2.8) was dominated by adjustment of the artificial initial conditions to a more realistic temperature distribution. By 1 ms (Figure 2.9) the radiation diffusion from the interior air had spread through the outer air and begun to affect the steel, and the pressure had fallen to 6.91 MPa. The one-second pressure was 1.72 MPa, and the final calculated pressure was 1.13 MPa at two seconds.

The pressure dropped smoothly except for a period of faster decay between 0.5 and 0.7 seconds. The temperature profiles in Figures 2.10 and 2.11 show the qualitative change that occurred in that interval. At 0.5 seconds, there is an opaque layer of steel vapor at about 1 eV, but by 0.7 seconds the maximum temperature is 0.36 eV and all of the vapor is relatively transparent.

Figure 2.12 is a sketch of the steel opacity model as a function of temperature along a 6.5 MPa isobar. Near the boiling point, the opacity model is dominated by scattering, giving a Rosseland opacity of $0.02 \text{ m}^2/\text{kg}$. But at temperatures above 0.6 eV, excitation of bound electrons becomes important. At 1 eV, the opacity is about $90 \text{ m}^2/\text{kg}$, and the mean free path in the vapor is about 6 mm.

Ionization affects the mechanical properties of the gas as well. Figure 2.13 shows the increase in specific heat above 0.7 eV as electron excitation begins. The ionization potentials of the three steel components range from 6.8 to 7.9 eV.

2.2.4 Melt Growth

The growth of the liquid layer is shown in in Figure 2.14. For comparison, the maximum vapor mass is shown at the appropriate time. The liquid mass was comparable to the vapor mass during the first half-second, but later the liquid layer continued to grow while the vapor was condensing. After 0.7 seconds, the layer grew in both directions, the melt line advancing into the solid while recondensation created more liquid at the inside surface.

DEWILL (Unverified Prototype)

Ref.Calc.#2 - 100 ton steel vessel (r=1434 d=25)

Figure 2.8 Pressure History, Reference Calculation #2.

DEMFAU. (Unverified Prototype)

Ref.Calc.#2 - 100 ton steel vessel (r=1434 d=25)

Time = 1.00×10^3 seconds

Figure 2.9 Temperature Profile, Reference Calculation #2, 1 ms.

UWILL (Unverified Prototype)

Ref.Calc.#2 - 100 ton steel vessel (r=1434 d=25)

Time = 5.00×10^{-1} seconds

Figure 2.10 Temperature Profile, Reference Calculation #2, 0.5 s.

DEWALL (Unverified Prototype)

Ref.Calc.#2 - 100 ton steel vessel ($\rho=1434$ d=25)

Time = 7.00×10^1 seconds

Figure 2.11 Temperature Profile, Reference Calculation #2, 0.7 s.

Figure 2.12 ANEOS Opacity Model for Steel.

Figure 2.13 ANEOS Specific Energy Model for Steel.

011111.1. (Unverified Prototype)

Ref.Calc.#2 - 100 ton steel vessel (r=1434 d=25)

Figure 2.14 Melt Growth, Reference Calculation #2.

The irregularities shown in Figure 2.14 occurred because the integration grid was relatively coarse at the melt line. The initial width of the innermost steel element was six microns, but the integration mesh was progressively coarser at depth. By 1.0 seconds, the melt line had reached the forty-sixth steel element, which had a width of 1 mm. This one element represented a mass of 17 Mg.

The liquid increased in mass throughout the calculation, exceeding 110 Mg at 2.0 seconds. This constituted a 6 mm melt layer.

2.2.5 Wall Heating

Figure 2.15 shows the temperature profile in the wall after one second had elapsed. The slope changes at the melting point because the energy flux at that point must be discontinuous, the jump determined by the heat of fusion and the melting rate.

The role of radiative transfer increases with temperature. At room temperature there is negligible energy transfer by radiation. As the solid approaches the melting point, radiative transfer increases; by the onset of melting, radiation is over 10% of the total energy flux. The relative contribution of radiative transfer increases in the liquid phase, reaching about 60% of the flux near the boiling point. In the vapor phase virtually all of the energy transfer is radiative.

2.3 CONCLUSIONS

Two factors limit confidence in this particular prediction after one second. One is that DEWFALL is not designed to treat the clouds of steel liquid that began to appear after 1.0 second. The second is that the melt line was traversing a relatively coarse portion of the grid. Nevertheless, we learned that simple initial conditions could produce interesting and relevant calculations, and we discovered some important features of the phenomena.

DUMFALL (Unverified Prototypel

Ref. Calculated - 100 ton steel vessel (c-1434 d-25)

Time - 1.00×10^0 seconds

Figure 2.15 One-Second Wall Temperatures, Reference Calculation #2.

Radiation is the dominant energy transfer mechanism at the liquid-vapor interface. Therefore accurate models of thermal conductivity are irrelevant at temperatures near or above the boiling point.

The rate of cooling of the interior gases is limited by the high opacity of steel above 0.7 eV. The effect is that the interior radiates like a 0.7-eV black body. Using 14 m as the radius of the black body, the cooling rate is 608 GJ/s. At this rate, the 418 GJ of excess heat would dissipate in 0.7 second. This is in good agreement with the calculation, which cooled the gas below 0.7 eV in 0.6 second.

3.0 CHART-D CONTINUATION WITH LINER

(Reference Calculation #1)

3.1 INPUT

3.1.1 Initial Conditions

Reference calculation #1 predicted the response of a system similar to that of Section 2. There were two major differences, namely:

- 1) the steel was 0.2 m thick with a 10-mm aluminum liner on the inside wall and
- 2) the heat source was modeled as a cold central core surrounded by high explosive and beryllium, with energy added to the core at a constant rate for two microseconds.

LANL personnel used Chart D to predict the response of this system. The Chart D calculation was continued for 993,222 cycles to reach an elapsed time of 8.26 milliseconds, consuming six hours of Cray computer time. We developed the input for Reference Calculation #1 (Figure 3.1) from the Chart D output at one millisecond. The elements in the DEWFALL input correspond to the zones in the Chart D calculation. The nineteen steel zones were graded in width from 0.7 to 35 mm. The outermost aluminum zone was 1.8 mm, matching the mass of the adjacent steel zone. The 33 aluminum zones graded down to a width of 30 microns at the inner surface. The interior mesh included 22 zones in the air, 7 zones in beryllium, one zone in high explosive, and 4 zones in the core.

At one millisecond, the Chart D output reported 2.2 GJ of kinetic energy, less than one percent of the source energy. For comparison, the error in energy conservation had reached 8 GJ. To create the DEWFALL input (Figure 3.1), we calculated the total specific energy for each zone as

$$M_i[E_i + (V_i^2 + V_{i+1}^2)/4],$$

where M is the mass, E is the specific internal energy (including the radiation field), and the V's are the velocities at the zone boundaries.

```

***** DEWFALL Input File *****
* Problem ID
$problem
* probid is the problem id - 40 characters in single quotes.
  probid = ' Scarab Case - 100 ton, steel vessel (r=1434, d=20)',
$end
* Invariants
$invar
* nelmnt is the number of elements (integer <= 100)
nelmnt = 87.
* totvol is the total volume (cm3)
totvol = 1.236e+10.
* mass is the array of element masses (grams)
mass =
      1085.      1042.6      1000.9      960.82      1002.1,
      941.      1129.2      1355.      1626.      1951.3,
      2341.5      2809.8      3378.4      4054.      4864.8,
      5837.8      7005.4      8406.4      10088.      12105,
      14526.      17432.      20918.      25101.      30122,
      36146.      43375.      52050.      62460.      74953,
      89943.      107930.      129520.      155420.      206660,
      227320.      250050.      275060.      302570.      332820,
      366100.      402710.      442990.      487280.      536010,
      589610.      648580.      713430.      784780.      863250,
      949580.      1044500.      1149000.      1263900.      1390300,
      1529300.      1682200.      1850500.      2035500.      1989100,
      2585900.      3361600.      4370100.      5681200.      7385500,
      9601200.      12482000.      14393000.      17992000.      22490000,
      28112000.      35140000.      43925000.      54907000.      68634000,
      85792000.      1.0724e8      1.3405e8      1.6287e8      1.9544e8,
      2.3453e8      2.8144e8      3.3772e8      4.0527e8      4.8632e8,
      5.8358e8      7.003e8.
* isubid is the array of element substance IDs - integer
isubid = 4*6. 5. 7*4. 22*3. 33*1. 20*2.
$end
* Distribution
$distrib
* eltime is the elapsed time (secs) - here the initial problem time.
eltime = 0.001,
* dteos is the max. time step because of eos discontinuities
dteos = 1.e-7.
* energy is the array of element energies (ergs)
energy =
      1.683e15      1.153e15      1.093e15      1.038e15      6.78e15,
      1.504e16      1.785e16      2.126e16      2.536e16      3.027e16,
      3.614e16      4.319e16      3.583e16      4.240e16      4.997e16,
      5.871e16      6.869e16      7.995e16      9.333e16      1.084e17,
      1.247e17      1.416e17      1.594e17      1.793e17      2.017e17,
      2.272e17      2.523e17      2.720e17      2.820e17      2.899e17,
      2.965e17      2.892e17      2.580e17      2.496e17      9.665e16,
      3.689e15      3.823e15      3.953e15      3.831e15      2.883e15,
      2.887e15      2.857e15      2.790e15      2.692e15      2.578e15,
      2.468e15      2.384e15      2.349e15      2.384e15      2.489e15,
      2.664e15      2.930e15      3.223e15      3.545e15      3.900e15,
      4.290e15      4.719e15      5.191e15      5.710e15      5.580e15,
      7.254e15      9.430e15      1.226e16      1.594e16      2.072e16,
      2.693e16      3.501e16      1.955e16      2.444e16      3.055e16,
      3.818e16      4.773e16      5.966e16      7.457e16      9.322e16,
      1.165e17      1.457e17      1.821e17      2.212e17      2.654e17,
      3.185e17      3.822e17      4.587e17      5.504e17      6.605e17,
      7.926e17      9.511e17.
* vol is the array of element volumes (cm3)
vol =
      10574488.8      458688.957      445636.687      433778.781      5170794.63,
      10271804.3      12485625.8      15166778.5      18456299.6      22503748.1,
      27424455.3      33473909.9      17687958.1      21472457.6      26070739.5,
      31624052.0      38364731.6      46341786.1      56326074.8      76324085.7.

```

Figure 3.1 Input for Reference Calculation #1.

```

109795918., 158185117., 222224583., 301585966., 397387862.,
509601015., 638149183., 793324188., 966873065., 1162062015.,
1322885718., 1393724173., 1360075606., 1411625794., 604799531.,
98406.9264, 107225.557, 116847.918, 125391.628, 128501.930,
140537.428, 153647.462, 168053.869, 183809.883, 201129.455,
220332.585, 241466.865, 264920.163, 291090.504, 319959.229,
351826.602, 386995.183, 425713.227, 468284.549, 515116.709,
566617.265, 623267.876, 685624.305, 754168.210, 736976.658,
958095.590, 1245498.33, 1619155.24, 2104927.72, 2736383.84,
3557317.52, 4624675.80, 1833970.43, 2292558.61, 2865698.26,
3582059.12, 4477573.90, 5596967.38, 6996304.79, 8745412.84,
10931702.3, 13664627.9, 17080784.9, 20753058.1, 24903160.0,
29884046.8, 35861365.9, 43032619.7, 51639908.2, 61967380.2,
74360346.5, 89232925.5,

$end
* Material Parameters
$matpar
* nsubst is the number of substances (integer <= 10)
nsubst = 6,
* msubid is the ordered array of possible substance IDs
msubid = 1, 2, 3, 4, 5, 6,
* Al Steel Air Be HE core
* k0 is the 1st array of solid conductivities (erg/cm-s-eV)
k0 = 328.e9, 126.e9, 1., 1., 1., 1.,
* k1 is the 2nd array of solid conductivities (erg/cm-s-eV-eV)
k1 = 1197.e9, 903.e9, 1., 1., 1., 1.,
* lmvol is the array of liquid molar volumes (cm3/mole)
lmvol = 0.02, 7.105, 1., 1., 1., 1.,
* molwt is the array of molecular weights
molwt = 26.98, 55.85, 2., 2., 2., 8.,
* sigma is the 1st array of Lennard-Jones constants (Angstroms)
sigma = 2.63, 2.34, 2., 2., 2., 2.,
* ek is the 2nd array of L-J constants of form e/k (eV)
ek = .271, .299, .3, .3, .3, .3,
$end
* Requests
$reqsts
* nreqst is the number of solution times requested (integer <=100)
nreqst = 30,
* soltim is the array of solution times requested (secs)
soltim = .001, .00101, .0011, .0012, .0015,
.002, .005, .01, .02, .05,
.1, .2, .3, .4, .5,
.6, .7, .8, .9, 1.0,
1.1, 1.2, 1.3, 1.4, 1.5,
1.6, 1.7, 1.8, 1.9, 2.0,
* profilg is the array of profile flags (logical: .t. or .f.)
profilg = 3*.true., 2*.false.,
.true...false...true...false...false.,
.true...false...false...false...true.,
.false...false...false...false...true.,
.false...false...false...false...true.,
.false...false...false...false...true.,
$end
***** end of DEWFALL input file *****
* equation of state input
* for the aluminium liner
aneos1 -1 'aluminium from library' lib=6 type=4 rhug=-1 thug=-1
* for the steel vessel
aneos2 -2 'steel vessel'
aneos2 3 4 7.85 -1 0 -4.58e05 2.0 0
aneos2 1.49 0 7.3e10 0.15 0 0 0 0

```

Figure 3.1, continued

```

aneos2 -1 0 0 0 0 0 -1 0
aneos2 26.0 -0.70
aneos2 24.0 -0.19
aneos2 28.0 -0.11
* for the air layer
aneos3 -3 'air layer' lib=1 type=2 rhug=-1 thug=-1
* for the HE inner layer
aneos4 -4 'HE inner layer'
aneos4 6 2 0.413 -1 0 0 00 0
aneos4 0 0 0 0 0 0 0 0
aneos4 0 0 0 0 0 0 0 0
aneos4 12.0 -0.24245
aneos4 1.0 -0.24491
aneos4 7.0 -0.24148
aneos4 8.0 -0.24148
aneos4 9.0 -0.01474
aneos4 17.0 -0.00494
* for the beryllium layer
aneos5 -5 'beryllium from library' lib=8 type=2 rhug=-1 thug=-1
* for the NE core
aneos6 -6 'ne core'
aneos6 1 2 20.55 -1 0 0 0 0
aneos6 0 0 0 0 0 0 0 0
aneos6 0 0 0 0 0 0 0 0
aneos6 92 -1.00

```

Figure 3.1, continued

3.1.2 Material Properties

Section 2.1.2 describes the models for steel and air.

At the temperatures in the DEWFALL calculation, beryllium and the core were modeled as monatomic ionized gases. The high explosive model was a mixture of nearly equal numbers of hydrogen, nitrogen, oxygen and carbon atoms, with 1.5% fluorine and 0.5% chlorine.

Aluminum was represented by the built-in ANEOS parameters for the pure metal, which was a mistake because the library model had a non-zero thermal conductivity which was incorporated into the calculated opacity. The effect was to make the thermal conductivity higher than intended by 233 J/m-s-K. Consequently, the solid phase was based on a reference density of 2.7 Mg/m^3 , a thermal conductivity of 516 J/m-s-K (instead of 283 J/m-s-K), a bulk modulus of 76.3 GPa (763 kbar), and a Gruneisen coefficient of 2.06. Melting occurred at 928K (0.08 eV), required a heat of fusion of 330 kJ/kg, and lowered the thermal conductivity to about 380 J/m-s-K (instead of the intended 150 J/m-s-K).

3.1.3 Initial Pressure Equalization

DEWFALL adjusted the initial volumes to establish a uniform pressure of 7.08 MPa. Before adjustment, gas pressures had varied from 4 to 55 MPa with 70% of the volume having pressures below 7 MPa.

The adjustments heated some elements by compression and cooled others by expansion, resulting in the irregular temperature distribution shown in Figure 3.2. For reference, Figure 3.2 also shows the temperatures before pressure equilization. Because the peak pressures at one millisecond were at the center of the sphere, that region was cooled significantly to reduce its pressure.

3.1.4 Restarts

DEWFALL stopped after 1.118 seconds, because the splitting interval determined at 1.1 seconds was no longer small enough. Because two hours of Cray computer time had been consumed, we restarted the calculation at 1.1

Aluminum Reference Calculation

DEWFALL vs CHARTD at 1 ms.

Figure 3.2 Temperature Distribution after Pressure Equalization.
Reference Calculation #1.

seconds, using the calculated energy and volume distributions to create a new input file. We added solution times at 1.115, 1.116, 1.117, 1.118, and 1.119 seconds.

The calculation reached 2 seconds of elapsed time with about one more hour of Cray computer time.

3.2 CALCULATED PHENOMENA

3.2.1 Comparison with Chart D

Within 0.1 milliseconds, the temperature irregularities had dispersed, leaving the profile shown in Figure 3.4. The center of the sphere still showed the effects of pressure equilization.

By 2 milliseconds (Figure 3.3) there were no longer any qualitative differences between the DEWFALL and Chart D results. At the diffusion front the two methods are in excellent agreement.

However, by 5 milliseconds the predictions deviated. Figure 3.5 shows that DEWFALL has a much steeper temperature gradient and predicts significantly higher temperatures in the liquid aluminum.

The difference between the two predictions is associated with the innermost aluminum zone in Chart D. Between two and five milliseconds, Chart D lowered the energy in the interior gases by 30 GJ, consistent with the flux reported at the material boundary. In the same period, the interior aluminum zones gained 10 GJ, which is consistent with the flux at the outside of the innermost aluminum zone. It appears that the remaining 20 GJ should be in the innermost aluminum zone, but that zone only gained 14 GJ; Chart D reported a 6 GJ error in energy conservation during this period.

An energy sink at the material interface would account for the lower Chart D temperatures that appear in Figure 3.5. However, the behavior in this region is so complex that no conclusions should be drawn without further examination by Chart D experts.

Aluminum Reference Calculation

DEWFALL vs CHARTD at 1.1 ms.

Figure 3.3 Temperature Profile, Reference Calculation #1, 1.1 ms.

Aluminum Reference Calculation

DEWFALL vs CHARTD at 2 ms.

Figure 3.4 Temperature Profile, Reference Calculation #1, 2 ms.

Aluminum Reference Calculation

DEWFALL vs CHARTD at 5 ms.

Figure 3.5 Temperature Profile, Reference Calculation #1, 5 ms.

3.2.2 Evaporation/Condensation

The vapor mass (Figure 3.6) reached 22 Mg after 1.7 seconds. This came from vaporization of a 3.2-mm layer of aluminum.

The model requires a minimum of 8.4 MJ/kg to vaporize room-temperature aluminum, including the 5.6 MJ/kg heat of vaporization. The source could vaporize at most 50 Mg of aluminum. The calculated peak is 44% of this maximum.

When this calculation was stopped, at 2.0 seconds, the interior had not yet cooled to the vaporization temperature of aluminum. Therefore no interior condensation had occurred.

3.2.3 Vapor Energy Removal

The anomalies in the vapor energy plots (Figure 3.7) can be traced to the problems in the DEWPOST approximation that were described in Section 2.2.2. A correct summary of the DEWFALL output would show the energy decaying smoothly to 170 GJ, matching Reference Calculation #2 at 2 seconds.

3.2.4 Pressure History

The pressure dropped (Figure 3.8) from 7.08 MPa at 1.01 milliseconds to 2.67 MPa after one second and 1.22 MPa at two seconds. Although the starting and ending pressures were in good agreement with Reference Calculation #2, the one-second pressure with the aluminum was 50% larger than the one-second pressure with no liner.

The aluminum maintained an opaque energy containment layer nearly one second longer than the unlined container. Figures 3.9 and 3.10 show the aluminum becoming transparent between 1.5 and 1.6 seconds.

The ANEOS model for aluminum (Figure 3.11) lets the vapor become relatively transparent below 0.6 eV. The dominant factor is the ionization potential,

DEMIFILL (Unverified Prototype)

Scorab Case - 100 ton steel vessel ($r=1434$ $d=20$)

Figure 3.6 Ablation History, Reference Calculation #1.

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DEWFALL (Unverified Prototype)

Scarb Case - 100 ton steel vessel (r=1434 d=20)

Figure 3.7 Energy Containment, Reference Calculation #1.

DIFFILL (Unverified Prototype)

Scarab Case - 100 ton steel vessel ($r=1434$ $d=20$)

Figure 3.8 Pressure History, Reference Calculation #1.

DEWFALL (Unverified Prototype)

Scarab Case - 100 ton steel vessel (r=1434 d=20)

Time = 1.50×10^0 seconds

Figure 3.9 Temperature Profile, Reference Calculation #1, 1.5 ms.

DEWFALL (Unverified Prototype)

Scrab Case - 100 ton steel vessel (r=1434 d=20)

Time = 1.60×10^0 seconds

Figure 3.10 Temperature Profile, Reference Calculation #2, 1.6 s.

Figure 3.11 ANOES Opacity Model for Aluminum.

which is 6.0 eV for aluminum as compared with 6.8 eV for the chromium component of the steel and larger values for its other constituents.

3.2.5 Melt Growth

The predicted conduction in the aluminum is exaggerated by the inadvertent inclusion of thermal conduction in the ANEOS opacity in addition to the explicit model in DEWFALL.

By 0.3 seconds, all ten millimeters of aluminum had melted (Figure 3.12). It took another 0.4 seconds for the interface temperature to reach the steel melting point so that the liquid mass could increase again.

The steel integration grid, starting with a 0.7-mm element having the mass of a 2-mm aluminum element, was too coarse to track the motion of the melt line. The increase in liquid mass at about 1.0 seconds represents the melting of that one element.

At the end of the calculation, about 0.8 millimeter of steel had melted.

3.2.6 Wall Heating

Figure 3.13 is a temperature profile in the wall at 2.0 seconds. There is a discontinuity in temperature gradient at the material interface to compensate for the discontinuity in conductivities.

3.3 CONCLUSIONS

Comparison with Chart D predictions suggests a problem in Chart D. That software appears to have significant numerical energy losses in a region of complex material response.

The DEWFALL predictions of heat transfer in the condensed region are distorted by inadvertently high conductivity in the aluminum and the relatively coarse zoning at the metal-metal interface.

DEWFALL (Unverified Prototype)

Scarab Case - 100 ton steel vessel (r=1434 d=20)

Figure 3.12 Melt Growth, Reference Calculation #1.

DEWFALL (Unverified Prototype)

Scarb Case - 100 ton steel vessel (r=1434 d=20)

Time = 2.00×10^0 seconds

Figure 3.13 Two-Second Wall Temperature, Reference Calculation #1.

There was no interior condensation in Reference Calculation #1 during the first two seconds. If the time of interior condensation scales with the time that the metal vapor becomes transparent, then interior condensation would be expected at 2.2 seconds.

It appears that the aluminum liner lowered the effective radiating temperature from 0.7 to 0.6 eV, which lowered the radiative flux by nearly a factor of two. This accounts, at least qualitatively, for the longer time scale in Reference Calculation #1.

Inasmuch as the differences between the two calculations are all explainable by the presence or absence of the aluminum liner, it appears that the simple initial conditions are adequate. The long CHART-D calculation and the conversion of CHART-D output to DEWFALL input may not be necessary. This should be verified by repeating Reference Calculation #1 with simple initial conditions.

The time scale for heat transfer out of the vapor is sensitive to details of the optical behavior of liner vapor. Using the ANEOS model, the time scale may vary inversely with the fourth power of the ionization potential. However, the ANEOS model is not expected to be accurate at temperatures near the boiling point.

In conclusion, the DEWFALL heat transfer model appears satisfactory, even with crude initial conditions. However, the ANEOS model is being used outside of its range of validity; it should be checked against more detailed EOS calculations and experimental data. Finally, the input should be altered, both to provide better material parameters and to refine the integration grid in the region of interest.