Los Alamos Technical Associates, Inc.

Water-Molten Uranium Hazard Analysis

LATA Report No. 92

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NOTICE

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1.0 SUMMARY

The Los Alamos Technical Associates, Inc. (LATA) has investigated the hazard potential of cooling water leakage into the crucible of molten uranium in the MARS laser isotope separation experiment. The findings of this investigation are contained in this report.

1.1 Objectives

The primary objective of this investigation is to answer the question, "What is the significance of the hazard of a cooling water leak into the molten uranium?"

Specific objectives are to:

1. assess the likelihood of a liquid-liquid (vapor-phase) explosion resulting from a cooling water injection into or onto the molten uranium or resulting from molten uranium falling into water that has collected in the bottom of the vacuum vessel;

2. determine the severity of postulated H_2O-molten uranium accidents;

3. investigate the vulnerability of the proposed vacuum containment vessel; and

4. formulate design and operational recommendations to facilitate safe operations for MARS.

1.2 Summary of Approach

The approach taken on this investigation was to:

1. review and synthesize the pertinent literature on molten metal/water hazards;

2. discuss the postulated accidents with experienced foundry personnel, laboratory researchers, designers of explosion containment vessels, and recognized experts on liquid-liquid explosions (more commonly called vapor-phase explosions);

3. review experimental data and actual accidents that have occurred in both industry and research laboratories;

4. synthesize all pertinent information and perform a hazard assessment for MARS;

5. investigate the vulnerability of the postulated vacuum containment vessel, assuming a worst case and the maximum credible accident, if the H_2O-molten uranium mixing does result in a vapor-phase explosion; and

6. apply engineering judgment to draw conclusions from the investigation and make design and operational recommendations.

1.3 Current Status

This final report documents the findings of this investigation and constitutes the final deliverable under the current level-of-effort contract. There are several issues remaining before a design package can be completed and operational procedures finalized. One task remaining is to define the peak internal pressure over all portions of the vacuum vessel. A second task is to determine if internal vessel components present a shrapnel or missile hazard under the conditions of the operating basis accident (OBA). These issues can be resolved in a timely fashion through a combination of in-house and contracted efforts.

The unique circumstances of the postulated MARS accident scenarios made it advisable to consult experts for the current investigation. Consequently, Drs. Hans Fauske and Robert Henry of

Fauske, Grolmes, Henry & Theofanous, Ltd., were employed as subcontractors to define the accident likelihood and the energy release source terms. Their final report is included in its original form as Appendix A. After the energy release was defined, the LATA project team performed the necessary thermodynamic and compressible flow gas dynamic calculations to derive the resultant pressure loading on the vacuum vessel walls. LATA has analyzed the vacuum vessel vulnerability to this pressure loading by performing a preliminary stress analysis. These results were compared to American Society of Mechanical Engineers (ASME), Section VIII design criteria. Concurrently, a hazard analysis was being performed to put the postulated accidents into perspective. This analysis considered the credible hazards and consequences associated with the postulated accidents.

1.4 Conclusion Highlights

1. The necessary conditions for a vapor-phase explosion are not fully met in any of the scenarios defined for MARS, i.e., a vapor-phase explosion is highly unlikely. The chief factors that act to reduce the likelihood of a vapor-phase explosion in this instance are as follows:

    a. the very high temperature of the molten uranium;

    b. the very high solidification temperature of the uranium;

    c. water into molten metal is much less of a hazard than is molten metal into water;

    d. the vacuum environment; and

    e. lack of essential explosion trigger mechanisms.

2. Based upon practical experience and experimental simulation, the MARS U-H_2O configuration would require an external trigger to achieve a significant explosion probability; however, no such trigger is present in the design as planned.

3. If water should leak into or onto the uranium melt, it is highly likely that some uranium will be blown or splashed out of the crucible. This presents (1) a potential burn-through hazard in the bottom of the vacuum vessel, and (2) a potential vapor-phase explosion hazard if molten uranium traps water against the vessel wall.

4. To conduct a worst-case safety analysis, the probability of a water leak and a violent reaction is taken as unity. On this premise, conclusions of the analysis are summarized as follows:

   a. for the OBA, the gas pressure transient experienced by the vessel wall is 544 psia peak pressure with a duration of 200 μs;

   b. the OBA would result in a peak hoop stress of about 20,000 psi in a 1/2-in. thick vessel wall -- this is well below the material yield stress.

1.5 Recommendations

The following list of recommendations is the result of the LATA hazard analysis of the postulated molten uranium-cooling water accidents for the current MARS configuration. These recommendations are categorized between hardware design and procedures.

1.5.1 Design Recommendations - Personnel Safety

1. The vacuum vessel should be designed to sustain a worst-case short-term transient pressure loading of 500 psia peak gas pressure, with a total impulse of 0.05 psi-sec.* It should be able to sustain this OBA loading without rupture; however, it is judged to accept plastic deformation and other permanent damage for this extremely rare occurrence.

2. The MARS system should be designed to sustain a worst-case static pressure build-up of 75 psia in 48 sec resulting from the slow steam generation as water cools the uranium; a pressure relief valve may be used.

3. Design considerations should be given to minimizing the hazard of blast-driven fragments and missiles from internal system components.

4. Protection should be provided from a molten uranium splash-out, which could damage the vessel wall and various pipes, ducts, conduits, electrical cables, etc. Figure 1-1 illustrates conceptual design modifications to the MARS vacuum vessel.

1.5.2 Design Recommendations - Hazard Reduction

1. The utility of including a vacuum vessel internal pressure relief valve is subject to debate. From an explosion point-of-view, a relief valve (in the near vicinity of the explosion) would not be advised. However, a valve to relieve a quasistatic or static pressure would be advisable to protect other systems components that would be sensitive to static pressure, e.g., the vacuum pumps. In addition, it is

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* LATA is currently conducting more detailed gas dynamics calculations in the project's second phase to refine this conservative pressure loading.

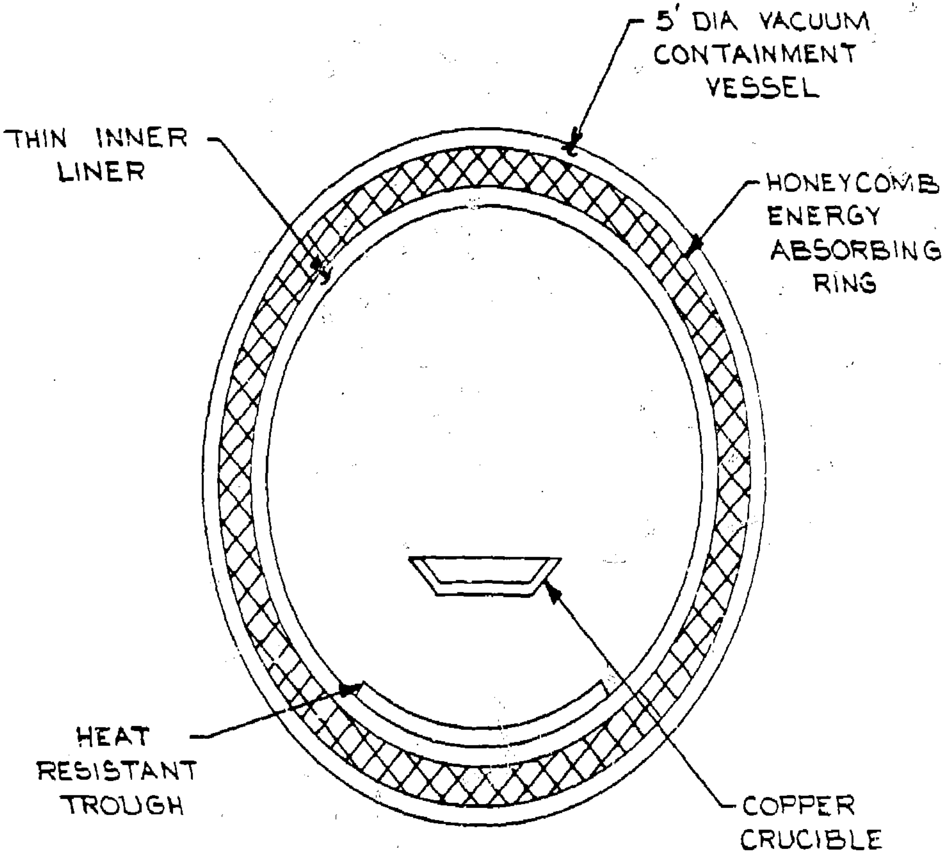


Figure 1-1. Cross section of vacuum vessel showing recommended design changes.

psychologically attractive to have a relief valve in any pressure system. If such a valve is deemed advisable, it should be designed to relieve the slow steam build-up.

2. Techniques to minimize the quantity of injected water are recommended, because more water increases the explosion magnitude and internal pressure hazard.

3. A porous, heat-resistant trough or shield is recommended to be placed beneath the crucible. It should allow water to pass through but should stop any splashed out molten uranium. This would eliminate the hazard of a vapor-phase explosion possibly caused by the uranium falling into trapped water following a cooling water failure.

1.5.3 Procedural Recommendations - Hazard Reduction

1. Concerning the slow steam generation, the roughing pumps will greatly reduce the slow build-up of internal pressure; however, this steam may damage the pumps. The vessel can easily withstand the expected internal pressure; therefore, it is recommended that the pumps not be operated if a water leak occurs.

2. A pressure (vacuum) sensor should be provided to (1) shut down the E-beam source, and (2) sound an alarm if the internal pressure exceeds an abnormal operating pressure, such as 10^{-3} torr. Even though the E-beam will likely shut down when the hard vacuum is lost, the electrical potential should be eliminated.

3. Procedures should be established to minimize the flow of water once a leak has occurred; in all cases a small water quantity is preferable. A slow leak may be difficult to detect; however, the presence of steam may be the most likely indicator.

4. When the uranium is in a molten state, personnel involvement near the MARS vacuum vessel should be minimized, or the system should be operated remotely.

2.0 INTRODUCTION

It has been known for years that the contact between hot and cold liquids can produce violent interactions in the general category of liquid-liquid explosions, more commonly called vapor-phase explosions. A vapor-phase explosion occurs when the vapor produced cannot be relieved quickly enough to prevent pressurization and the formation of shock waves. Some examples of these interactions are shown in Table 2-1[1].

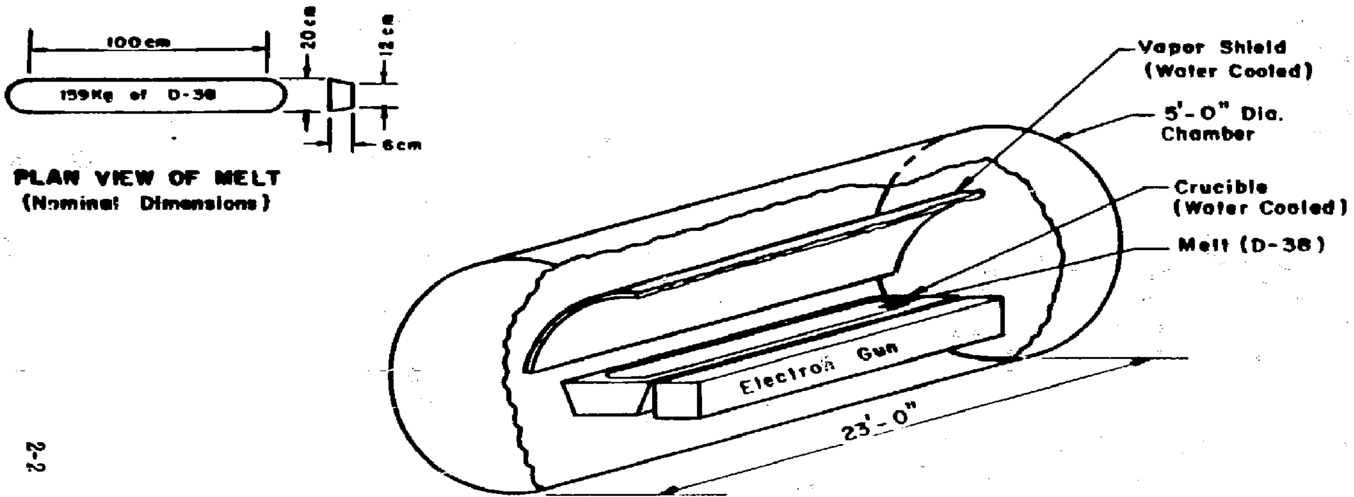
TABLE 2-1

EXAMPLES OF VAPOR-PHASE EXPLOSIONS[1]

Area	Hot Fluid	Cold Fluid
Reactors (SPERT-1, SL-1, BORAX-1)	Aluminum	Water
Steel Industry	Steel	Water
Aluminum Industry	Aluminum	Water
Kraft Paper Industry	Smelt (Na_2CO_3 + Na_2S)	Water
Liquid Natural Gas (LNG) Industry	Water	LNG
Volcanic Eruptions	Lava	Water

2.1 Background

The MARS experiment is a part of the demonstration of feasibility for Lawrence Livermore Laboratory's (LLL's) laser isotope separation technique. The experimental setup consists of molten uranium heated by an electron beam as shown in Figure 2-1. The molten natural uranium or depleted uranium is contained in an open copper crucible that is water cooled and mounted in a vacuum chamber. The vapor shield surrounding the crucible is also water cooled. The purpose of this study is to evaluate the likelihood and severity of an accidental uranium-cooling water interaction.



OPERATING CONDITIONS

1. **Chamber Pressure ~ 10^{-6} Torr**
2. **Crucible Cooling ~150gpm @ 80psi**
3. **Vapor Shield Cooling ~80 gpm @ 80psi**
4. **Electron Gun Cooling ~40 gpm @ 80psi**

Figure 2-1. Chamber/source configuration.

2.2 Statement of Problem

The temperature of the molten uranium in the crucible (2,000 ± 500°C) is well above the melting point of uranium (2,500° C was used to be conservative). In the event of a crucible water line failure or a vapor shield water line failure, water could be (1) injected into the uranium, (2) sprayed onto the uranium from above, or (3) molten uranium could be splashed out of the crucible, as the result of circumstances (1) or (2), and fall into water that has collected in the bottom of the vacuum vessel. A reaction between the uranium and water could theoretically result in an explosion that could possibly damage the equipment, breach the vacuum confinement, and spread some radioactive contamination to other areas of the building. In the past, this type of explosion, from much larger systems, in the foundry industry has damaged buildings and injured people. The problem here is to ascertain the likelihood of such an explosion and the extent of the damage that might result.

The cooling system failure scenarios are summarized in Table 2-2, in the order of likelihood mutually agreed upon between LLL and LATA.

Detailed accident scenarios for MARS are discussed later in Subsection 4.1. Detailed, worst-case analyses of these unlikely accidents are provided in Section 5.0, with a very conservative approach taken in all cases.

TABLE 2-2

COOLING FAILURE SCENARIOS

Scenario for U/H_2O Contact	Result	Order of Likelihood
1. Failure of primary cooling water system and electrical power systems	Same as No. 2.	1
2. Crucible coolant boiling	Melt through and water injection at 4 gpm for 1 to 3-1/4 in tubes (12 gpm total). Velocity of 10 to 15 ft/sec. E-beam shuts down, cooling water continues to flow.	2
3. Crucible coolant boiling	Same as No. 2 except water shuts off within 10 sec. Maximum water input is 2 gal.	3
4. Failure of overhead cooling line	Ejects up to 10 gal onto surface of molten uranium. Cooling water and E-beam shutdown.	4
5. Crack in crucible	High-velocity water jet injects 0.1 gpm into molten uranium. E-beam shuts down, water does not.	5

REFERENCES FOR SECTION 2.0

1. Hans K. Fauske, "Some Aspects of Liquid-Liquid Heat Transfer and Explosive Boiling." Proceedings Fast Reactor Safety, USAEC CONF-740401-P2, (1974).

3.0 VAPOR-PHASE EXPLOSIONS

The contact of a hot and a cold liquid can sometimes produce a rapid thermal interaction in which a significant fraction of the thermal energy of the hot liquid is converted to mechanical work. This thermal interaction is usually called a vapor-phase explosion. Although the foundry industry has been aware of these interactions for years, the precise details of the phenomenon are still unknown. One of the liquids must be significantly above the boiling temperature of the other liquid in order to lead to vapor formation on a millisecond time scale. Another prerequisite for a vapor-phase explosion is destabilization of film boiling, leading to large area liquid-liquid contact. Other details of the physical processes involved depend on the nature of the two liquids and are bound up in theories that will be discussed in the following section.

3.1 Theory

The physics of vapor-phase explosions is not precisely understood, although many theories have been advanced. These explosions are thought to result from the sudden conversion of liquid to vapor and are thus physical rather than chemical reactions. In order to produce vapor in the short time period required for shock generation, the hot and cold liquids must be in intimate contact over large areas. The condition of film boiling between two liquids does not fulfill this condition: the heat transfer rates are orders of magnitude below those required for a thermal explosion. Thus, it is generally believed that fragmentation of the hot liquid (molten uranium in this case) must be achieved in order to produce intimate contact over large surface areas resulting in increased heat transfer. A number of concepts have been proposed for the fragmentation mechanism. Experiments have shown that several of these mechanisms may be operable in different physical situations. All of these theories are difficult to verify experimentally because of the short time scale of the mixing process ($<10^{-4}$ sec). Some of the fragmentation theories (triggering mechanisms) follow.

Violent Boiling Theory - This hypothesis states that the fragmentation is vapor induced by the violent boiling behavior of the cold liquid. The theories of Board[1] and Fauske[2] fall under this heading. Three basic processes have been identified for violent boiling fragmentation.[3]

In the first process, the highly superheated cool liquid vaporizes so quickly that an energetic high-pressure pulse is generated and fragments the hot liquid. This high superheating is caused almost instantaneously because the liquid-liquid direct contact temperature is close to the homogeneous nucleation temperature. This is the spontaneous nucleation criterion of Fauske and will be discussed in more detail in Subsection 3.1.2.

The second process is fragmentation caused by vapor film collapse or bubble growth and collapse. During the collapse, coolant microjets are produced with sufficient kinetic energy to produce fragmentation of the hot liquid directly.[4]

In an extension of the second process, the microjets (discussed for process two) have sufficient energy to penetrate into the hot liquid leading to dispersion and entrainment of coolant.[5] Further fragmentation is then induced by spontaneous nucleation.

Entrapment Hypothesis - When a layer of cool liquid is trapped between a hot molten material and a solid surface or wall, vapor may be produced quickly enough to cause a thermal explosion. Long[6] demonstrated this by dumping large quantities of liquid aluminum into water. In these experiments, it was determined that the wall played an essential role in the initiation of explosive events, since violent explosions were observed when bare metal or rusted containers were used for the water (aluminum was poured into the water) and no explosions were witnessed when the wall was painted or covered with grease. It was theorized that the bare metal surface was well wetted by the water and that this permitted some water to be entrapped by the aluminum. This entrapped water expanded rapidly and provided the trigger for the explosion. When the wall was greased or painted, the water no longer wetted the surface and the cascading aluminum merely pushed the water aside as it approached the wall, i.e., no trigger was available. The mechanism is illustrated in Figure 3-1.

Liquid Entrainment Hypothesis - In this theory, cold liquid trapped inside a molten mass of metal produces steam and a pressure pulse causing fragmentation of the metal drop and subsequent thermal explosion.[7] The experiments of Flory et al.[8] with lead support this liquid entrainment theory. A Helmholtz instability was postulated as a mechanism for enclosing a small amount of liquid water in the metal drop. The water then instantly vaporizes, driving the enclosing metal outward. This would cause fragmentation of the metal and an explosion under the right temperature conditions (spontaneous nucleation temperature).

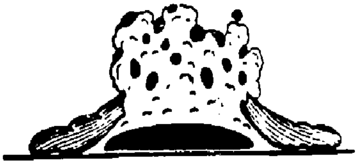
Shrinking Shell Hypothesis - This theory postulates that the pressure from the shrinking of solidifying outer layers of a molten drop causes bursting of the drop and, hence, fragmentation. However, experiments with bismuth, which expands upon freezing, show a fragmentation similar to that of contracting metals such as tin and lead.[8] This theory has been discounted for the most part, but is similar to the next theory that will be discussed.

Local Stress Theory - This theory states that, when the molten metal reaches its temperature of solidification, the sharp change in crystal structure produces stresses that cause fragmentation and subsequent thermal explosion. Stress-induced fragmentation by the rapid solidification of hot material has been demonstrated by the rapid cooling of Al_2O_3 in an argon atmosphere.[9] The model has been further developed by Zyszkowski.[10,11]

Chemical Reaction Theory - Free hydrogen is released from water during its chemical reaction with hot molten metal. An explosion or explosive fragmentation could result upon recombination with oxygen. Kinetic calculations have shown that hydrogen production could not be

(A) WATER IS TRAPPED,

(B) BOILING BEGINS,



(C) STEAM EXPANDS.

Figure 3-1. Entrapment mechanism.

responsible for the extent of fragmentation. Thus chemical reactions are not thought to be responsible for vapor-phase explosions.

Hydrodynamic Fragmentation Hypothesis - Hydrodynamic fragmentation is caused by the nonuniformity of forces resisting the motion of a deformable body in a fluid.[12,13] This has been demonstrated by the fragmentation of mercury in water under isothermal conditions. This theory is similar to the liquid entrainment hypothesis.

Impact Fragmentation - An impact or an externally applied shock can cause vapor film collapse with intimate liquid-liquid contact. Spontaneous nucleation then leads to a vapor-phase explosion.[14] In experiments by Wright,[15] a column of water, held in a tube, impacted upon a hot metal at the bottom of the tube and produced fragmentation. Other experiments demonstrated that vigorous interactions were observed only when artificially induced pressure transients were applied. This resulted in pressures significantly higher than those applied.[16]

3.1.1 Liquid-Liquid Heat Transfer

For the familiar water boiling case (solid-liquid heat transfer), there are basically three heat transfer regimes: pure convection, nucleate boiling, and stable film boiling. In addition, the so-called transition boiling regime separates the nucleate and film boiling regimes. This is shown in Figure 3-2. In the nucleate boiling regime, vapor bubbles form and grow on a number of favored sites or imperfections on the solid heating surface. The formation of these bubbles forces hot liquid from the vicinity of the surface into the colder bulk of the cooler liquid. In addition to this liquid-vapor exchange action, microconvection currents are set up as vapor bubbles are emitted from the nucleation sites and colder liquid rushes to the hot, solid surface to fill the void. When the excess temperature is raised to a certain point, the heat flux reaches a maximum. The maximum heat flux occurs at the critical excess temperature of the cool liquid. A further increase in temperature then causes a decrease in the heat flow rate, and this is called the transition region.

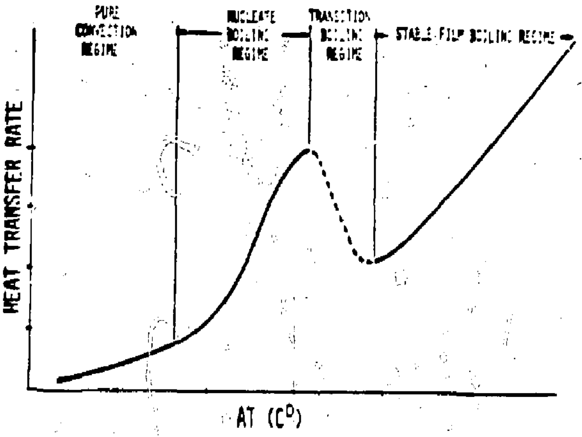


Figure 3-2. Typical boiling curve where ΔT is the excess temperature above boiling point.

As the critical excess temperature is reached, the number of sites at which bubbles form is increased and the number of vapor columns increases. The limit to the number of vapor columns that can be accommodated is reached when the space between these columns is no longer sufficient to accommodate the streams of liquid that must move toward the hot surface to replace the liquid that evaporated to form the columns. In the transition boiling regime, nucleate and stable film boiling occur alternately. In the stable film boiling regime, a vapor film blankets the hot solid surface.

In the liquid-liquid system, there are no surface imperfections and the nucleate boiling regime does not exist. Instead there is homogenous nucleation heat transfer. The nucleation is a result of density fluctuations rather than nucleation from preexisting nucleation sites. All three heat transfer regimes can exist in a liquid-liquid system simultaneously, that is, the convective, homogeneous nucleation, and film boiling regimes. These are shown in Figure 3-3. Of particular interest is the homogeneous nucleation regime, because the vapor generation rate is sufficiently fast to produce shock waves. In this regime, gas is not trapped at the interface and direct liquid-liquid contact is made.

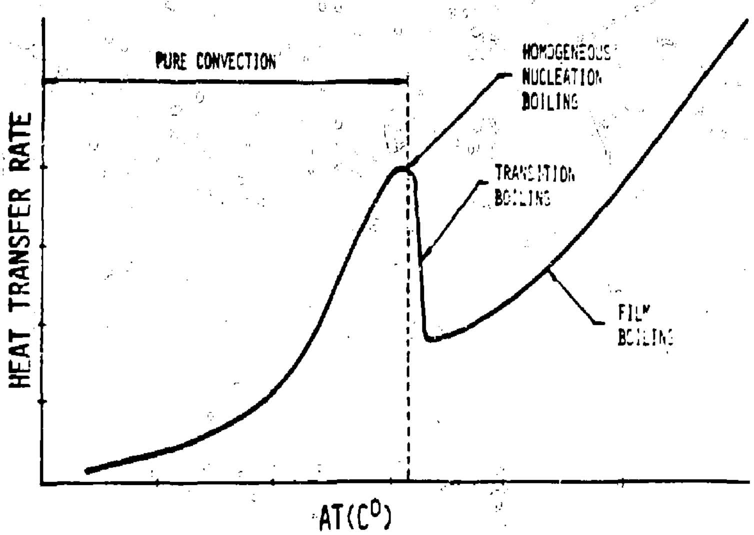


Figure 3-3. Liquid-liquid boiling curve.

It can be noted from Figure 3-3 that the transition from homogeneous nucleation to film boiling is quite sharp. The most violent boiling exists around the transition region. Imagine the contact of two liquids in which one liquid is extremely hot. The conditions initially favor film boiling on the right of the curve. The two liquids are separated from each other by a layer of vapor from the cool liquid. As the hot liquid cools, the temperature difference between the two liquids decreases and the heat transfer rate decreases, moving left along the curve. As the temperature approaches the transition region, the vapor film becomes unstable and collapses, allowing contact between the two liquids. The transition regime (and increased heat transfer) continues until conditions allow homogeneous nucleation boiling. Homogeneous nucleation is a bulk effect in which vapor is formed spontaneously throughout the superheated liquid. As stated before, the nucleation is a result of density fluctuations and does not depend on preexisting nucleation sites. For the uranium-water system the heat transfer process over the entire molten uranium range will be film boiling. The transition region will be reached only after the uranium is in the solid phase.

3.1.2 Interface Temperature, Spontaneous Nucleation Model

It is interesting to pursue this theory in more detail because it adds to the list of necessary, but not sufficient, conditions that have been compiled for vapor-phase explosions. Also this theory, of all those reviewed, seems to apply best to the case at hand--the MARS experiment. Two of the necessary conditions have already been discussed: (1) two liquids, one at a temperature higher than the boiling point of the colder liquid, must come into contact, and (2) the contact must be intimate. The spontaneous nucleation model says that the hot liquid temperature, and, thus, the interface temperature between the liquids, must be greater than some minimum value. In fact, a definite temperature threshold, below which no explosive interactions occur, has been observed in many experiments.[14, 17]

The spontaneous nucleation model requires that the interface temperature upon contact between two liquids be greater than or equal to the spontaneous nucleation temperature of the liquid-liquid system. A further requirement is that the thermal boundary layer must be sufficiently thick to support a critical size vapor cavity. The frequency of formation of critical size vapor cavities is given by the classical equation for nucleation

$$J = \omega N_L \quad \exp \frac{W}{kT_s} \, f(\sigma) \qquad (3\text{-}1)$$

where

ω = constant $\cong 10^{10}$ sec^{-1}
N_L = number of molecules per unit volume of liquid
W = the reversible work of formation of the critical embryo from the liquid
k = Boltzman constant
T_s = spontaneous nucleation temperature

and

$f(\alpha)$ = a function dependent on the liquid-liquid contact angle α (measurement of interfacial tension as a function of time).

The variable J is the frequency of formation of nucleation sites per unit volume at a given temperature and pressure. The work of formation W is given by

$$W = \frac{16\pi\,\sigma^3}{3(P_v - P_\ell)^2} \tag{3-2}$$

where

σ = liquid surface tension
P_v = vapor pressure

and

P_ℓ = pressure in the cold liquid.

The value of T_s, the spontaneous nucleation temperature, can be estimated from the previous equation and is sometimes estimated as approximately 90% of the bulk homogeneous nucleation temperature.

Spontaneous nucleation is primarily a surface effect and describes the homogeneous or gas-free heterogenous nucleation that results from density fluctuations rather than nucleation from preferred sites. In either case, the critical size cavities, which initiate the vaporization process at or near the interface, are produced by these local density fluctuations within the cold liquid. For spontaneous nucleation with homogeneous conditions, the two liquids represent a well-wetted system, i.e., perfect surface contact with the vapor embryos produced entirely within the cold liquid. Spontaneous nucleation with heterogeneous conditions represents poor or imperfect wetting at the liquid-liquid interface. In this case, the critical size cavities are created at the interface with a somewhat lower temperature requirement. Perfect wetting implies $\alpha = 0$, which corresponds to $f(\alpha) = 1$. In this case, the spontaneous nucleation temperature corresponds to the homogeneous nucleation temperature of the cold fluid. The imperfect wetting case, heterogeneous nucleation, yields a spontaneous nucleation threshold somewhat below the homogeneous nucleation temperature of the bulk fluid. The two temperatures are not appreciably different, nowever, because the increase in nucleation sites in "impure" water is not great. Thus, spontaneous nucleation is a surface or interface boiling phenomenon that is similar in nature to the homogeneous nucleation of liquid-liquid heat transfer that is a bulk phenomenon in the cold liquid. In homogenous nucleation, the bulk liquid is superheated to a uniform temperature. In spontaneous nucleation, a thin region of liquid at the interface is superheated on a very short time scale.

It is important to note that spontaneous nucleation cannot proceed until a sufficiently thick thermal boundary layer has been developed to support vapor embryos of the critical size. The interface temperature can rise from the bulk temperature of the cold liquid to the spontaneous nucleation temperature in approximately 10^{-12} sec. The instantaneous interface temperature developed upon contact of two semi-infinite masses can be estimated by the following equation:

$$T_i = \frac{T_h + T_c(R)^{1/2}}{1 + R^{1/2}} \tag{3-3}$$

where

T_h = initial temperature of hot liquid
T_c = initial temperature of cold liquid
R = $\dfrac{k_c \rho_c C_c}{k_h \rho_h C_h}$
h = subscript representing hot liquid
c = subscript representing cold liquid
k = thermal conductivity
ρ = density

and

C = specific heat.

The spontaneous nucleation theory predicts a threshold condition that has been seen in a number of experiments and appears to be satisfied for all known occurrences of large-mass vapor-phase explosions.[17] This theory applies to the free-contacting mode (hot and cool liquid mixed) and not to vapor-phase explosion modes requiring solid surfaces or externally applied shock waves to inititate the explosion. In summary, the theory proposes the following necessary conditions:

1. initial stable film boiling with a vapor film separating the two liquids,
2. liquid-liquid contact due to breakdown of the vapor film,
3. spontaneous nucleation upon contact, which implies $T_i \geq T_s$ for a thermal boundary layer of adequate thickness to support formation of vapor embryos of critical size, and
4. adequate physical and inertial constraints to sustain a shock wave.

The theory also predicts a high-temperature cutoff for the free-contacting mode near the thermodynamic critical temperature. This is because the system pressure must be sufficiently low to allow explosive boiling processes on a significant size scale, i.e., 1.0 MPa or less for a system in which water is the exploding fluid. Thus, for high pressures at very high interface temperatures, the theory eliminates explosive interactions. Experiments thus far have shown that no large-scale vapor-phase explosions occur when the interface temperature exceeds the thermodynamic critical temperature. For example, the spontaneous nucleation model predicts that the liquid aluminum-water system is not explosive in the free-contact mode.

Experiments have shown that violent explosions were observed only when the molten aluminum reached the bottom bare metal or rusted surface of the water container. No explosions were produced if the walls were painted or covered with grease, indicating that the well-wetted, cool solid surface produced the water entrapment and explosion triggering mechanism. Aluminum-water shock tube experiments also produced explosions, but again no explosive interactions have been witnessed for aluminum-water systems in the free-contacting mode.

3.2 Experimental Evidence and Incidents

In an effort to develop general background information, data were sought from incidents involving molten uranium/water events occurring under conditions similar to those possible in the MARS experiment. While these events are rather rare, there have been instances at the EBI E-beam source at the Oak Ridge Y-12 facility in which cooling water was accidently injected into molten uranium. Only slow steam generation resulted, and no explosions occurred. A meeting was held with knowledgeable Union Carbide employees to discuss the circumstances surrounding three specific events that occurred over the last 20 yr.[18]

The first event occurred when cooling water was injected through a failed cooling water tube into approximately 60 kg of molten uranium metal. At the time of the cooling tube failure, the vessel was operating in a 1.5 x 10^{-5} torr environment. Sufficient steam was generated to cause approximately 26 kg of liquid metal to be ejected from the crucible and to cause the pressure within the containment system to rise to a pressure of 1 x 10^{-3} torr. At this pressure, the roughing vacuum pumps were automatically activated and no further pressure rise was noted.

A second and similar event involved approximately 180 kg of molten uranium metal. The results were essentially those of the first event, with the exception that the pressure appeared to have reached a slightly positive gage pressure (less than 1/2 atmosphere). While no actual pressure measurements are available, a pressure relief plate showed evidence of having shifted its position slightly, but permitted none of the contents of the vacuum chamber to escape. The pressure plate has been sealed with a spring force equaling a static equivalent pressure of 7 lb/sq. in.

The third event occurred with approximately 10 kg of molten uranium metal and 4.5 kg of water. This event caused a failure of the exterior vacuum vessel and was estimated to have generated an internal static equivalent pressure in excess of 100 psi in a vacuum chamber volume of approximately 25 cubic ft. Of the three, this is the only incident to occur in a vessel with no pressure relief mechanism.

In the Oak Ridge Y-12 incidences, there was no evidence that vessels were damaged by uranium metal particles ejected by the generated steam, or any proof that a significant shock wave was generated, as would be the case for a chemical or tamped steam explosion. In each case, it appears that a slow heat exchange and steam generation mechanism were totally responsible for the pressures involved, with very inefficient energy conversion.

There are numerous arc furnaces and electron beam facilities in production use by the foundry metals industry. These installations are significantly similar to the MARS equipment; however, they are used to process Ni, Ta, Ti, Cb, Mo and other refractory metals.[19] Categorically, the safety record with these facilities has been excellent. Conversations with furnace operators indicate that they have experienced incidences of cooling water leaks into the melts resulting in only a slow steam generation, not vapor-phase explosions. One facility is particularly similar to MARS. This is the 1,200 KW electron beam furnace operated by Viking Metallurgical Corporation in Verdi, Nevada. This facility is used to produce ingots of titanium 18 in. by 9 ft. They periodically have cooling water leaks into the melt but have never had a vapor-phase explosion.[20] In fact the occurrence of a water leak is only looked upon as an operational inconvenience and a hazard only to the diffusion pumps.

While this limited experience is not the basis upon which future accident predictions can or should be made, it is presented here as an example of specific events to provide some experience basis from which criteria developed for the MARS vessel may be judged.

3.3 Application to the MARS Experiment

After researching the subject of vapor-phase explosions with respect to theory, experimental evidence, and history of accidents. LATA, and its subcontractor FGH&T, Ltd., conclude that the potential for a vapor-phase explosion in the event of a cooling system failure in the MARS experiment is extremely unlikely. However improbable, it cannot be categorically ruled out due to the complicated nature of the interaction. This section will discuss the important mixing parameters identified by LLL in the statement of work and will then address the probability of a vapor-phase explosion in this setting based upon the theory and evidence presented in the previous sections.

3.3.1 Vacuum Environment

The vacuum environment affects a possible vapor-phase explosion in two ways. First, the lack of atmospheric pressure causes water injected from the vapor shield cooling system above the crucible to flash to steam. This would reduce the probability of a water-molten uranium interaction. Water injected onto the melt surface presents a less hazardous situation. This is particularly true in the absence of an identifiable triggering mechanism.

The second way in which the vacuum affects the potential accident is the manner in which the shock wave is produced and the resulting characteristics of the shock loading on the pressure vessel wall. If a vapor-phase explosion occurs in a hard vacuum, it is a shockless explosion with pressure profile defined by

$$P(r) = K \rho^{\gamma}\left(1 - \frac{r^2}{R^2}\right) \frac{\gamma}{\gamma-1} \tag{3-4}$$

The *equation variables will be defined in Section 5.0; nevertheless,* this means that the highest pressure is at the center and lowest at the gas cloud front; this is the opposite of the pressure profile for an explosion in a shock supportive medium such as air or steam. The net result of the vacuum is to reduce the damage potential to the containment walls.

3.3.2 Crucible Geometry

With the size of this crucible, the crucible geometry does not play a significant part in the development of an accident scenario in this situation. Its only relevance is the quantity of uranium that it holds. Higher crucible walls would reduce the amount of uranium that would be splashed out or blown out with the injection of water. However, a very confining geometry would increase the potential of a vapor-phase explosion and increase the chance of exploding such a crucible into potentially damaging fragments.

If the crucible system was designed to include a solid material (e.g., graphite) between the copper and the uranium melt, the vapor-phase explosion hazard would be reduced. The cold liquid must come in contact with the hot liquid and, if a solid liner were present, the water would more likely be converted to steam before it could reach the uranium.

3.3.3 Temperature of Uranium

The temperature of uranium is extremely important in this system. Its high temperatures from initial melt to the postulated operating temperature suggest an extremely small potential for producing an explosive reaction with water. This would also tend to make the uranium/crucible interface temperature high enough that appreciable crucible wall wetting from injected water could not occur, thus reducing potential for the entrapment mechanism.

The interface temperature between the uranium and water must be greater than the spontaneous nucleation temperature of the system. Considering the high initial temperature of the uranium metal, as well as the high thermal conductivity, the contact interface temperature is not only above the homogeneous nucleation limit, but it is far greater than the thermodynamic critical temperature of the water. Experiments utilizing a free-contacting mode (no external trigger) and with no potential for chemical interaction have shown that large-scale explosions do not occur when the interface temperature exceeds the thermodynamic critical temperature (see Appendix A).

For the conditions of 16°C (60°F) water and molten uranium metal at 2,500°C, the interface temperature developed upon contact is 2,170°C, more than 3.5 times the thermodynamic critical temperature of the water (on an absolute temperature base). Even when the uranium cools to the freezing point, the interface temperature is still 1,000°C, or twice the critical temperature. Therefore, the uranium-water system satisfies the stable liquid-liquid film boiling criterion throughout the molten uranium temperature range. In light of the available data, these extremely high interface temperatures make a vapor-phase explosion in a free-contacting mode impossible and very unlikely even in the presence of an external trigger. Consequently, the probability of having a vapor-phase explosion with these two materials is small even if a cooling system failure should occur (see Appendix A).

The high solidification temperature and high thermal conductivity of the uranium are also advantageous because the water will quickly solidify the uranium in the vicinity of the water injection point. This will reduce the situation to one of film boiling and eliminate the vapor-phase explosion potential.

3.3.4 Quantity of Uranium

The quantity of uranium influences the problem in several ways. The mass of uranium determines the amount of water that can be turned into steam.

In the event of a vapor-phase explosion, the energy available to the explosion is a function of and approximately proportional to the heat or energy content of the uranium, which is proportional to the mass. For an energetic but nonexplosive interaction, the quantity of uranium splashed out of the crucible and onto the floor of the containment vessel will directly affect the possibility of melt-through or possible vapor-phase explosion by an entrapment mechanism if water has collected at the vessel bottom.

3.3.5 Temperature of Water

The temperature of the cooling water has a negligible effect on the present problem as specified; however, if higher temperature cooling water were used and a leak occured, it would more readily flash to steam in the vacuum environment. This would reduce the vapor-phase explosion hazard.

3.3.6 Quantity of Water

The quantity of water determines the ultimate steam pressures at the containment wall. It also influences the magnitude of a vapor-phase explosion and determines how much uranium can be splashed out of the crucible in the case of a less energetic boiling type interaction. As the quantity of water becomes very large, the hot metal is quenched, the vessel interior is cooled, the steam recondenses, and the pressure stabilizes to the vapor pressure of water at essentially room temperature, ($\sim$ 4 mm of Hg).

3.3.7 Uranium/Water Ratio

The ratio of hot metal to water or fuel to coolant is more important than the absolute quantities just discussed.

The amount of steam generation is proportional to the combined quantity of water and hot metal. For a fixed amount of water, the worst case is vaporization of all the water. This requires a mass ratio of about 5.6 kg of uranium and copper crucible to 1 kg of water. More hot metal will not increase the quantity of steam and will only slightly increase its pressure by superheating and retarding condensation.

Considering the postulated vapor-phase explosion and the specific energy levels for fuel and water (as derived in Appendix A), each gram of water requires 7.1 g of uranium metal for an optimum mixture. Since the constraint of how much can be mixed is determined by the volume of the crucible, this mass ratio should be cast as a volume ratio. Assuming a density of 16 g/cm^3 for molten uranium at 2,500°C and a density of unity for the water, the volume ratio is 0.44 cm^3 of metal per cubic centimeter of water or a water-to-metal volume ratio of 2.25. Therefore, the most energetic interaction would result from an intimate metal-water mixture in the crucible volume in which 70% of the volume was occupied by water. With the reference design, the crucible volume is approximately 10,000 cm^3, so an optimum interation would involve 7,000 cm^3 (7,000 g) of water and the resultant mechanical work could be 3 x 10^6 J. The remaining 3,000 cm^3 would be occupied by the 48 kg of molten metal that drives the interaction (reference analysis by Fauske and Henry in Appendix A).

For mixtures less than optimum, the likelihood and severity of a vapor-phase explosion will be less; however, a quantitative measure would require extensive computer simulation and probably a series of experiments.

3.3.8 Uranium/Water Density Ratio

From the vapor-phase explosion theory, it is not clear how this would affect the probability or the extent of an explosion. Water injected from above would tend to float on the surface of the uranium, possibly reducing the potential for any entrapment mechanism. We feel that a large density ratio, as in this case, helps keep the liquids separated and reduces the chance of entrapment and a vapor-phase explosion.

If the water is injected into the melt, a Rayleigh-Taylor instability could lead to intimate mixing and entrapment.

3.3.9 Water Entrapment in Uranium

Water entrapment does not appear to be a problem for the scenarios of water into or onto the uranium because of the extremely high temperature differential and the lack of an identifiable triggering mechanism. Most of the experimental and accidental vapor-phase explosions between molten metals and water occurs when the metal is poured into the water.

The bare-wall entrapment mechanism would not fit the conditions of a cooling line failure in the vapor shield since water would be sprayed on the molten uranium surface. In this configuration, a vapor-phase explosion is highly unlikely since only limited amounts of water could penetrate the molten metal and no trigger can be identified to initiate this interaction.

3.3.10 Injection of Water into Uranium

A subsurface release of water in the event of a cooling line rupture within the crucible would perhaps be the only mechanism by which one could approach explosive conditions. In this case, the wall is available, but it is at a temperature that is far greater than the value at which the water could wet the surface. The water could melt the wall only if the wall temperature is essentially less than the local boiling temperature. In this vacuum vessel case, this temperature would be quite low. Therefore, here again a wall-induced trigger and the resultant vapor-phase explosion would seem very improbable.

3.3.11 Molten Uranium into Water

Pouring molten uranium into a vat of water would have a higher probability of producing a vapor-phase explosion than is the case for water into the uranium. Several triggering mechanisms can be postulated for this case. The liquid entrainment theory postulates that, due to instabilities, a drop of uranium could surround and envelop some water as it passes to the bottom of the vat. This water would superheat and subsequently change to vapor, producing a pressure sufficient to fragment the uranium drop. This fragmentation and increased heat transfer could then produce the conditions for a vapor-phase explosion. Also a large mass of molten uranium could fall to the bottom of the vat and entrap a portion of the water wetting the bottom surface of the vat. The trapped water could produce steam on a time scale sufficient to cause high pressures, fragmentation, and subsequent explosion. This is the so-called liquid entrapment mechanism. In the sixth scenario of uranium splashing out of the crucible, the entrapment mechanism might be present if the vessel wall were wetted with sufficient water.

3.3.12 Pressure Transient in the Molten Uranium

An externally applied pressure wave can, in some instances, produce a vapor-phase explosion in a case where one would not normally be produced. Typically, this trigger pressure is on the order of 1 MPa. It is theorized that the pressure overcomes the resistance of the vapor layer at the liquid-liquid interface, producing increased heat transfer and fragmentation, and a subsequent vapor-phase explosion. For the MARS experiment, it is difficult to see where such an initiating pulse could be generated for the accident in question, especially since the very low-pressure environment would not transmit such pulses efficiently.

3.3.13 Violent Boiling Theory

This theory appears to be the most applicable for MARS. Any of the three processes discussed under the violent boiling theory could possibly occur in this case. Even though the molten uranium temperature is above the spontaneous nucleation temperature of water, it is so far above it that intimate contact between the two liquids is unlikely. For instance, water injected from above would tend to be *held off the uranium by a vapor film much like a drop of water on a* hot stove (Leiden-Frost phenomena). Of course, this film boiling would occur only if all the water did not flash to steam. Any water injected from below would tend to float to the surface of the uranium because of density differences. The water would be surrounded by water vapor because of the extremely high uranium temperature. In both cases, benign film boiling appears likely. Only the presence of an externally applied pressure wave could possibly increase the probability of an explosive reaction. Even with film boiling, there is a good chance of a violent, but not explosive reaction, such as a pressure increase inside the vessel or significant splashing of uranium out of the crucible.

3.3.14 Entrapment Hypothesis

The bare wall entrapment mechanism would not fit the conditions of a cooling line failure in the vapor shield since water would be sprayed on the molten uranium surface. In this configuration, a vapor-phase explosion is highly unlikely since only limited amounts of water could penetrate the molten metal and no trigger can be identified to initiate the interaction.

A subsurface release of water in the event of a cooling line rupture within the crucible would perhaps be a mechanism by which one could approach explosive conditions. In this case, the wall is available, but it is at a temperature that is far greater than the value at which the water could wet the surface. Therefore, here again a vapor-phase explosion would seem very improbable.

The last possibility would involve the scenario in which water flooded the pressure vessel floor and molten uranium subsequently splashed out of the crucible onto the wetted floor. Although this sequence of events is extremely unlikely, it is the most probable mechanism for a vapor-phase explosion in the MARS configuration.

3.3.15 Liquid Entrainment Hypothesis

If water were in the crucible and uranium droplets poured in, this hypothesis could potentially be operable. The uranium droplet would penetrate the surface and begin its descent to the bottom of the crucible. An instability could cause a pit-like formation on the bottom of the drop and a subsequent envelopment of water in the pit by forces acting on the outside of the molten metal. After complete entrainment, the water superheats and then vaporizes explosively causing fragmentation of the metal drop. However, because the water is being injected into the uranium, this mechanism is not likely to be operable.

For the single scenario of water on the vessel floor and a crucible spillage, this mechanism could be operable. The same argument applies here as in the entrapment hypothesis.

3.3.16 Shrinking Shell Hypothesis

This mechanism would not be operable for the original five accident scenarios because of the same reasons given for the entrainment hypothesis; however, it could apply to the sixth scenario of U into H_2O.

3.3.17 Local Stress Theory

Not much evidence is available to support this theory. The temperature threshold would still exist and be met in this case, but the temperatures should be high enough that only minimal quantities of uranium would be solidified.

3.3.18 Chemical Reaction Theory

Free hydrogen will be released with water-metal contact. In the absence of oxygen, however, it is unlikely that any appreciable explosive reaction could occur. The reaction rate is not fast enough to be responsible for vapor-phase explosions and any potentially hazardous effects should be eliminated by the vacuum. This would be a subject for consideration in a hazard analysis.

3.3.19 Hydrodynamic Fragmentation Hypothesis

This mechanism is analogous to the entrainment theory and would be ruled out for the same reasons in all but the sixth scenar

3.3.20 Impact Fragmentation

For the MARS experiment, no origin can be identified for an externally applied initiating pulse. Should such a pulse be generated with the required timing, a vapor-phase explosion could not be ruled out. Thus, even though no mechanisms or triggers can be identified for vapor-phase explosion in connection with the MARS facility, the unpredictable nature of accidents, and of the vapor-phase explosion in particular, prevents the exclusion of such an occurrence. A small probability of a vapor-phase explosion does exist, and for this reason, ways of avoiding cooling failure should be considered.

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4.0 HAZARD ASSESSMENT FOR MARS

During conceptual design of a facility or major experiment, a preliminary hazard analysis (PHA) is usually developed. An early assessment of significant hazards and the establishment of feasible alternatives for their successful mitigation assure project management that potential economic and safety pitfalls are avoided to permit the orderly development of project activities. The present study is not to be construed as a PHA, since the purpose of it is to evaluate the potential for one hazardous condition, namely the vapor-phase explosion. However, in the course of the project, other potential hazardous conditions and possible mitigating factors were identified. These potential conditions will be briefly discussed in Subsection 4.1 and should be useful as input to any future hazards or safety analyses.

4.1 Hazards and Hypothetical Accidents

In order to assess the likelihood of a vapor-phase explosion, it is necessary to define the conditions surrounding uranium-water contact. Several basic scenarios have been developed to account for crucible failure and for cooling shield failure. These failures result in water injection into the uranium from below and water ejection onto the uranium from above, respectively.

4.1.1 Coolant System Failure

A localized, high-heat flux could produce boiling in one or more of the crucible cooling passages. Boiling would severely degrade the heat transfer capacity causing possible melt of the cooling passage wall. It is estimated that melt-through of one to three 1/4-in. diameter water passages would expose the molten uranium to a water injection rate of 10 gpm (each passage) at velocities of 10 to 15 ft/sec.

Another source of water injection could result from the occurrence of a small crack in the crucible wall due to a material defect or thermal stress. This could possibly produce a high-velocity jet of water with a small flow rate ($\leq$ 0.1 gpm) that mixes with the molten uranium inside the crucible. A complete failure of the primary cooling water system would also result in heat transfer degradation, melt-through, and subsequent water-uranium mixing.

The same scenarios could lead to failure of the overhead cooling line (3/8-in.) for the vapor shield. It is assumed that up to 10 gal of water could be ejected onto the molten uranium surface. For any of these scenarios, a likely assumption would be cooling water and E-beam shutdown at some point after cooling water system failure. However, because the sensing devices and safety systems are not defined at this point, the amounts of water mixing with the uranium will be estimated arbitrarily using conservative assumptions (see Section 5.0).

4.1.2 Hypothetical Violent Interactions

Given that the cooling system fails, there are several interactions that could result. The most critical would be a high-order vapor-phase explosion. This could occur due to water injection or could result from the external application of a pressure pulse simultaneously with water injection, which could cause impact fragmentation and subsequent vapor-phase explosion. The uranium-water contact could also result in a less violent reaction that would produce steam and splash some of the uranium out of the crucible. The last reaction would be a no-impact condition, which would cause no appreciable steam pressure generation and would not disturb the uranium at all. The possibility of this benign interaction between water and molten uranium is negligible.

4.2 Evaluation of Relative Probabilities

Under the assumed accident conditions, the interface temperature developed upon contact of water (16°C) and molten uranium (2,500°C) is 2,170°C. This is far above the spontaneous nucleation temperature and is more than 3.5 times the thermodynamic critical temperature of water. Even when the uranium cools to its freezing point, the interface temperature is 1,000°C, about twice the critical temperature.

Experiments utilizing a free-contacting mode have shown that large-scale explosions have not occurred when the interface temperature exceeds the thermodynamic critical temperature. The uranium-water interface in the MARS system satisfies the stable liquid-liquid film boiling criterion throughout the molten uranium temperature range. Therefore, these high interface temperatures make a vapor-phase explosion extremely unlikely in the event of a cooling system failure.

A vapor-phase explosion initiated by an external trigger is also highly unlikely, although some tests have shown that normally benign conditions resulting in no interaction could lead to an explosion with the addition of an externally applied pressure pulse (roughly at a magnitude of 1 MPa). An initiating pulse of this kind would be unlikely in the case of a cooling water accident for the MARS system. Triggering by wall or surface entrapment would be impossible for cooling line failure in the vapor shield since the water would be sprayed on the molten uranium surface. In the event of a cooling line rupture within the crucible, a subsurface release of water could theoretically produce wall entrapment conditions. However, the high wall temperature there is far greater than the value at which the water could wet the surface and be trapped. Therefore, no external triggering mechanisms can be identified, and the vapor-phase explosion is improbable.

The most probable event resulting from cooling system failure would be a less energetic, boiling. This boiling reaction could splash much of the uranium out of the crucible, forming a molten pool in the bottom of the containment vessel. Given a cooling system failure, the probability of this occurrence is considered to be quite high and melt-though should be considered as a possibility. Previous experience with this type of system indicates that a reaction in the range between the explosion and the no-impact condition will occur.

Table 4-1 summarizes the hazards analysis by listing the courses, the consequences, the controls, and the relative probability of occurrence.

TABLE 4-1

HAZARDS ANALYSIS TABLE FOR LIQUID-LIQUID INTERACTION

Event	Causes	Effects and Potential Consequences	Prevention Measures and Controls	Relative Probability*
Vapor-phase explosion	Cooling shield failure	1) Ejection of water onto molten uranium surface. Explosive transient.**	Quality control, water pressure detector or vacuum pressure detector and automatic shutoff operational procedures. Containment vessel design for maximum credible explosion. Same as above above. Mesh under crucible to prevent molten uranium from reaching the vessel floor.	1
		2) Flooding of pressure vessel floor. Subsequent splashing of uranium into water. Explosive transient.**		2
	Crucible failure	1) Injection of water into molten uranium. Explosive transient.**	Quality control, water pressure detector and automatic shutoff, operational procedures, containment vessel design for maximum credible explosion. Same as above. Mesh under crucible to prevent molten uranium from reaching vessel floor.	2
		2) Flooding of vacuum vessel floor. Subsequent splashing of uranium into water. Explosive transient.**		2
Energetic reaction (non-explosive)	Cooling system failure	Water-uranium contact. Splashing of uranium against vacuum vessel walls. Possible damage to vessel bottom from molten uranium.	Quality control, water pressure detector or vacuum pressure detector and automatic shutoff, containment vessel design for moderate steam pressures, including pressure relief valve. Mesh under crucible to prevent molten uranium from reaching vessel floor. High melting point burn through in bottom in vessel.	3

TABLE 4-1
(Concluded)

HAZARDS ANALYSIS TABLE FOR LIQUID-LIQUID INTERACTION

Event	Causes	Effects and Potential Consequences	Prevention Measures and Controls	Relative Probability*
No reaction	Cooling system failure	No water-uranium contact or small amount of water vaporized. All molten uranium remains intact in crucible.	Quality control. Moderate containment.	3

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*Relative probability -- 1) Impossible -- will not occur.
2) Remote -- very unlikely to occur.
3) Infrequent -- may occur occasionally or during life of facility.
4) Frequent -- will occur on a regular basis.

** Given that proper mixing conditions exist.

5.0 CONTAINMENT VESSEL INTEGRITY

As a worst-case safety analysis, the occurrence of a cooling water leak was assigned a probability of 1.0; consequently, the theoretical analysis sequence was as follows:

1. derive the source terms, i.e., the initial source energy release;
2. transport the energy to the walls of the vacuum vessel;
3. calculate the gas dynamics of the vapor-wall interaction;
4. calculate the vulnerability of the vessel through a stress analysis.

The five major U/H_2O failure conditions are postulated in LLL letter EBS 79-10[1] and updated in subsequent conversations.[2] They were discussed in Section 4.0 as being either a crucible failure or a cooling shield failure. They are reproduced here for added clarification.

1. A high, localized, heat flux produces boiling in the water cooling passages, which blocks the flow. The resulting crucible failure exposes the melt to a breach in one to three 1/4-in. diameter water passages that have a combined flow rate of up to 12 gpm at velocities of 10 to 15 ft/sec. When this occurs, the E-beam gun shuts down, quenching the heat source; the cooling water does not shut off.
2. The crucible fails as in No. 1 above, except the cooling water and E-beam gun both shut off within about 10 sec. This results in 2 gal of water mixing with the melt, at velocities of 10 to 15 ft/sec.

3. A small crack occurs in the crucible, which results in a high-velocity jet of water with a small flow rate (<0.1 gpm) that mixes with the melt. The E-beam gun shuts down, and the cooling water remains on.

4. A complete failure of primary cooling water and electrical power systems occurs during operation. Consider only the damage that might occur to the crucible, which would, in turn, result in a water-melt mix.

5. A failure of a 3/8-in overhead cooling shield water cooling line that ejects up to 10 gal of water onto the melt. The cooling water and E-beam gun will shut down when this occurs.

Midway through this study, a sixth scenario was supplied by LLL lead project personnel.[3] This scenario considers the situation of a water leak into or onto the uranium melt (as in the previous five scenarios), water accumulation at the bottom of the vacuum vessel, then molten uranium being blown or splashed out of the crucible and falling into the water.

Two cases or types of reactions were considered as necessary to explore the consequences of these six scenarios. The two cases consist of a quasistatic steam generation and an explosive steam release.

5.1 Two Cases for Analysis

The vacuum confinement vessel for the MARS experiment must be designed to function satisfactorily over its range of expected service. The vessel will be required to serve its normal function of providing a vacuum jacket for the experiment and to provide containment in the event of a possible operating accident or to confine its contents and protect operating personnel in the event of the occurrence of an improbable accident condition.

5.1.1 Case 1: Operating Basis Accident (Quasistatic Pressure)

The design criteria for the vacuum vessel must allow for routine operation at service loads. As a starting point, ASME vacuum vessel codes[4] were assumed for the MARS vessel design. Appendix B presents the engineering analysis for determination of the minimum vessel wall thickness to operate under hard vacuum conditions. As described in Appendix B, the conceptual vessel was to be 23 ft long and 5 ft in diameter and manufactured from Type 304L stainless steel. Based upon this analysis, which satisfies the very conservative ASME code, the minimum wall thickness should be 1/2 in.

The allowable code internal pressure would be about 315 psig with an ultimate burst pressure of about 1,260 psig. These values should be kept in mind as the expected internal pressures for two consequences of mixing molten uranium and water are subsequently developed.

Accidents that may occur a few times during the service life of the vessel are classified for this purpose as OBA's and must be confined in such a manner as not to impair personnel safety. Design criteria for this service should also be imposed that provide a vessel with sufficient reserve strength to resist conditions of failure that would result in an energy release of sufficient magnitude as located so that it would create a hazard to operating personnel. In situations where personnel safety would be compromised by a structural failure, it is recommended that stresses approaching but not excluding the material yield strength be permitted. In other situations where personnel safety is not a governing criteria, yielding may be permitted and the amount of plastic deformation permitted by design should be governed by the programmatic consequences of such a rare event.

From the start, the ground rules established by LLL was to allow the structure to yield but not rupture. The accident postulated for Case 1 is a slow (quasistatic) steam generation as water contacts the hot uranium. This is designated as the OBA quasistatic condition.

The chemical reaction equation is given by

$$U + (n + 2)\ H_2O \rightarrow UO_2 + 2H_2 + nH_2O + E \qquad (5\text{-}1)$$

where

E = exothermic reaction of 133,000 cal/mole of U
n = number of moles of H_2O in excess of stoichiometric ratio.

If there is a water leak into the crucible during MARS operations, it is highly likely that the above reaction will take place with a simple generation of steam and a modest quantity of hydrogen. This is certainly the case prior to U liquification during initial melting or postoperations cool down. The UO_2 and H_2 are not considered to present significant hazards and will be dropped from further consideration (see discussion in Section 4.0).

The expected quasistatic steam pressure pulse is discussed in Subsection 5.3.

5.1.2 Case 2: Operating Basis Accident (Vapor-Phase Explosion)

The accident postulated for this case is an extreme condition of a highly unlikely vapor-phase explosion resulting from a mixing of water with molten uranium. Paraphrasing the previously described scenarios, the water could enter the melt from a below-surface breach in the crucible, could be sprayed onto the melt surface, or the melt could spill out into water resting on the bottom of the vacuum vessel.

The approach taken here was to

1. define the initial explosive energy (source terms) for a worst-case credible vapor-phase explosion;
2. transport the expanding steam cloud to the vessel walls via an adiabatic expansion;

3. impact the steam with the rigid vacuum vessel wall, 30 in. away, using one-dimensional, planar shock interaction relationships to predict the pressure transient seen by the wall; and

4. load the wall with the very conservative pressure transient using an elastic response model to predict peak hoop tension stresses--this stress analysis is discussed in Subsection 5.4.

This approach is admittedly not elegant and not truly consistent; however, it is a reasonable engineering approximation using conservative, worst-case assumptions. These assumptions and their rationale will be explained in Subsection 5.3.

5.2 Fragment Effects

In some explosive environments, notably those involving high explosives and contained steam explosions, fragments are ejected at high velocities from or near the point of detonation. Data on liquid-liquid explosions, while sparse, show evidence that the fragment particle size and momentum are sufficient to be of some concern from the damage standpoint. There exists a possibility for fragment generation from the destruction of the crucible and crucible support mechanism and other components located within the vacuum chamber. These mechanisms should be designed in a manner to prevent them from being propelled against the vessel wall with sufficient velocity to cause penetration. Alternatively, a missile shield may be employed.

5.3 Transient Pressure Effects

The various situations considered are based upon the two cases defined in Subsection 5.1. The transient steam pressure on the containment vessel wall is derived as the independent variable needed for the preliminary stress analysis presented in Subsection 5.4.

5.3.1 Case 1: Quasistatic Steam Generation

The quasistatic steam generation is a likely occurrence whenever the cooling water contacts the hot copper crucible and uranium. The highest postulated leak rate occurs in scenarios 1 and 2 with the melt-through of three 1/4-in. diameter cooling water passages for a total flow rate of 12 gpm.

The analysis for this case utilized the following heat balance equation:

$$m(t)_{cu}\, C\,(t)_{cu}\;\; \Delta T_{cu} + m(t)_{u}\, C\,(t)_{u}\;\; \Delta T_{u} + E = m\,(t)_{H_2O}\;\; \Delta h_{H_2O} \tag{5-2}$$

where the time dependent variables are:

m_{cu}, m_u are masses of copper and uranium giving up thermal energy;

m_{H_2O} is mass of water absorbing thermal energy;

C_{cu}, C_u are respective specific heats:

ΔT_{cu}, ΔT_u are temperature decreases for the cooled masses of copper crucible and uranium;

E is exothermic thermal energy from the chemical reaction; and

Δh_{H_2O} is the enthalpy change as water is converted to steam.

This equation was utilized with constant average specific heats over the entire temperature range. Two subcases were analyzed: (1) steam generation is restricted by a gradual uranium solidification starting at the point of water injection, and (2) steam generation is maximized by perfect heat transfer from all 159 kg of uranium and the entire copper crucible instantaneously.

- First Subcase -- Gradual U/H_2O Heat Transfer

For a worst case, imagine a water leak directly under the center of the crucible, such that the water spurts vertically upward and separates the molten metal into two equal halves. It could be visualized as two parallel vertical walls of molten metal, a short distance apart, with liquid water filling the space between. If such a leak should occur, it is more likely that the water would make a circular (or approximately circular) hole in the metal rather than planar. But the planar geometry gives more surface area, a higher heat transfer rate, and hence a more conservative approach. Figure 5-1 illustrates this solidification concept.

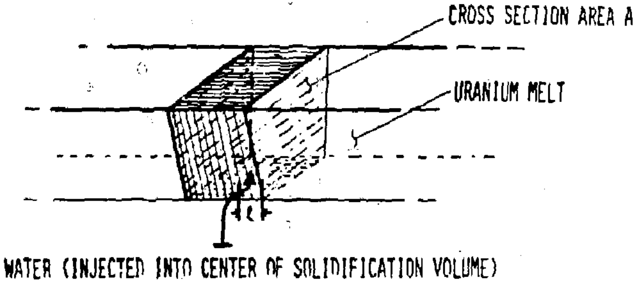

Figure 5-1. Idealized melt solidification.

The molten metal forming the two parallel vertical walls will begin to solidify and become self-supporting. The heat transfer rate between the water and the metal will probably be governed by film boiling because the metal is considerably above the Lieden-Frost temperature for water[5]. The heat transfer in film boiling is almost entirely by radiation from the uranium through the vapor film to the liquid water. An estimate of the maximum rate of heat flux to the water is given by the following expression.

$$q''(\max) = \varepsilon\, \sigma\, (T_m^4 - T_w^4) \qquad (5\text{-}3)$$

where

ε = surface emissivity = 1.0 for maximum
σ = Stefan-Boltzman constant = 5.67×10^{-8} W/m²-K
T_m = maximum metal temperature = 2,273 K
T_w = *minimum water temperature = 0 for maximum q"*

substituting

$$q''(\max) = 1.5 \times 10^6 \text{ W/m}^2 \qquad (5\text{-}4)$$

$$= 0.48 \times 10^6 \ \frac{\text{Btu}}{\text{hr-ft}^2}$$

It should be noted that in steam boilers[5], the maximum heat flux is typically $10^5 \ \frac{\text{Btu}}{\text{hr-ft}^2}$. For conservatism, the maximum heat flux is assumed to be $10^6 \ \frac{\text{Btu}}{\text{hr-ft}^2}$ for the case being analyzed.

For conservatism, it is assumed that the molten metal is cooled on one side only, i.e., at the water interface. All other surfaces are adiabatic.

Reference 6 and 7 consider the uniform, convective cooling of a plane, semi-infinite body, initially at t_o. Reference 7 includes the effects of the finite heat capacity of solidified phase, and assumes that

t_0 equals the solidification (i.e., melting) temperature t_d. The results are summarized in Reference 8 and are presented (in Figure 55 of that reference) as a function of dimensionless variables.

The solidified mass is given by

$$U_{solid} = \rho A(2\ell) \qquad (5\text{-}5)$$

where

A = melt cross-sectional area of 96 cm^2
ρ = density of 16.63 gm/cc
ℓ = solidification depth in cm.

Based upon the previous heat transfer rate discussion, ℓ is plotted as a function of time as given in Figure 5-2. Again a conservative approach was taken by assuming that heat transfer to the water provided the only cooling mechanism for the uranium. That is, the solidification length (ℓ) is conservatively low, the times will be long and the generated quasistatic steam pressure will be high (as a worst-case).

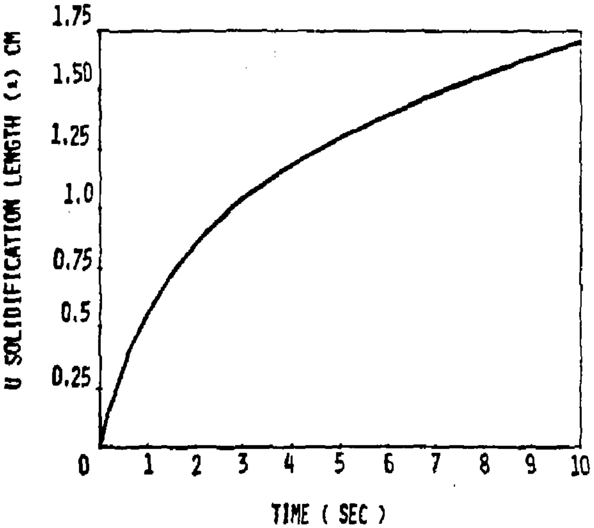

Figure 5-2. Idealized uranium melt solidification history.

The mass of solidified uranium and an appropriate mass of copper crucible were then included in the heat balance equation. This process was then repeated at increasingly later times as more water entered more heat transfer took place, and more steam was generated. The results are shown in Figure 5-3, with a peak pressure of 74 psia after 1,060 sec.

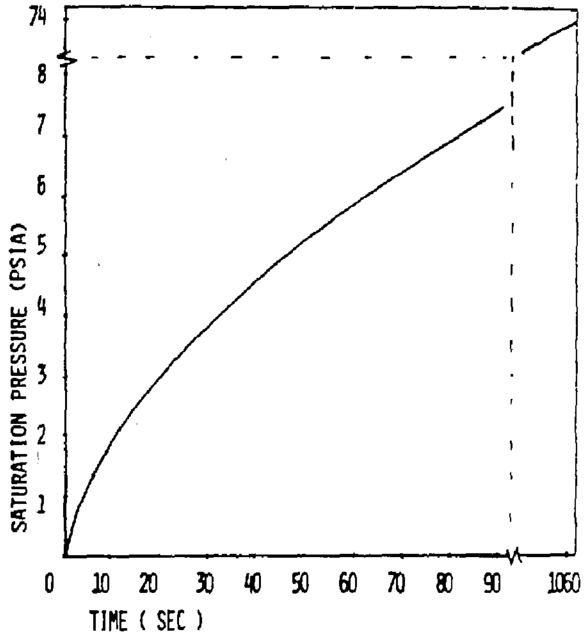

Figure 5-3. Case 1: Steam generation history.

Engineering judgment dictates that the peak pressure is realistic, but the rate is much too slow. If such long times were involved, much of the steam would recondense and the pressure would not be so high. In addition, use of the vacuum roughing pumps should keep up with such a slow steam generation and maintain a vacuum. A more realistic pressure rise is computed for the second subcase.

- Second Subcase -- Upper Limit

This analysis assumes that all of the crucible and all of the melt are instantaneously involved in an optimal heat transfer. This situation results in the steam pressure generation shown in Figure 5-4, with a peak pressure of 78 psia at 48.3 sec. Note that this pressure is similiar to that for the first analysis, but the time is much shorter.

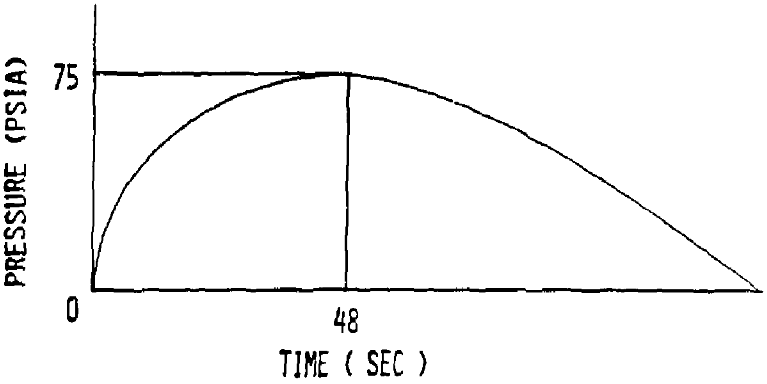

Figure 5-4. Case 1: Idealized quasistatic steam pressure history.

Any actual accident situation is expected to generate a quasistatic peak pressure of no more than 75 psia. This is the loading function to be used for the Case 1 stress analysis discussed in Subsection 5.4.

5.3.2 Case 2: Vapor-Phase Explosion

This case considers a conservative analysis of the intensity of a postulated vapor-phase explosion. This might be called a worst-credible-case analysis in that considerable conservatism is applied to all the variables; however, the assumptions are tempered by experimental evidence and empirical data so that the final results are reasonable estimates of the real-world physics.

- Source Terms

The source terms for this accident were derived by Fauske and Henry as given in Appendix A. These two researchers have performed vapor-phase explosion experiments in support of nuclear power reactor development. They have also conducted investigations into vapor-phase explosion accidents in industry. Even though this previous research has not considered mixing molten uranium and water, there is a considerable and analogous data base of molten metal into water and water into molten metal for such metals as steel, aluminum, and titanium (refer to previous Subsection 3.2). This background factual evidence is necessary to derive a credible estimate of the initial pressure, volume, and temperature source terms for our case of molten uranium (D38) and water mixing.

To provide a frame of reference for the reader, rough rules-of-thumb for vapor-phase explosion properties are based upon considerable experimentation.[9] The source pressure is expected to be about 100 atmospheres (1,500 psia). This low-order explosion or deflagration usually occurs after a short delay from initial water/metal contact. This delay might be tenths of seconds to a few seconds. Typically the heat transfer (explosion efficiency) is low, (2 to 40% of optimum; 10% is typical). Peak pressures of about 10 atmospheres (150 psi) would be expected at distances of a few feet in a rarified atmosphere such as our vacuum vessel condition. With these generalities as a perspective, the specifics of the MARS experiment are addressed (see analysis by Fauske and Henry in Appendix A.)

As a maximum heat transfer case, the uranium is assumed to cool to the homogeneous nucleation temperature of the water, which is much lower than the average final temperature in an actual explosion. With these approximations, the specific energy released from the fuel is given by

$$q = 0.167 \text{ J/g/°C } (2,500 - 300) = 367 \text{ J/g} \qquad (5\text{-}6)$$

This energy release, which is an overestimate of the specific energy available from the fuel in an explosive event, is then compared with the specific energy required to vaporize the water in order to determine the optimum mixture of water and uranium.

The liquid, liquid/vapor, and vapor states are assumed to follow an equilibrium thermodynamic path as shown in Figure 5-5 taken from Appendix A. The final state is one of saturated vapor.

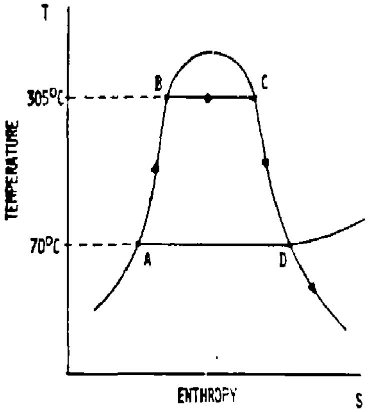

Figure 5-5. Thermodynamic path for an exploding liquid (Reference Appendix A)

Energy addition for the thermodynamic path shown is the summation of the three processes

$$q_T = q_{AB} + q_{BC} + q_{CD} \cdot \qquad (5\text{-}7)$$

Or assuming equilibrium thermodynamics

$$q_T = q_{AD} \, , \qquad (5\text{-}8)$$

which can be computed from the change in specific heat to the final state D. This is approximately 2,600 J/g. The first law of thermodynamics gives

$$q_T = \Delta U + w \qquad (5\text{-}9)$$

where the change in internal energy Δu can be found from the change in enthalpy less the $\int PdV$ work going from state A to state D. This results in an internal energy change of about 2,170 J/g. Therefore the work per unit mass, $\dot{w}$, is 430 J/g. This represents the specific energy received by the water. The "explosion efficiency" can be estimated as

$$\frac{430 \text{ J/g}}{2{,}600 \text{ J/g}} = 0.165 \text{ or } 16.5\% \; . \qquad (5\text{-}10)$$

An optimum U/H_2O mix can be estimated by determining how much U must give up its heat to supply the required specific energy change of the H_2O of 2,600 J/g. This

$$\frac{2{,}600 \text{ J/g}}{367 \text{ J/g}} = 7.1 \quad , \qquad (5\text{-}11)$$

which means that each gram of water that follows the specified thermodynamic path requires 7.1 g of uranium metal. Thus, an idealized mixture will have this ratio of fuel and coolant.

Following the analysis from Appendix A for a crucible volume of 10,000 cm^3, the optimum interaction would involve 7,000 cm^3 (7,000 g) of H_2O. For this water to react within the confines of the crucible, 7,000 cm^3 of uranium must be displaced. Based upon the maximum water leak rate postulated in the scenarios (Section 4.0) of 12 gpm (0.757 kg/sec), the time required would be

$$\frac{7 \text{ kg}}{0.757 \text{ kg/s}} = 9.25 \text{ sec} \qquad (5\text{-}12)$$

to achieve this optimum mix, (should reference be made to the comparable calculation in Appendix A, the longer 23-sec delay is based upon a flow rate of only 4.7 gpm). It should be recognized that extreme conservatism was exercised here; it is highly unlikely that this much water could be accumulated in the crucible for such an optimum vapor-phase explosion because it would be flashing to steam due to the high temperatures and the vacuum environment.

Based upon the discussion in Appendix A, the steam vapor flow will cause the water, and/or the metal, to "boil-up" and increase the void fraction until something equivalent of the churn-turbulent flow occurs and allows the vapor to escape more freely. When such a flow transition takes place, the average void fraction will be approximately 0.40. Therefore, the maximum volume of liquid that would be available at the time of interaction is given by

$$Q_\ell = 0.60(V)0.70 \qquad (5\text{-}13)$$

where V is the 10,000 cm^3 crucible volume and the 0.7 multiplier is the volume fraction of coolant in the reacting mixture, i.e., 7,000/10,000 from before. So the liquid volume to be analyzed as a source term would be 4,200 cm^3 and this would interact with 1,800 cm^3 of fuel (28.8 kg).

Fauske and Henry evaluated two different source terms. one assuming the absolute maximum amount of liquid (7,000 cm^3) and the other using a realistic assessment of the optimum liquid-fuel mixture considering the flow stability (4,200 cm^3). These source terms were analyzed in the same way and only differ because of the masses of liquids involved.

According to experiments, cited in Appendix A, the maximum pressure generated by the interaction is essentially equivalent to the saturation pressure corresponding to a homogeneous nucleation condition at one atmosphere. Consequently, an upper estimate of the pressure-volume behavior would be one in which the liquid is heated to this pressure as essentially all liquid; the heat transfer continues at this pressure until all the liquid is vaporized and sufficient energy transfer continues to maintain a saturated vapor condition as the pressure decreases. Using this thermodynamic path and a liquid volume of 7,000 cm^3, the pressure-volume behavior is tabulated in Table 5-1 and illustrated in Figure 5-6. The results for a similar calculation using 4,200 cm^3 of water are also listed in Table 5-1 and shown in Figure 5-6. These adiabatic PV expansions are based upon an initial source pressure of about 1,350 psi (9.3 MPa). It should be pointed out that these source terms were derived irrespective of the vacuum vessel environment. That is, the source terms are independent of the initial condition of 10^{-6} torr and the final "ambient" pressure.

Table 5-1 provides some insight into the sensitivity of the pressure as a function of the quantity of water involved in the reaction. That is, the pressure at expansion to the vessel wall is higher for the 7,000 cm^3 case than for the 4,200 cm^3 case. Specifics to the MARS system are discussed on page 5-21.

TABLE 5-1

EXPANDING STEAM CLOUD PRESSURE-VOLUME RELATIONSHIPS

	Water Volume	
Pressure	7000 cm^3	4200 cm^3
P MPa	V m^3	V m^3
9.3	0.007	0.004
9.3	0.138	0.082
6.9	0.195	0.117
5.0	0.278	0.167
3.0	0.468	0.281
2.0	0.697	0.419
1.0	1.360	0.817
0.5	2.620	1.575
0.3		2.546

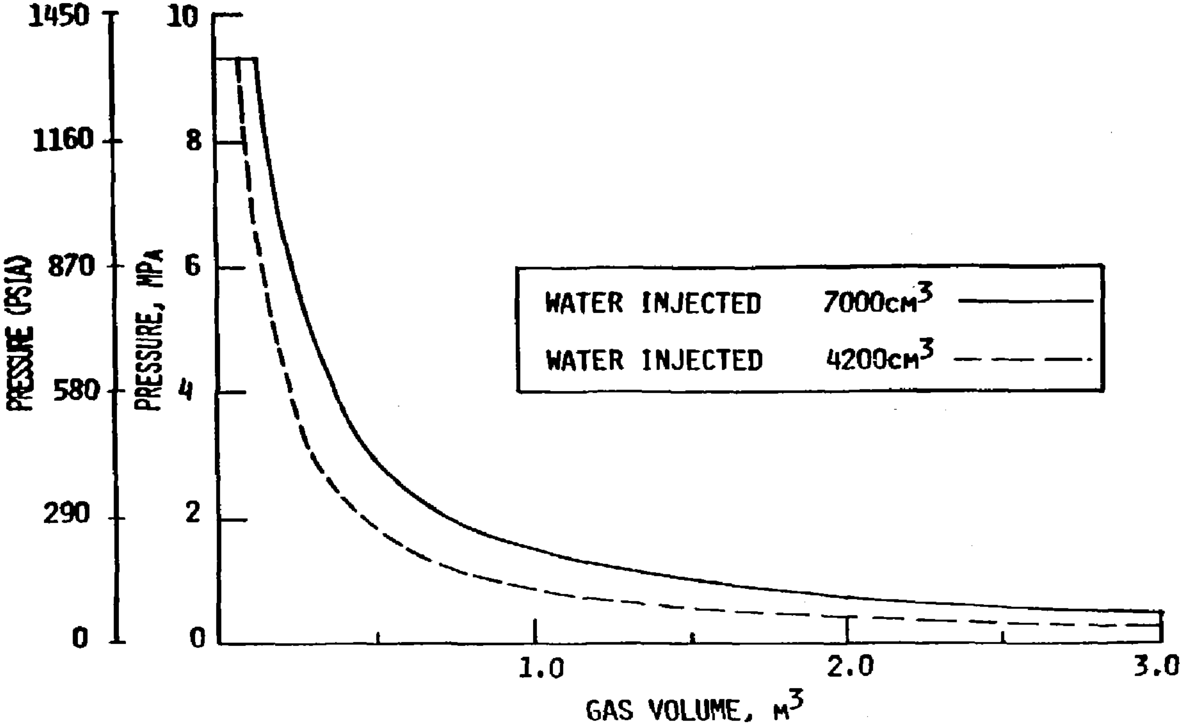

Figure 5-6. Pressure-volume relationships for explosive source term.

Pressure Transient At Vessel Wall - General

As mentioned in Section 3.0, if the vapor-phase explosion occurs in a hard vacuum, the expanding steam pressure-profile would look similar to that shown by Figure 5-7.

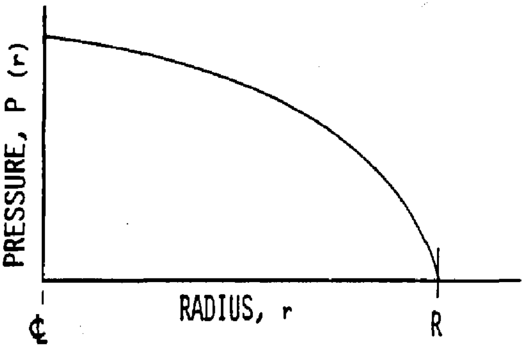

Figure 5-7. Expanding steam pressure-profile; shockless explosion into a vacuum.

where the pressure-profile is defined by[10]

$$P(r) = K \rho^{\gamma} (1 - \frac{r^2}{R^2}) \frac{\gamma}{\gamma-1} \qquad (5\text{-}14)$$

where

P = instantaneous pressure of expanding gas

r = instantaneous radius within the profile from explosion source

R = instantaneous radius of leading edge of profile
K = isentropic constant
ρ = density
γ = ratio of specific heats for the expanding gas.

This means that the highest pressure is at the center and lowest at the gas cloud front; this is opposite the pressure profile for an explosion in a shock supportive medium such as air or steam. The net result of the vacuum is to reduce the damage potential to the containment walls. However, experience has shown that vapor-phase explosions usually occur after some period of liquid mixing. This would cause low-pressure steam to be produced and the vacuum would be lost. Consistent with a conservative approach, the MARS system vacuum pumps are not considered to help remove the generated steam and maintain the vacuum. Therefore, a steam atmosphere is generated prior to the vapor-phase explosion. This atmosphere would support a shock wave so that the pressure profile, just prior to contact with the vessel wall, would probably resemble a steam piston. The actual profile is changing with time and radius and would decay from the peak at the shock front if the vapor-phase explosion source decays rapidly with time. However, the only practical method to predict this time-dependent phenomena is by use of a hydrodynamic computer program. This is beyond the scope of this study, so the profile is taken as the simple shape shown in Figure 5-8.

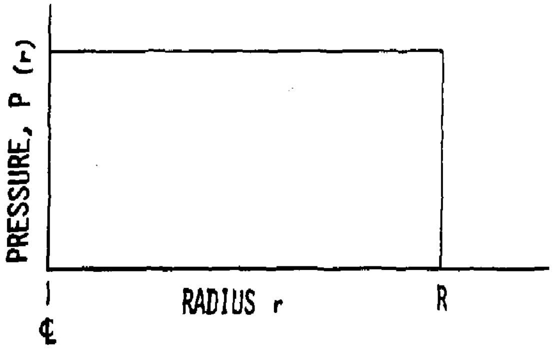

Figure 5-8. Assumed pressure-profile for MARS vapor explosion.

Concerning the pressure rise-time of the vapor-phase explosion, experiments with gas explosions (e.g., methane, hydrogen, etc.) show that the source pressure rises slowly compared to a high explosive detonation. Typically, rise times of about 10 ms are experienced.[11] This relatively slow reaction rate would tend to retard the pressure decay behind the shock front and substantiate the assumption of a steam piston analogy. Nevertheless, it must be kept in mind that the pressure experienced by the vessel wall will be a short-lived decaying transient.

The portion of the vessel wall that is of paramount interest is that closest point directly opposite the crucible, where the explosion is postulated to occur. The pressure transient will be most severe in this area, which can be envisioned as a circumferential ring around the cylindrical vacuum vessel. The area taken for analysis is the wall opposite the crucible at a mean distance of 30 in. from the explosion source. This area would be impacted normally by the radially expanding spherical blast wave. Fauske's analogy of a cylindrical expansion (Appendix A) was not considered as being representative of what should be essentially a point source explosion.

Following initial wall contact, the steam cloud will reflect from the rigid wall and expand down the axis of the cylindrical vessel. This means that the pressure transient at the nearest wall will be amplified by shock reflection then decay rapidly as the steam expands into the entire vessel. The net result is a transient pressure loading of the type illustrated by Figure 5-9.

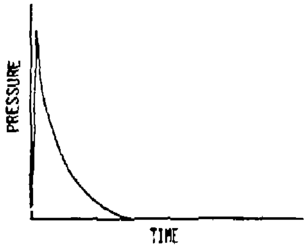

Figure 5-9. Estimated pressure-profile seen by nearest vessel wall.

- Pressure Transient at Vessel Wall--MARS Specific

As applied to the specific MARS configuration, the analysis of source terms and expanded steam volume for 4,200 cm^3 of water was derived in the preceeding subsection. The conditions are outlined as follows:

1. 7,000 cm^3 of water is leaked into or onto the melt in 9.25 sec, when a vapor-phase explosion occurs;
2. 4,200 cm^3 of water are involved in the vapor-phase explosion source;
3. 2,800 cm^3 of water (remainder) is available for generation of low-pressure steam, which very quickly fills the vessel and diminishes the vacuum;
4. the vapor-phase explosion generates a shock wave in the low-pressure steam atmosphere; and
5. the shock wave reflects from the vessel walls yielding a high-pressure short-duration shock loading.

In order to estimate the peak shock amplification as the blast wave strikes the vessel wall, an estimation of the atmosphere between the source and the wall must be made. Fauske's analysis (Appendix A) shows that steam will be produced at 50 g/sec. The previously discussed quasistatic steam generation used steam production values of about 200 g/sec to a maximum of 757 g/sec (this ultraconservative approach means that all incoming water is instantaneously vaporized). Fauske's vaporization rate was used in the vapor-phase explosion analysis because the 50 g/sec represents a more realistic heat transfer rate for the film boiling situation. This results in a vaporized steam mass of 462 g after the 9.25-sec delay time prior to the vapor-phase explosion. This mass of steam would negate the vacuum and provide a quasistatic saturated steam atmosphere at 0.74 psia.

The conservative approach taken to estimate the peak pressure at the wall was to (1) begin with the adiabatically expanded pressure from Fauske's analysis (see Figure 5-6) taken at a spherical volume that is tangent to the 30-in. radius vessel wall, (2) compute plane shock wave reflections (actually spherical onto cylindrical geometry would result in lower reflection factor), (3) multiply the incident pressure by the plane wave reflection factor.

From Figure 5-6 the incident pressure is interpolated as 64.5 psia (0.445 MPa). The reflection factor equation (from any classical gas dynamics text) is

$$\frac{P_3}{P_2} = \frac{\frac{3\gamma - 1}{\gamma + 1} \cdot \frac{P_2}{P_1} - \frac{\gamma - 1}{\gamma + 1}}{\frac{\gamma - 1}{\gamma + 1} \cdot \frac{P_2}{P_1} + 1} \qquad (5\text{-}15)$$

where

P_3/P_2 is the ratio of reflected pressure to incident pressure

P_2/P_1 is the ratio of incident pressure to ambient (steam atmosphere) pressure

γ = ratio of specific heats for steam at the appropriate temperature.

For the conditions stated above,

$$P_2/P_1 \approx 64.5/0.74 = 87.16 \qquad (5\text{-}16)$$

$\gamma \approx 1.3265$ for steam at 297°F, which is the saturation temperature for P_2

this results in a reflection factor of

$$P_3/P_2 = 8.43$$

and peak reflected pressure of

$$P_3 = 544 \text{ psia}.$$

Experimental evidence shows that the duration of this pressure transient should be expected to be on the order of a 100 ms according to Fauske.[9] The duration in our case was determined by calculating the rate at which the shock wave strikes the wall and then reflects back on itself toward the source. An iterative approach was taken: (1) calculate shock velocity, (2) calculate particle velocity behind shock, (3) increment time, (4) calculate new expanded volume, (5) calculate new decayed shock pressure, (6) repeat procedure following reflected shock back toward source. This procedure of hand calculations utilized the following formulas and shock Hugoniots.[12]

$$u_s = v_2\ ((P_3 - P_2)/(v_2 - v_3))^{1/2} \tag{5-17}$$

$$\frac{V_3}{V_4} = 1 - \frac{\Delta t(u_s - u_p)\ 4\pi r^2}{\frac{4}{3}\pi(R^3 - r^3)} \tag{5-18}$$

$$PV^{\gamma} = \text{constant (adiabatic, isentropic expansion behind shock)} \tag{5-19}$$

$$u_p = u_s(1 - v_3/v_2) \tag{5-20}$$

where

u_s = shock velocity

u_p = particle velocity

v_2, v_3 = specific volumes

r = radius to shock front (moving back towards center)
R = 30 in. vessel radius
Δt = time step
V_3, V_4 = volume of expanded steam
P = pressure
γ = ratio of specific heats

Through an interative solution, it was found that the shock reflects toward the source center and the pressure at the wall decays exponentially. This occurs in about 200 μs.

Therefore the predicted pressure transient on the wall (at nearest approach) can be characterized by a pulse of 544 psia peak and 200 μs duration. The pressure decay is exponential (as expected); however, the response (stress) of the vessel wall is not a strong function of the precise decay shape. Therefore, a linear ramp decay was assumed for subsequent use in the stress analysis. Figure 5-10 shows the resultant pressure profile.

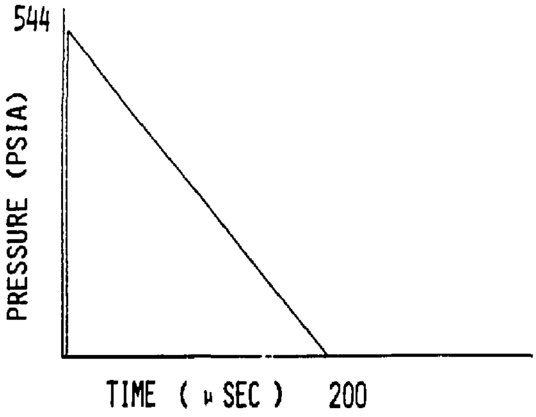

Figure 5-10. Idealized transient pressure loading seen by vessel wall.

It should be pointed out that this is a worst case, at a point directly opposite the postulated explosion. Other areas of the vessel will experience a reduced pressure loading. Also, it is important to recognize that a great deal of conservatism went into this estimate of the wall loading. The primary points of conservatism are delineated in the next subsection. When the cumulative effects of these conservative assumptions are integrated, it is judged that the peak pressure is high by a factor of 2 to 5 and the impulse [$\int P(t)dt$] is high by a factor of 1.5 to 2.

5.3.3 *Areas of Conservatism*

Our conservatism in this analysis is contained in the following assumptions:

1. For a worst case quasistatic steam generation, perfect heat transfer was assumed to estimate the most rapid generation of the largest mass of steam.

2. The MARS system vacuum pumps would help diminish the slow steam pressure build-up (loss of vacuum); however, for conservatism they are not considered to help. This makes both the quasistatic steam pressure (Case 1) and the vapor-phase explosion (Case 2) situations worst case.

3. Excess energy is supplied to the water by the molten uranium by assuming it cools to the homogeneous nucleation temperature of the water, even though the melt would long since have solidified, precluding a liquid/liquid type of vapor-phase explosion reaction.

4. The vapor-phase explosion does not occur until the optimum U/H_2O mix has been obtained; this requires about 9 sec. Experiments indicate that vapor-phase explosions occur more quickly than this, so optimum mixing is conservative.

5. The estimated explosive source terms represent essentially complete thermal interactions with an optimum quantity of fuel. Energy releases resulting from large-scale vapor-phase explosions vary from a few percent to seldom more than 10% (reference Appendix A) of that which could be derived from the optimum quantities. Consequently, experimental systems yield considerably less energy than the optimum values derived above, thus these estimates involve considerable conservatism.

6. The approach of using plane wave shock reflection factors is conservative because most of the steam particles would actually strike the wall at an angle as the cloud expands down the axis of the cylinder.

5.4 Vessel Wall Stress Analysis

As a trial configuration, one may assume that a vessel is designed to operate in a normal service mode without consideration of accident conditions. The resulting system may be a cylindrical vessel 60 in. in diameter with 0.5 in. walls as developed in Appendix B. This as a result of imposing the service load (vacuum) as the sole design criteria. The resulting vessel is capable of containing working static pressures up to 315 psi when conforming to ASME code requirements.

Imposing the accident condition in the vessel and using a suitable dynamic analysis. The following stress and conditions result.

- OBA (Quasistatic Steam Generation)

  It is postulated that the internal pressure environment resulting from a slow stress pressure build-up will be as shown in Figure 5-4. Because the natural period of the cylindrical shell is extremely short, with respect to the rise time of the pressure shown in Figure 5-4, the shell will respond as if the pressure at any time is a statically applied load. The peak pressure of 75 psi will be contained; that is, the peak pressure experienced during the event will be less than the allowed maximum working pressure of 315 psi.

- OBA (Vapor-phase explosion)

A second condition, considered a remote possibility, could produce a steam pressure excursion as was shown in Figure 5-10. This pressure time history is assumed to be applied to a segment of the cylinder surrounding the vacuum crucible and application of this load would result in the development of dynamic circumferential stresses in the midsection of the cylinder. The analysis of the stress conditions follows.

Because the arrival of the pressure pulse causing circumferential stresses will proceed the lower longitudinal stress, resulting from pressures impinging upon the ends of the cylindical vessel, it is assumed that the circumferential stresses will control and may be treated independently of the longitudinal effects. Choosing a unit element from a segment of the vessel, a single-degree-of-freedom system, as shown in Figure 5-11 may model the vessel wall and be analyzed for response to the transient load.

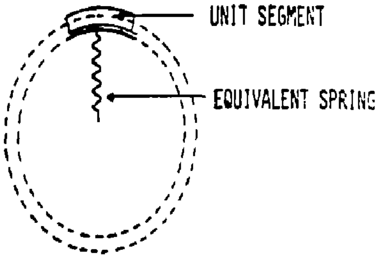

Figure 5-11. Idealized single-degree-of-freedom model for circumferential stress calculation.

The characteristic of the equivalent spring and mass of the segment are calculated as follows.

Assuming the cylinder qualifies as a thin-walled pressure vessel, the circumference, change in circumference, radius and change in radius may be related as

$$c + \Delta c = 2\pi(r + \Delta r) \tag{5-21}$$

and

$$\varepsilon(\text{unit strain}) = \Delta c/c \quad . \tag{5-22}$$

Then the circumferential stress related to a change in radius may be expressed as

$$\sigma = E\ \Delta r/r \tag{5-23}$$

where

σ = stress
E = Young's modulus
r = radius of the vessel
Δr = change in vessel radius.

Using the circumferential stress formula for internal pressure

$$\sigma = Pr/t \tag{5-24}$$

where

P = internal pressure
t = wall thickness of vessel

combining Equations (5-24) and (5-25),

$$P = t\ E\ \Delta r/r^2 \tag{5-25}$$

an equivalent spring constant (K) results if $\Delta r = 1$,

$$P(1) = K = tE/r^2\ . \tag{5-26}$$

A unit element is selected with thickness "t;" this mass is calculated in in - lb - sec units as

$$m = 7.33 \times 10^{-4}\ t\ . \tag{5-27}$$

The natural period of the system is then

$$\tau = 3.11 \times 10^{-5}(r)\ . \tag{5-28}$$

Thus it can be shown that the natural period of this system can only be changed by altering the size of the cylinder and no change in natural frequency will result from changing the wall thickness. Solving the above Equations (5-27), (5-28), and (5-29) for r = 30 in., t = 0.5 in., and $E = 30 \times 10^6$ psi

$$K = 16667 \text{ lb/in.}$$

$$m = 3.67 \times 10^{-4} \text{ (mass, in-lb-sec)}$$

$$\tau \text{ (period)} = 931 \times 10^{-6} \text{ sec.}$$

Using an energy concept and response curve[13], the solution of maximum response to the given transient may be accomplished. The ratio of load duration to natural period T/τ for this condition results in a value of 0.2148, indicating that the system is relatively slow to respond to the applied loading, which will permit a larger fraction of the applied impulse to be converted to kinetic energy. The maximum kinetic energy that can be imparted to a system under impulsive loading is given by

$$W_p = H^2/2m \tag{5-29}$$

when

W_p = work done without system reaction
H = impulse
m = system mass.

For the transient shown in Figure 5-10, W_p = 4.03 lb-in. In an elastic system, the ratio of elastic stored energy to maximum work done (W_p) is given[13] for the preceeding conditions as 0.90. Thus the elastic strain energy W_e = 3.63 lb-in. Displacement associated with this energy is given as

$$W_e = 1/2\ K(\Delta r)^2 = 3.63\ . \tag{5-30}$$

Then Δr = 0.0208 in., which results in a maximum wall stress of 20,800 psi. Based on a material yield strength of 40,000 psi and on ultimate tensile strength of 60,000 to 80,000 psi, the peak circumferential stress of 20,800 would appear to be acceptable.

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6.0 CONCLUSIONS

1. For the operating conditions and configuration of the MARS laser isotope separation experiment, the occurrence of a steam explosion resulting from a cooling system failure is highly unlikely. This is due to the extremely high temperatures and to the lack of any identifiable triggering mechanisms. Although experiments have not been performed with molten uranium metal and water, experiments with molten UO_2 and water resulted in only mild reactions. Vapor-phase explosion theory also predicts this behavior. Operating experience with some cooling water accidents at a similar facility at Oak Ridge Y-12 plant also tends to support this conclusion. However, because there is a remote probability of such an event occurring, the potential energy source term of a vapor-phase explosion should be considered in establishing the structural design basis for the containment vessel. This results in a conservative design that will ensure the safety of the facility and operating personnel.

2. The most likely event in case of the various cooling system failures appears to be a rapid boiling of the water (film-type boiling), resulting in uranium splashing out of the crucible and the formation of a molten pool in the bottom of the containment vessel. The potential for melt-through of the vacuum vessel is minimal; however, the vapor-phase explosion hazard from molten uranium falling into waste should be prevented by design. Possible design features for preventing melt-through might be use of extra cooling, a double wall or thicker wall, addition of a graphite or refractory liner, or the inclusion of an emergency cooling system for the containment vessel. A study should be performed to assess the effectiveness of these safety design features for mitigating damage to the equipment and facility, as well as to compare their relative costs of materials, fabrication, and operation.

3. Given the OBA conditions, it is highly unlikely that the particles of uranium and uranium oxide will present a damaging shrapnel threat to the vessel, i.e., the expected finely divided particles will not be a serious consequence, except for cleanup.

4. Given the OBA conditions, the water-cooled copper vapor shield will very likely be blown apart and presents a threat to the vacuum vessel as a missile or fragments.

5. The pressure transient for the worst-case molten uranium-cooling water reaction will not damage the crucible, i.e., there is no shrapnel hazard from the copper crucible.

6. The use of the high-capacity (roughing) vacuum pumps will not mitigate the rapid pressure build-up from the OBA; however, they would mitigate the slow rate steam build-up as water is simply vaporized by the uranium. The possibility of a lift-off lid should be investigated; however, pressure relief valves or small blow-out ports will not relieve the OBA explosion pressure.

7. Considering the worst case of an OBA vapor-phase explosion, (1) the gas pressure transient experienced by the vessel wall is 544 psia peak pressure with a duration of 200 μs, and (2) the peak hoop stress in the vessel wall will about 20,000 psi, which is only about half the yield strength.

8. The hazard posed by the chemical reaction is insignificant; ie, the formation of hydrogen does not pose a problem.

9. The energy transformation is a very inefficient process with only 1 to 10% of the potential enthalpy change going into the kinetic energy of the vapor-phase explosion.

10. The utility of including a vacuum vessel relief valve is subject to debate. Such a valve or rupture disk will be of no benefit in protecting the vessel from the OBA explosion. However, a valve to relieve a quasistatic or static pressure would be advisable to

protect other systems components that would be sensitive to static pressure, e.g., the vacuum pumps. In addition, it is phychologically attractive to have a relief valve in any pressure system.

DRAFT
5-29-79

APPENDIX A

Subcontract Final Report FGH&T 78-6

from

Hans Fauske and Robert Henry

FGH&T 78-6

URANIUM-WATER VAPOR EXPLOSION HAZARD

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URANIUM-WATER VAPOR EXPLOSION HAZARD

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URANIUM-WATER VAPOR EXPLOSION HAZARD

I. INTRODUCTION

Vapor explosions have been responsible for numerous foundry accidents in which large quantities of hot molten metal inadvertently came into contact with water. These interactions present a considerable hazard to both the operating personnel and the facility itself. Extensive experimental evidence has shown that the occurrence of such events is strongly dependent upon the temperatures of the metal and water and the system pressure. The temperatures of the two liquids must be such that the interface temperature upon contact between water and the metal is greater than the spontaneous nucleation temperature of the system[1] (~305°C or less for water). In addition, the system pressure must be sufficiently low to allow violent boiling processes to occur on a significant size scale[2] (~1.0 MPa or less for a system in which water is the exploding fluid).

II. EXPLOSIVE POTENTIAL

A. Interface Temperature

Experiments have shown that the interface temperature upon contact, which is given by

$$T_i = \frac{T_h + T_c\sqrt{\dfrac{k_c\rho_c C_c}{k_h\rho_h C_h}}}{1 + \sqrt{\dfrac{k_c\rho_c C_c}{k_h\rho_h C_h}}} \qquad (1)$$

must be greater than or equal to the spontaneous nucleation temperature of the liquid-liquid system. For water, this temperature is 305°C (homogeneous nucleation) or less. Considering the high initial temperature of the uranium metal, as well as the high thermal conductivity, the contact interface temperature is not only above the homogeneous nucleation limit, but it is far greater than the thermodynamic critical temperature of the water. Experiments utilizing a free-contacting mode (no external trigger) and with no potential for chemical interaction[2] have shown that large scale explosions do not occur when the interface temperature exceeds the thermodynamic critical temperature. However, additional experiments with external triggers have demonstrated that systems which are not explosive in the free contacting mode can be made to explode with an external trigger.

No experimental data is available for uranium metal and water, but large scale tests at Ispra[3] and Grenoble[4] have shown that no explosive interactions result when kilogram quantities of molten UO_2 ([illegible]°C) are dropped into water. Large scale tests (a few kilograms)[3] with stainless steel dropped into water have also shown only benign interactions, and in fact, limited scale experiments[5] with molten stainless steel and a strong (1.0 MPa) external trigger have only shown fragmentation with no explosions.

For the conditions of 16°C (60°F) water and molten uranium metal at 2500°C, the interface temperature developed upon contact is 2170°C, more than 3.5 times the thermodynamic critical temperature of the water (on an absolute temperature base). Even when the uranium cools [illegible] the freezing point, the interface temperature is still (1000°C [illegible] twice the critical temperature. Therefore, the uranium-water system satisfies the stable liquid-liquid film boiling criterion throughout the molten uranium temperature range. In light of the available data, these extremely high interface temperatures make a vapor explosion in a free contacting mode impossible and very unlikely even in the presence of an external trigger. Consequently, the probability of having a vapor explosion with these two materials is small even if a cooling system failure should occur.

B. System Pressure

A broad range of experimental studies has shown that explosive interactions can be eliminated by elevated system pressures.[5,6,7] This termination of explosive conditions, even in the presence of an external trigger, can be related to a suppression of the propagation mechanism for the interaction. For systems in which water has been the exploding liquid[6,7] the experiments have demonstrated that an ambient pressure of 1.0 MPa (145 psia) is required to suppress an explosion. Since this is far greater than the ambient pressure in the vacuum chamber, this suppression mechanism would not be applicable under the conditions of interest.

C. External Trigger

As discussed above, this metal-water combination will not be explosive without the addition of an external trigger. This is one aspect of explosive vapor formation that has not been carefully documented or closely controlled in the past. Only recently have attempts been made to quantify the magnitude of the trigger and specifically to determine the requirements for a sufficient trigger. However, a survey of experimental data will provide some indication of possible mechanisms for this apparatus.

Some experimenters have provided an external pressure pulse[5,8,9] to initiate the interaction, and the results of Ref. 5 showed that a trigger pulse of 1.0 MPa was sufficient to begin the interaction. Later experiments in this apparatus revealed that those conditions which would not explode with a trigger pulse of 1.0 MPa were also nonexplosive when the magnitude of the pulse was increased to 10.0 MPa.[10] However, in this system it is difficult to see where such an initiating pulse could be generated for the accident in question, especially since the very low pressure environment would not transmit such pulses efficiently.

A more likely triggering condition would be the wall induced initiation that has been observed in the large scale molten aluminum-water vapor explosion studies.[11] In these experiments it was determined that the wall played an essential role in the initiation of explosive events since violent explosions were observed when bare metal or rusted containers were used for the water (aluminum was poured into the water, and no explosions were witnessed when the wall was painted or covered with grease. It was theorized that the bare metal surface was well wetted by the water and this permitted some water to be entrapped by the aluminum. This entrapped water exploded and provided the trigger for the explosion. When the wall was greased or painted, the water no longer wetted the surface and the cascading aluminum merely pushed the water aside as it approached the wall, i.e., no trigger was available.

The bare wall-entrapment mechanism would not fit the conditions of a cooling line failure in the vapor shield since water would be sprayed on the molten uranium surface. In this configuration a vapor explosion is highly unlikely since only limited amounts of water could penetrate the molten metal and no trigger can be identified to initiate the interaction.

A subsurface release of water in the event of a cooling line rupture within the crucible would perhaps be the only mechanism by which one could approach explosive conditions. In this case, the wall is available, but it is at a temperature which is far greater than the value at which the water could wet the surface. Therefore, here again a wall induced trigger and the resultant vapor explosion would seem very improbable, but it cannot be categorically ruled out.

III. ENERGETICS

Since an explosive interaction cannot be ruled out for all postulated accident conditions, the energy release from such events must be considered. The relative specific energies release from the fuel and absorbed by the water will be considered first and then the total amounts pertinent to quantities and the geometry in question will be evaluated.

A. Energy Released from the Fuel

During the thermal interaction, the energy released from the fuel can include the sensible heat of the metal above the melting point, the latent heat of fusion of the uranium, and the sensible heat of the solid metal above the water temperature. Compared to the sensible heats in the liquid and solid states considered, the latent heat of fusion is negligible and will not be included. As an additional simplifying feature, the metal will be assumed to cool to the homogeneous nucleation temperature of the water which is much lower than the average final temperature in an actual explosion. With these approximations, the specific energy released from the fuel is given by:

$$q = 0.167\ \text{J/g}^\circ\text{C}\ (2500 - 300) = 367\ \text{J/g} \qquad (2)$$

This energy release, which is an overestimate of the specific energy available from the fuel in an explosive event, is then compared with the specific energy required to vaporize the water in order to determine the optimum mixture of water and uranium.

In an explosive interaction, once the metal cools sufficiently to solidify, the fragmentation process would be essentially terminated and the multiplication of area would cease. Therefore, the meaningful fragmentation occurs when the metal is molten. Uranium metal at the solidification temperature, and for values down to levels corresponding to spontaneous nucleation temperatures upon contact, would develop stable film boiling following intimate contact, and the energy transfer would, for all intents and purposes, be stopped. These considerations alone mean that the calculation given in Eq. 2 is a conservative estimate (overestimate) of the energy that would be released by the metal in an actual explosion.

B. Energy Received by the Water

A vapor explosion results when thermal energy is extracted from the high temperature metal and deposited in the water as latent heat of vaporization at a rate which exceeds the acoustical response of the surrounding environment, i.e., the resultant vapor cannot be accommodated without pressurization. As the liquid receives this energy, it follows a thermodynamic path similar to that shown in Fig. 1; heating in an all liquid state to the homogeneous nucleation temperature, complete vaporization at this temperature and pressure, and additional energy transfer to maintain saturated vapor during the depressurization. The latter term is included since liquid could be generated by spontaneous condensation if the vapor expanded isentropically from point C. Minute droplets formed in the condensation process would be an efficient source of additional vapor if they contacted hot metal. Therefore, this additional energy transfer is included but heat transfer with the vapor itself is negligible on an explosive time scale, so the final state is one of saturated vapor.

Energy addition for the thermodynamic path shown is the summation of the three processes.

$$q_T = q_{AB} + q_{BC} + q_{CD} \qquad (3)$$

The first, which is all liquid heating, is given by

$$q_{AB} = C_\ell (T_B - T_A), \qquad (4)$$

the second process, high pressure vaporization is

$$q_{BC} = h_{fg} \tag{5}$$

and the last, maintaining saturated vapor is approximated by

$$q_{CD} = \bar{T}(s_{gD} - s_{gC}) \tag{6}$$

Combined, the specific energy received by the water can be calculated from

$$q_T = C_L(T_B - T_A) + h_{fg} + \bar{T}(s_{gD} - s_{gC}) \tag{7}$$

For an expansion to a final pressure of 0.6 MPa (90 psia) in the reference containment volume, the specific heat addition is 2600 J/g. From the first law,

$$q_T = \Delta u + w \tag{8}$$

the work per unit mass can be evaluated for the thermodynamic path considered, and for the final pressure designated this is 430 J/g.

C. Optimum Metal-Water Mixtures

Given the specific energy levels for fuel and water, each gram of water that follows the path shown requires 7.1 g of uranium metal. Thus, an idealized mixture will have this ratio of fuel and coolant. Since the constraint of how much can be mixed is determined by the volume of the crucible, this mass ratio should be cast as a volume ratio. Assuming a density of 16 g/cm^3 for molten uranium at 2500°C and a density of unity for the water, the volume ratio is 0.44 cm^3 of metal per cm^3 of water or a water to metal volume ratio of 2.25. Therefore, the most energetic interaction would result from an intimate metal-water mixture in the crucible volume in which 70% of the volume was occupied by water. With the reference design the crucible volume is approximately 10,000 cm^3, so an optimum interaction would involve 7000 cm^3 (7000 g) of water and the resultant mechanical work would be 3 x 10^5 J. The remaining 3000 cm^3 would be occupied by the 48 kg of molten metal which drives the interaction.

As the above calculations clearly show, the optimum mixture of metal and water requires that a considerable amount of uranium is displaced before the explosion is initiated. This displacement would have to occur as the result of a coolant line rupture in the crucible for which the maximum credible volume flow rate would be 300 cm^3/sec (0.01 ft^3/sec). With these conditions, a 23 sec delay time between the failure and the explosive interaction would be required for sufficient water to enter the crucible. This is an order of magnitude greater than the one or two second delays that have been observed to date, but it certainly represents the maximum amount of water that could be exploded in an optimum manner. However, given the extremely high temperature of the crucible at failure, the vapor produced by film boiling off the walls will cause much of this liquid to be removed from the cavity.

D. Film Boiling

At inception of the failure, the chamber pressure is at high vacuum. As the water is released into the crucible it will be flashing as a result of the depressurization, and it will also begin receiving heat from the walls through radiation dominated film boiling. In order to assess the role of this vapor production, the vapor generation at the end of the delay time will be calculated.

Assuming the molten metal and water are intimately mixed, the water will receive energy, via film boiling, from the crucible walls and from the metal as well. For a dispersed mixture, the latter is generally the most important, but for this demonstrative calculation, only the former will be considered. A typical film boiling heat transfer coefficient for water is 0.023 w/cm^2 °C and, if anything, could be expected to be somewhat greater for the high wall temperatures involved in this case. This coefficient would be applicable over the entire surface area of approximately 2400 cm^2. If the wall temperature is taken to be 2500°C, the saturation temperature of the liquid is of little consequence and the energy transfer rate would be about 1.3 x 10^5 J/sec or a heat flux of about 50 w/cm^2. This energy input to the liquid vaporizes the water at a rate of 50 g/sec, and after 23 sec 1150 g of steam would be produced. With this amount of vapor, and assuming no condensation, the static pressure would be 30 kPa (~4.4 psia). At this pressure, the vaporization rate produces a vapor superficial velocity, based on the horizontal cross-sectional area of the crucible (2000 cm^2), of approximately 135 cm/sec. This velocity far exceeds the value for which bubbly flow could be sustained in the liquid as given by

$$U_v = 0.3\sqrt[4]{\frac{g\sigma}{\rho_\ell}} \tag{9}$$

and is equal to 5.3 cm/sec. Consequently, the vapor flow will cause the water, and/or the metal, to "boil-up" and increase the void fraction until something equivalent of the churn-turbulent flow pattern occurs and allows the vapor to escape more freely. When such a flow transition takes place, the average void fraction will be approximately 0.40. Therefore, the maximum volume of liquid that would be available at the time of interaction is given by

$$0.60(V)0.70 = Q_\ell \tag{10}$$

where V is the 10,000 cm^3 crucible volume and the 0.7 multiplier is the volume fraction of coolant in the reacting mixture. So the liquid volume to be analyzed as a source term would be 4200 cm^3 and this is interacting with 1800 cm^3 of fuel (~28.8 kg).

E. Pressure-Volume Relationship

Two different source terms will be evaluated, one assuming the absolute maximum amount of liquid (7000 cm^3) and the other using a realistic assessment of the optimum liquid-fuel mixture considering the flow stability (4200 cm^3). These source terms will be analyzed in the same way and will only differ because of the masses of liquid involved.

Experimental measurements[2,5,7,8] have shown that the maximum pressure generated by the interaction is essentially the saturation pressure corresponding to homogeneous nucleation at one atmosphere. This was utilized in part B to calculate the energy received by the water during the explosion. Consequently, an upper estimate of the pressure volume behavior would be one in which the liquid is heated to this pressure as essentially all liquid, the vaporization continues at this pressure until all the liquid is vaporized and sufficient energy transfer continues to maintain a saturated vapor condition as the pressure decreases. Using this thermodynamic path and a liquid volume of 7000 cm^3 the pressure-volume behavior is tabulated in Table I and illustrated in Fig. 2. The results for a similar calculation using 4200 cm^3 of water are also listed in Table I and shown in Fig. 2.

If the explosion is assumed to expand in a radial manner, as depicted in Fig. 3, which ignores the expansion towards the end caps of the chamber, then the pressure-volume relationships given in Fig. 2 can be translated to the pressure-radius dependencies illustrated in Fig. 4 for both quantities of water. This source term is a conservative representation of the source term since the axial expansion is not considered.

F. Realistic Energy Release

The above estimates both represent essentially complete thermal interactions with an optimum quantity of fuel, the first is based upon the entire crucible volume while the second considers the maximum liquid which could be retained in the crucible in the presence of film boiling. Energy releases resulting from large scale vapor explosions vary from a few percent to about 10%[9,10] of that which could be derived from the optimum quantities. Consequently, experimental systems yield considerably less energy than the optimum values derived above, and thus, these estimates involve considerable conservatism.

IV. SUMMARY

For all the accident conditions of interest, the most likely system failure to result in a vapor explosion is a rupture of the crucible cooling system. This would inject water beneath the molten uranium pool at a rate of 300 cm^3/sec. As water flows into the crucible, uranium metal will be displaced and will overflow. This is assumed to continue until an optimum quantity of metal and water is available which requires at least 23 secs. During this time, not only will water displace the uranium, but the significant quantities of vapor produced in film boiling will displace both water and metal. The vapor flow will generate a void fraction of at least 40% which decreases the amounts of materials available to explode.

Pressure-volume and pressure-radius calculations are presented for both the optimum mixtures considering no film boiling and for the optimum quantities considering the "boiled-up" condition resulting from film boiling. Both of these are conservative estimates of the energy release, since an optimum metal-water mixture would require approximately 23 sec of coolant water flow after failure, and generally speaking, experimental delay times vary from fractions of a second to a few seconds. In addition, even with optimum quantities, vapor explosion experiments demonstrate an energy release that is 10%, or less, of the theoretical maximum.

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NOMENCLATURE

C - specific heat

g - acceleration of gravity

h_{fg} - latent heat of vaporization

k - thermal conductivity

Q - volume flow rate

q - energy addition

s - specific entropy

T - temperature

$\overline{T}$ - average temperature

U - velocity

u - specific internal energy

V - volume

w - work per unit mass

Δ - difference

ρ - density

σ - surface tension

Subscripts

c - cold

h - hot

i - interface

ℓ - liquid

T - total

TABLE I. PRESSURE-VOLUME AND RADIUS RELATIONSHIPS

Pressure	Water Volume			
	7000 cm^3		4200 cm^3	
P MPa	V m^3	r m	V m^3	r m
9.3	0.007	0.05	0.004	0.04
9.3	0.138	0.21	0.082	0.16
6.9	0.195	0.25	0.117	0.20
5.0	0.278	0.30	0.167	0.23
3.0	0.468	0.39	0.281	0.30
2.0	0.697	0.48	0.419	0.37
1.0	1.360	0.67	0.817	0.52
0.5	2.620	0.93	1.575	0.72
0.3			2.546	0.92

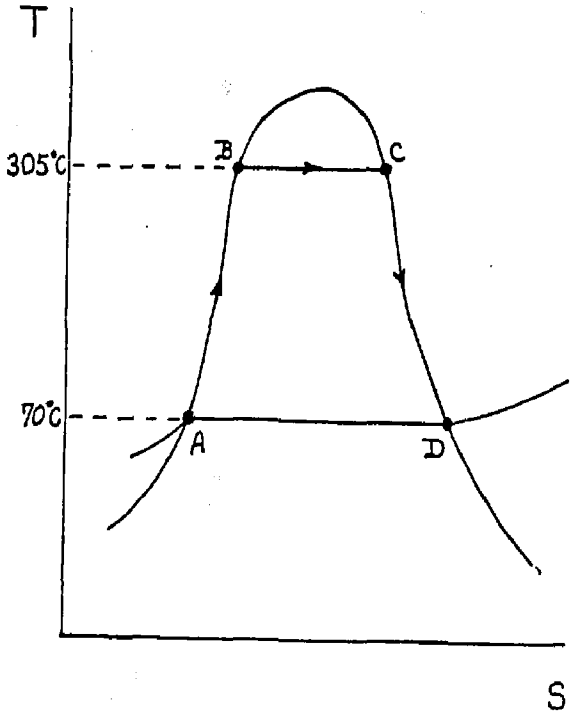

Fig. 1. Thermodynamic Path for an Exploding Liquid

1MPa = 145 psi

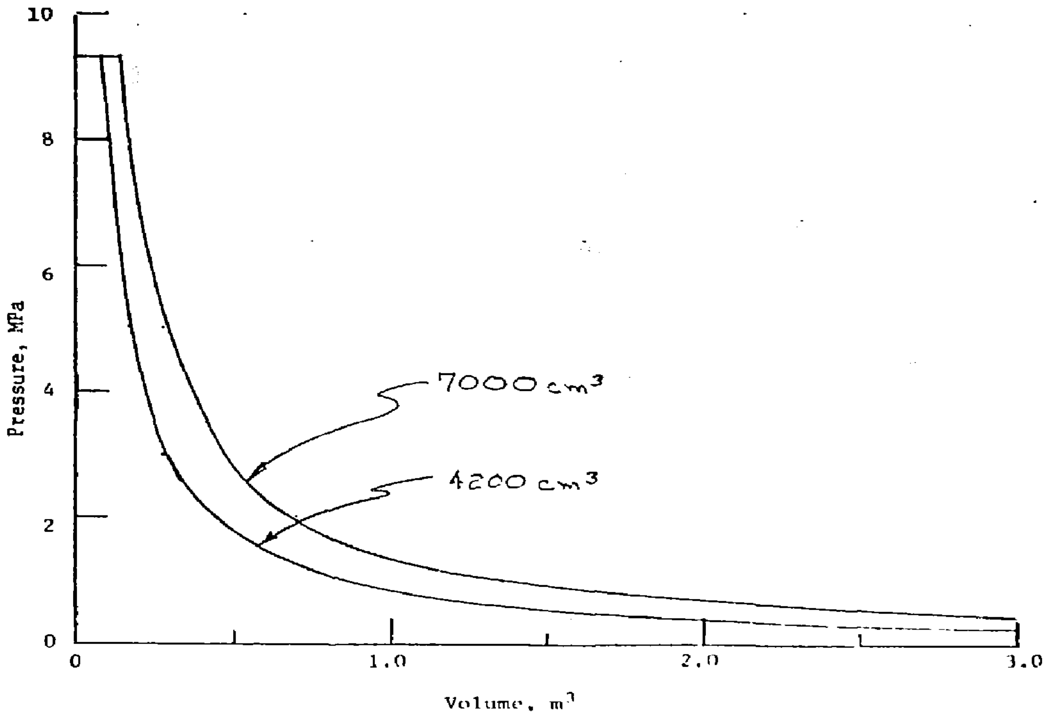

Fig. 2. Pressure-Volume Relationships for Explosive Source Term

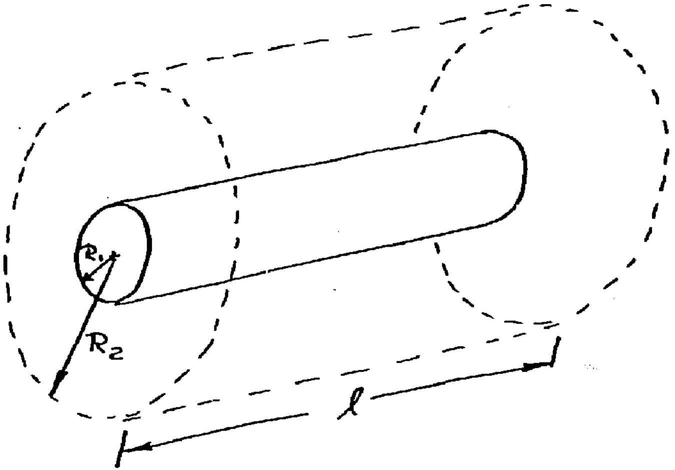

Fig. 3. Radial Expansion of the Explosive Mixture.

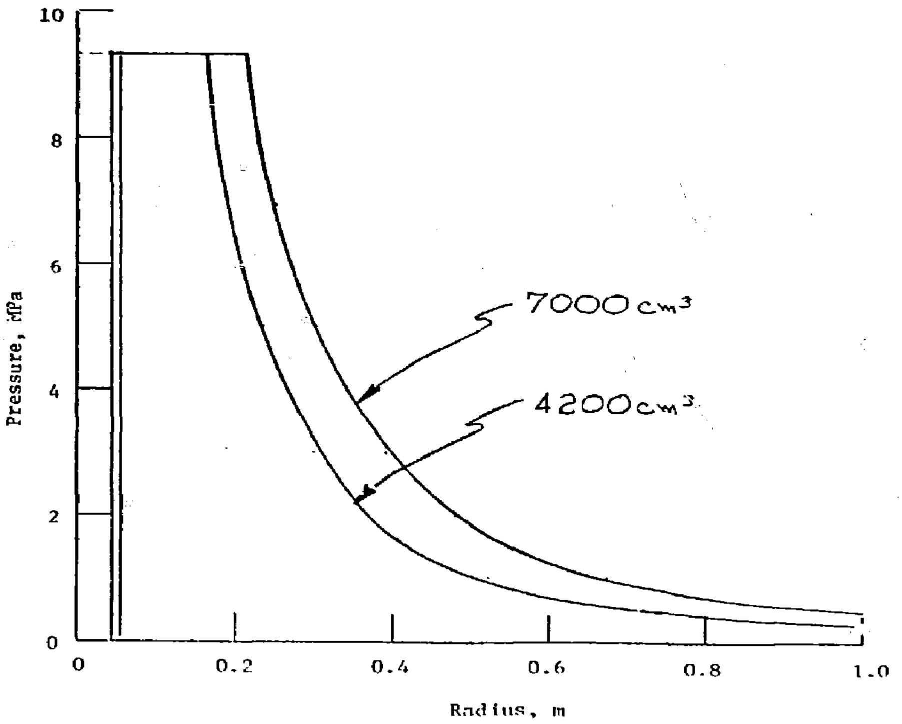

Fig. 4. Pressure-Radius Relationships for Explosive Source Term

APPENDIX B

VACUUM VESSEL WALL THICKNESS DETERMINATION

The vacuum vessel overall geometry was supplied by LLL in updated conceptual drawings. As illustrated by Figure B-1, the updated concept is a 23 ft long vessel. This is a considerable volume expansion over the 8 ft long vessel specified in the original statement of work.

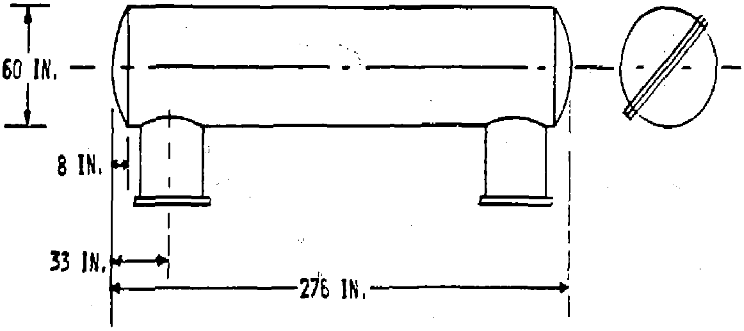

Figure B-1 Sketch of conceptual MARS vacuum vessel.

The intent of this appendix is to

1. Calculate the wall and head thickness to meet ASME Section VIII code, and

2. calculate the internal burst pressure, using the thickness found in 1. above.

Part 1: Calculation of Code Required Wall

Trial 1:

let $t = 1$ in.

P = 15 psi external pressure

D_o = 60 in. outside diameter

P_a = ? allowable external pressure

L = Design length

$L/D_o = 4.47$

$D_o/t = 60$

B = 7,200 (factor from figure UHA-28 of code)

$$P = \frac{B}{D_o/t} = 120 \text{ psi}$$

Trial 2:

let t = 1/2 in.

$D_o/t = 120$

$B = 3{,}000$

$P_a = 25$ psi

Trial 3:

$D_o/t = 160$

$B = 2{,}100$

$P_a = 13$ psi

therefore use 1/2-in. wall.

Part 2: Calculation of Code Required Head Thickness

For ellipsoidal heads

P = 1.67 x external design pressure

D = I.D. of head skirt

E = joint efficiency

S = allowable stress.

Trial 1:

$$t = \frac{PD}{2SE - 0.2P}$$

$$= \frac{(24.55)\ (59)}{(2)(18750)(1) - (0.2)(24.55)}$$

= 0.4 in.

Trial 2:

for t = 0.5 thickness (from Part 1)

from code design procedures $L_1 = K_1\ D_o$

$K_1 = 0.90$ and $L_1 = (0.90)\ (60) = 54$

then

$L_1/100\ t = 108$ and $B = 9{,}200$

$$P_a = \frac{B}{L_1/t} = 85 \text{ psi}$$

so 1/2 in. head thickness is conservative.

Part 3: Calculation of Allowable Internal Pressure

For t = 0.5 in.

(1) Circumferential stress

P = allowable pressure
S = allowable stress
t = thickness
E = joint efficiency (assumed = 1)
R = inside radius

$$P = \frac{SEt}{R + 0.6t}$$

$P = 315$ psig

(2) longitudinal stress

$$P = \frac{2SEt}{R - 0.4t}$$

$P = 640$ psig

(3) Heads under internal pressure

$$P = \frac{2SEt}{D + 0.2t}$$

$P = 317$ psig

Part 4: Calculation of Burst Pressure

For a minimum tensile strengh of 75,000 psi

(1) Shell

$$P_{burst} = \frac{315}{18,750} \times 75,000 = 1,258 \text{ psig}$$

(2) Heads

$$P_{burst} = \frac{317}{18,750} \times 75,000 = 1,268 \text{ psig}$$

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