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SUBJECT: Hazard to HRT Containment Cell from Zirconium-Water Reaction or D₂ Explosion

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SUMMARY

An analysis has been made of some circumstances which may lead to excessive pressures within the HET containment cell. Rupture of the high-pressure system would release hot D₂O, deuterium, and oxygen into the cell. The resulting pressure would depend on the amount of fluid released, its energy content, and the possible occurrence of a zirconium-water reaction.

In this study the energy release, explosion hazard, and cell pressures developed with and without an explosion have been examined for a number of situations involving rupture of the high-pressure system. Analysis of the effects of a metal-water reaction reveals that more than 10% of the zirconium must react before the static cell pressure (without an explosion) is increased appreciably by the additional energy release. If uniformly dispersed, the gas in the cell would be explosive only if reaction of more than 10% of the zirconium occurred and if this was accompanied by condensation of all steam present.
INTRODUCTION

The high-pressure system and all other components of the HRT which contain fuel solution are located within a steel cell designed to prevent the escape of radioactivity in the event the reactor develops a leak or ruptures. This cell, normally to be maintained at a negative pressure of 7.5 psia, has been tested hydrostatically and found to be capable of withstanding a uniform internal pressure of 45 psia.

Rupture of the high-pressure system would result in the release of hot fluid into the containment cell. Under this circumstance the maximum cell pressure attained would depend on the mass of hot liquid exposed to cell conditions, the energy stored in the system, and the rate at which the fluid discharge occurs. Wood has computed the pressures which would exist in the cell following release of the hot liquid in the core and blanket plus the water on the shell side of one heat exchanger. The values below were obtained with the assumption of adiabatic steam expansion (with constant internal energy of the fluid) for the case of core and blanket being initially at 300°C and the heat exchanger at 244°C:

a. Core and blanket only .................. 35.5 psia
b. Core, blanket, and one heat exchanger .... 46.8 psia

Although the value for Case b is slightly higher than the test pressure for the cell, it should be noted that the initial core and blanket temperatures considered are higher than would exist under normal operating conditions. In addition, the expanding steam would contact the colder surfaces in the chamber, resulting in rapid heat transfer. Removal of
heat from the steam would lead to pressures lower than those computed using the adiabatic model. Wood concludes that because of protection of the reactor and both heat exchangers by blast shields, occurrence of simultaneous failures is extremely unlikely.

Two possible events which could increase the cell pressure attained after a rupture need to be considered: (1) release of energy by reaction of the Zircaloy-2 core tank with D$_2$O, and (2), explosion in the cell of radiolytic D$_2$ normally in the reactor plus any D$_2$ evolved from a metal-water reaction.

The effects of a Zr-D$_2$O reaction are considered in this memorandum and the possibility of a D$_2$-O$_2$ explosion occurring is investigated.
ZIRCONIUM-WATER REACTION

Studies of metal-water reactions have revealed that high temperatures and fine dispersions are necessary to achieve appreciable Zr-H₂O reaction. The results of one recent investigation² indicated that less than 5% reaction will occur if molten Zircaloy droplets of 2500 micron diameter are dispersed in water, and the particle size must be less than 100 micron to achieve 75% reaction. Negligible reaction will occur with large drops. Nevertheless, the behavior of Zircaloy-2 with fuel solution in a radiation field is at present uncertain.

If all of the zirconium in the reactor core tank (∼380 lb) were to react according to equation (1), about 10⁶ Btu of energy would be released.

\[ \text{Zr} + 2 \text{D}_2\text{O} \rightarrow \text{ZrO}_2 + 2 \text{D}_2 + \text{Energy} \quad (1) \]

Were the D₂ evolved to combine with O₂ in the reactor cell, an additional 10⁶ Btu would be released. Because of the improbability of a Zr-D₂O reaction when the metal is present in massive form, complete reaction does not appear to be a reasonable assumption. If 10% or 1% of the zirconium in the core reacted with D₂O, the energy release would be 10⁵ or 10⁴ Btu, respectively. These values can be compared to 1.5 x 10⁶ Btu, which is the thermal energy (above liquid at 100°C) stored in hot fluid in the core and blanket.

A sudden release of 10⁶ Btu uniformly throughout the fluid within the reactor pressure vessel would raise its temperature by about 120°C. This temperature increase, even if not extremely rapid, would result in a
pressure rise which possibly is sufficient to rupture the pressure vessel. On the other extreme, a 1% metal-water reaction would raise the temperature less than \(2^\circ\)C and no damage other than to the core tank itself is likely. At reaction percentages in between these extremes, the pressure increase would depend on the rate of chemical reaction, but it is likely that more than 10% reaction would be required to rupture the high-pressure system. If the metal-water reaction were caused by a rapid power excursion, the additive effects of the two events might, of course, be more destructive.

Accompaniment of a Zr-D\(_2\)O reaction by rupture of the reactor would release the heat of reaction into the cell in addition to the thermal energy normally stored in fluid in the system. The resulting cell pressure would depend on the fraction completion of the metal-water reaction. Assuming no heat transfer to the cell or its contents, and with the high-pressure system initially at 300°C, the following pressures would occur as a result of rupture of core and blanket:

a. No Zr-D\(_2\)O reaction ......................... 35.5 psia  
b. 100% reaction .............................. 55  psia  
c. 50% reaction ............................... 45  psia  
d. 10% reaction .............................. 38  psia  
e. 1% reaction ............................... 36  psia

The energy from recombination of D\(_2\) and O\(_2\) is not included in the preceding figures. As noted before, the higher-than-normal fluid temperature used, plus omission of heat transfer, tend to make the computed pressures higher than would actually occur.
EXPLOSION HAZARD IN REACTOR CELL

The concentrations of D₂ which would occur in the containment cell after rupture of the reactor have been computed for a number of situations. The gas concentration is dependent on the partial pressure of steam in the cell and on the extent to which a metal-water reaction has occurred. Values have been obtained for the cases of no heat transfer from the steam and for complete steam condensation. If the blanket were saturated with dissolved D₂ and there were no Cu⁺⁺ in the core, the following mol-percentages of D₂ would exist in the cell after a rupture:

Adiabatic Steam Expansion

a. No Zr-D₂O reaction ............................ 0.5% D₂
b. 100% reaction .................................. 7% D₂
c. 10% reaction .................................... 1.2% D₂
d. 1% reaction ..................................... 0.5% D₂

Complete Steam Condensation

a. No Zr-D₂O reaction ............................ 2% D₂
b. 100% reaction .................................. 2.4% D₂
c. 10% reaction .................................... 5% D₂
d. 1% reaction ..................................... 2% D₂

The lower explosive limit of H₂ is 4% in air⁴ and is in excess of 10% in steam.⁵ The lower explosive limit for D₂ in air has been found⁴ to be somewhat higher than that for H₂. It appears, therefore, that an explosion in the cell would not occur unless there had been at least a 10% zirconium-water reaction, and this would have to be accompanied by condensation of all steam present.
The above computations assumed complete mixing of gases in the reactor cell since circulation of air is afforded by space-cooler blowers having a combined capacity of about 20,000 cfm. However, it is conceivable that a D₂ leak from the reactor into a pocket in the insulation or elsewhere could result in accumulation of a combustible mixture.
The static pressure which exists in a fixed-volume, adiabatic system following a hydrogen explosion varies from 4 to 11 times the initial pressure over a wide range of hydrogen concentrations in diluents of air and steam. Although detonation cannot be sustained in a three-dimensional system, the impact pressure on a container wall from an ordinary explosion may be 2 to 4 times as great as the equilibrium static pressure, or between 8 and 44 times the pressure before the explosion. At the time of an explosion the pressure existing in the HRT cell could be between 7.5 and 55 psia, dependent on the amount of heat transfer and the fraction completion of a metal-water reaction. Thus the range of impact pressures which could occur extends far beyond what could be sustained by the cell without damage. However, the likelihood of an explosive mixture is less for the higher initial pressures.

The preceding values apply to explosions in a container filled with a uniform gas mixture. As indicated in the preceding reaction, attainment of an explosive mixture which fills the cell is unlikely. If a stoichiometric gas mixture with a volume equal to 1% of the reactor cell were to explode, the static pressure which would exist in the cell following an adiabatic expansion would be 1.2 times the initial pressure. For a volume of 5% the pressure rise ratio would be 2.0. The increased pressure on the wall from impact would probably be slight unless the explosion occurred at the wall itself.
All of the D$_2$ from the reactor following a 10% zirconium-water reaction would occupy 1.8% of the cell volume if accumulated as a stoichiometric mixture. If it were to explode before any steam condensation occurred elsewhere in the cell, the maximum static pressure would be about 50 psia. With no metal-water reaction the D$_2$ normally in the reactor (accumulated as a stoichiometric mixture) would occupy less than 0.5% of the cell, and the static pressure, if it were to explode, would be about 41 psia.
APPENDIX

Internal energy of high pressure system above liquid at 100°C:
Core at 300°C ........................................ 368,000 Btu
Blanket at 280°C ................................. 1,148,000

Dissolved deuterium in high-pressure system:
Core with no Cu⁺⁺ ................................. 0.129 lb-mol
Core with 80% recombination .................. 0.112
Blanket saturated at 2000 psia and 282°C .................................. 0.441

Deuterium released by zirconium-water reaction:
For 100% of core tank reacted ............... 8.38 lb-mol

Air content of reactor cell:
For volume of 24,700 cu. ft. at 7.5 psia
and 150°F ........................................... 28.3 lb-mol

Energy released by a zirconium-water reaction:
Zr(s, 280°C) + 2 H₂(ℓ, 280°C) →
ZrO₂(s, 100°C) + 2 H₂(g, 100°C) + ΔE_Zr

ΔE_Zr = 132.1 k cal/gm-mol Zr
= 1448 cal/gm Zr
= 2606 Btu/lb Zr

Energy released by combustion of hydrogen:
H₂(g, 100°C) + 1/2 O₂(g, 100°C) →
H₂O(ℓ, 100°C) + ΔE_H

ΔE_H = 67.7 k cal/gm-mol H₂
= 1.22 x 10⁵ Btu/lb-mol H₂
REFERENCES


