SEP 28 1994 35 Section 21					ENGINEERING DATA TRANSMITTAL					Page 1 of <u>1</u> 1. EDT 156780	
2. To: (Receiving Organization)			3. From: (Originating Organization)			4. Related EDT No.:					
DISTRIBUTION			Nuclear Fuel Evaluations			156780					
5. Proj./Prog./Dept./Div.:			6. Cog. Engr.:			7. Purchase Order No.:					
Nuclear Fuel Evaluations			J. W. Weber			N/A					
8. Originator Remarks: APPROVAL/RELEASE						9. Equip./Component No.:					
						N/A					
11. Receiver Remarks:						10. System/Bldg./Facility:					
						N/A					
						12. Major Assm. Dwg. No.:					
						N/A					
						13. Permit/Permit Application No.:					
						N/A					
						14. Required Response Date:					
						09/29/94					

15. DATA TRANSMITTED					(F)	(G)	(H)	(I)
(A) Item No.	(B) Document/Drawing No.	(C) Sheet No.	(D) Rev. No.	(E) Title or Description of Data Transmitted	Approval Designator	Reason for Transmittal	Originator Disposition	Receiver Disposition
1	WHC-SD-SNF-SARR-001		0	Review of Consequences of Uranium Hydride Formation in N-Reactor Fuel Elements Stored in the K-Basins	E,S,Q	1		

16. KEY					
Approval Designator (F)		Reason for Transmittal (G)		Disposition (H) & (I)	
E, S, Q, D or N/A (see WHC-CM-3-5, Sec.12.7)		1. Approval 2. Release 3. Information 4. Review 5. Post-Review 6. Dist. (Receipt Acknow. Required)		1. Approved 2. Approved w/comment 3. Disapproved w/comment 4. Reviewed no/comment 5. Reviewed w/comment 6. Receipt acknowledged	

17. SIGNATURE/DISTRIBUTION (See Approval Designator for required signatures)										(G)	(H)
(G)	(H)	(J) Name	(K) Signature	(L) Date	(M) MSIN	(J) Name	(K) Signature	(L) Date	(M) MSIN	Reason	Disp.
1	1	Cog.Eng. J. W. Weber	<i>J.W. Weber</i>	9/15/94	L5-01					1	1
1	1	Cog. Mgr. R. P. Omberg	<i>R.P. Omberg</i>	9/15/94	83-85					1	1
1	1	QA J. I. Diehl	<i>J.I. Diehl</i>	9/15/94	X3-78						
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1	1	B. J. Makenas	<i>B.J. Makenas</i>	9/15/94	L5-01					1	1

18. <i>J.W. Weber</i> Signature of EDT Originator Date: 9/15/94		19. <i>R.P. Omberg</i> Authorized Representative Date for Receiving Organization Date: 9/15/94		20. <i>R.P. Omberg</i> Cognizant Manager Date Date: 9/15/94		21. DOE APPROVAL (if required) Ctrl. No. ☐ Approved ☐ Approved w/comments ☐ Disapproved w/comments	
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RELEASE AUTHORIZATION

Document Number: WHC-SD-SNF-SARR-001, Revision 0

Document Title: Review of Consequences of Uranium Hydride Formation
in N-Reactor Fuel Elements Stored in the K-Basins

Release Date: September 28, 1994

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SUPPORTING DOCUMENT		1. Total Pages 73
2. Title Review of Consequences of Uranium Hydride Formation in N-Reactor Fuel Elements Stored in the K-Basins	3. Number WHC-SD-SNF-SARR-001	4. Rev No. 0
5. Key Words Uranium Hydride K-Basins N-Reactor Fuel	6. Author Name: J. W. Weber <i>J. W. Weber</i> 9.19.94 Signature 80510/KK5C1 Organization/Charge Code	
7. Abstract		
<p>8. PURPOSE AND USE OF DOCUMENT - This document was prepared for use within the U.S. Department of Energy and its contractors. It is to be used only to perform, direct, or integrate work under U.S. Department of Energy contracts. This document is not approved for public release until reviewed.</p> <p>PATENT STATUS - This document copy, since it is transmitted in advance of patent clearance, is made available in confidence solely for use in performance of work under contracts with the U.S. Department of Energy. This document is not to be published nor its contents otherwise disseminated or used for purposes other than specified above before patent approval for such release or use has been secured, upon request, from the Patent Counsel, U.S. Department of Energy Field Office, Richland, WA.</p> <p>✓ DISCLAIMER - This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, nor any of their contractors, subcontractors or their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or any third party's use or the results of such use of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof or its contractors or subcontractors. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.</p>		<p>10. RELEASE STAMP</p> <div style="border: 1px solid black; padding: 5px; margin-top: 10px;"> <p>OFFICIAL RELEASE BY WHC DATE SEP 28 1994 35 <i>Section 21</i></p> </div>
9. Impact Level E,S,Q		

⊛ **APPROVED FOR
PUBLIC RELEASE**
M. Boston 9/28/94
Information Release Administration

MASTER

REVIEW OF CONSEQUENCES OF URANIUM HYDRIDE FORMATION IN
N-REACTOR FUEL ELEMENTS STORED IN THE K-BASINS

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REVIEW OF CONSEQUENCES OF URANIUM HYDRIDE FORMATION IN
N-REACTOR FUEL ELEMENTS STORED IN THE K-BASINS

J. W. Weber

September 1994

EXECUTIVE SUMMARY

The 105-K Basins on the Hanford site are used to store uranium fuel elements and assemblies irradiated in and discharged from N Reactor. The storage cylinders in KW Basin are known to have some broken N reactor fuel elements in which the exposed uranium is slowly reacting chemically with water in the cylinder. The products of these reactions are uranium oxide, hydrogen, and potentially some uranium hydride. The purpose of this report is to document the results of the latest review of potential, but highly unlikely accidents postulated to occur as closed cylinders containing N reactor fuel assemblies are opened under water in the KW basin and as a fuel assembly is raised from the basin in a shipping cask for transportation to the 327 Building for examination as part of the SNF Characterization Program.

KE Basin fuel is stored in open cylinders; the fuel is continually submerged in water and any hydrogen that has been generated during storage has been released and the potential for developing significant amounts of uranium hydride is low. On the other hand, the KW Basin fuel is stored in sealed, water filled cylinders. Although the situation is unlikely and has not been found when opening KW Basin cylinders in the past, all or most of the water could have reacted with the uranium. As a result, a cylinder could contain hydrogen and uranium hydride, the latter being a source of additional heat and hydrogen when the cylinder is opened and refills with water. Because they present the greatest potential for uranium hydride buildup, this review concentrates on the sealed cylinders in the KW Basins.

The postulated accidents reviewed in this report are considered to bound all potential releases of radioactivity and hydrogen. These postulated accidents are:

- Opening and refill of a cylinder containing significant amounts of hydrogen and uranium hydride
- Draining of the single element can used to keep the fuel element submerged in water after the cask containing the can and element is lifted from the KW Basin

Analysis shows the release of radioactivity to the site boundary is significantly less than that allowed by the K Basin Safety Evaluation. Analysis further shows there would be no damage to the K Basin structure nor would there be injury to personnel for credible events.

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Review of Consequences of Uranium Hydride Formation in N-Reactor Fuel Elements Stored in the K-Basins

J. W. Weber

1.0 INTRODUCTION

The 105-K Basins on the Hanford site are used to store uranium fuel elements and assemblies irradiated in and discharged from N Reactor. Approximately 2100 tons of fuel is contained in two water filled basins, K-East (KE) and K-West (KW). The original intent was to recover the plutonium by reprocessing the fuel in PUREX in order to support defense production requirements. But with the diminishing need for weapons plutonium, the PUREX plant was shut down and by default the 105-K Basins became a form of interim storage.

The concern over possible uranium hydride formation within the fuel stored in the K Basins is not new and has been reviewed periodically. The purpose of this report is to document the results of the latest review of two potential, but highly unlikely accidents postulated to occur as closed cylinders containing N-Reactor fuel assemblies are opened in KW Basins and as a fuel assembly is raised from the basin in a shipping cask. The report discusses the events of these accidents and their consequences applying conservatism as deemed appropriate. The report is intended in part to support the Safety Evaluation at the K-Basins for Fuel Characterization shipments. The report describes the consequences of the highly unlikely events in terms of the physical damage to the K Basin structure and buildings and radiological releases to the environment. The expected chemical reactions and the quantities of reactants involved and the possible amounts of products are discussed for several postulated conditions in the KW Basins storage cylinders. Because the sealed cylinders in KW present the greatest potential for hydride buildup, this review will concentrate on them.

In addition to the potential for hydride which has formed in the KW fuel cylinders reacting with water on opening, there is a postulated highly

unlikely situation for hydride and uranium reacting with air as the shipping cask, containing an N-Reactor fuel assembly inside a water filled shipping container, is raised from the K-Basins. The assumption is made that the water in the canister somehow leaks out into the cask and on out the cask drain leaving the assembly "dry" and accessible to air. The postulated sequence of events leading to this situation will be described and its consequences shown.

The fuel is uranium metal in a tubular form clad with Zircaloy on the inner and outer diameter surfaces and sealed at both ends with Zircaloy end caps. An N reactor fuel assembly consists of two such tubular elements, the inner one smaller in diameter and centered by spacers within the larger outer.

The amount of fuel in the two basins is approximately equal, but the means by which it is stored in each basin is quite different. KE contains 1150 tons of fuel stored in 3668 open canisters while KW contains 958 tons stored in 3821 sealed water filled canisters (Bergsman 1994). A canister consists of two cylinders or barrels attached together to be handled as a unit. Regardless of the storage method, it is known that some number of the fuel elements in either basin are not intact, having been broken or the cladding damaged during the discharge from N-reactor. Although the exact amount is unknown, more than seven percent of the fuel elements may be broken or at least have broken cladding. There is a concern about the chemical reactions that have occurred between the basin water and the exposed uranium. (Bergsman 1994 and Swanson 1992).

Corrosion of exposed uranium in the storage cylinders would lead to formation of uranium dioxide, hydrogen, and perhaps a small amount of uranium hydride at the uranium-oxide interface. In the open cylinders of the KE Basin, the uranium hydride would soon react with water as the oxide film does not form a completely protective layer. Hydride would therefore be present in insignificant amounts at any one time in the KE basin and present no potential hazard. (Schmidt 1991).

In the sealed cylinders of KW basin, the same chemical reactions are likely. Although the cylinders are sealed to prevent added water ingress, the hydrogen gas can escape out through a vent system at a gauge pressure of

approximately 0.5 atmospheres. If the vent is plugged, the gas can leak out around the cylinder lid seal if the gauge pressure reaches 6 to 7 atmospheres.

Both the open and sealed cylinders contain up to seven fuel assemblies. The sealed cylinders in KW basin were originally filled with water to within a few inches of the top. The upper few inches initially contained a nitrogen cover gas. The fuel elements are not of the same length. This implies that the ratio of uranium to water in the sealed cylinders will vary from cylinder to cylinder and some of the 26 inch fuel elements will extend above the water interface into the vapor space from the start. Both a liquid and a vapor phase reaction could exist and the possibility that uranium hydride, uranium oxide and hydrogen may have been formed in the sealed cylinders cannot be dismissed.

In the K-Basin SNF Characterization program, it is planned to select one or more sealed canisters in the KW basin, open them, remove some of the fuel elements and ship them to the 327 Building for examination and characterization. Of particular concern is a "dry" cylinder in the KW basin in which all, or most of the water, has participated in possible reactions. Although this situation is unlikely and has not been found when opening KW Basin cylinders in the past, this cylinder could contain uranium oxide, uranium hydride, some or no water, and hydrogen. If this cylinder were opened under the basin, then water ingress could lead to the reaction with the uranium hydride, with a release of energy and additional hydrogen.

This document is assembled from the contributions and analyses of numerous WHC and contracted individuals.

2.0 CHEMICAL REACTIONS

2.1 Reactions of Concern

If the N-reactor fuel elements stored in the K-Basin have cladding which is not intact, then the metallic uranium will react with the basin or canister water. The most probable reaction is:

This reaction proceeds rather slowly at room temperature (McGillivray 1994) largely because, after the first oxide layer forms on the outside of the bulk metal, the water or its constituent species must diffuse through a layer of oxide or through microcracks to further react with the metal at the oxide/metal interface. This sluggishness is further confirmed by the fact that no rapid energetic oxidation reactions have been observed in the storage basins although it is certain that a significant fraction of the elements have failed cladding with exposed uranium metal. Corrosion rates (Baker 1966) show that temperature has a very strong effect on the corrosion rate. At the basin water temperature of approximately 10 C the corrosion rate is relatively low, between 2 and 4 mg/cm² - day.

Under some circumstances, where access to water or oxygen is limited, the following reaction can occur to produce a measurable quantity of hydride:

Any excess water will convert the hydride to an oxide by the reaction:

J. L. Swanson reviewed these various reactions in 1992. Theoretically, approximately half of the uranium metal can be converted to hydride with the remainder, of necessity, being oxide. For such large amounts of hydride to exist over long periods of time however, the hydride must be (1) adequately protected from additional water by the companion oxide or (2) the available water must be completely exhausted so that oxidation of the hydride does not commence. Perfect protection of the hydride from excess water (whether the hydride is a monolith or in particulate form) would require an oxide layer which is both adherent, uncracked, and thick enough to prevent water species from diffusing in quantity. Formation of a thick perfect layer of oxide on the metal is very unlikely given the very large density differences between the oxide and metal. However, the oxide and hydride are close in density so that some protection of the hydride may occur. The continued existence of hydride in an environment where all water has been exhausted pre-supposes that the water, which was present at one time, must have a decided preference to

form new oxide as per equation (1), rather than react with recently created hydride as per equation (3). In other words, once hydride has formed, the rate of the oxidation of fresh metal surface would need to be significantly greater than the rate of oxidation of the hydride. This is considered to be highly unlikely.

In Baker, 1966 the oxide/hydride forming reactions are reviewed in more mechanistic detail. The author suggests that water decomposes at the oxide surface to form hydrogen and hydroxyl ions and it is the OH^- which diffuses to the oxide/metal interface and is responsible for the formation of oxide and hydride. Further, he suggests that formation of uranium hydride is in direct competition with the formation of molecular hydrogen when atomic hydrogen is freed by the oxide forming reactions. In other words the hydride forming process is:

If this view is true, there is considerably less hydrogen available for hydride formation than equation (1) implies i.e. half of the hydrogen is left behind at the oxide/water interface before the oxide forming process starts.

(Baker, 1966) also reports that, after complete reaction of uranium samples with water, between 2 and 9 percent hydride was found (the remainder being oxide). This small amount of protected hydride within the oxide samples appeared to be stable both in the presence of excess water and in the proximity of a nearby ongoing reaction of uranium metal with water to produce more oxide. This same study also reports the observation that even in powder form only 20% of the uranium hydride reacted to uranium oxide and hydrogen in two weeks when exposed to water. This indicates the hydride/water reaction is indeed sluggish. Uranium hydride may therefore exist in small quantities in the fuel elements currently stored in the K-Basin closed cylinders.

Experimental observations bearing on the hydride question have been made during metallography of N-reactor fuel elements (Schmidt 1991). The hydride in this case is easily identifiable and has been found but never in large quantities.

Uranium and uranium hydride in dispersed powder form have been shown to ignite in air, in some cases even for room temperature starting conditions (Peacock, 1992 and Hartmann, 1951). However, if dry cylinders containing partial loadings of uranium hydride were to suddenly experience water entry, a similar rapid reaction of hydride with water (and instantaneous release of large quantities of hydrogen) would not occur. As discussed above, the hydride-to-oxide reaction has been shown to be sluggish in water. Furthermore, rapid reaction would require that the very mechanism such as an oxide layer which restricted the access of water to the hydride thus ensuring its long term survival would now be absent and that the hydride would now be in a high surface area particulate form quite unlike the monolithic fuel element.

Reports from the KW Basin operations during the opening of approximately 2000 canisters stored in KW for seven years indicated there was very little gas observed rising to the basin surface upon opening, handling and preparation for shipment to PUREX. These results indicate that the formation and/or reaction of uranium hydrides in the sealed canisters was an insignificant problem.

2.2 Reactions and Resulting Product Quantities

This section attempts to put the quantities of potential reactants in perspective and to derive product quantities which can be used in subsequent sections to evaluate consequences. Dimensions and fuel weights for N-Reactor fuel elements and assemblies are given in Appendix B. The fuel assemblies range from 15 to 26 inches long, and contain approximately 26 to 52 pounds of uranium fuel (including inner and outer elements), respectively. This translates into 49.2 to 98.4 moles of uranium per assembly. Since there can be up to seven assemblies per cylinder the total uranium loading per

cylinder ranges from 344 moles for the shortest assemblies to 689 moles for the longest assemblies.

An empty cylinder includes about 23,600 cm³ free space (8.07 inch ID, 28.125 inch length). The volume displaced by seven fuel assemblies can range from approximately 5400 to 10200 cm³. Two and one half inches of the cylinder at the top is assumed to initially be gas space with the remainder initially being water. The longest fuel assemblies therefore begin the storage period with a small segment, approximately 0.5 inch, uncovered by the water. The shorter assemblies begin the storage period completely covered by water. The volume of water in a cylinder with the 2.5 inch gas space and without any fuel assemblies is 21,500 cm³. Cylinders with seven of the smallest fuel assemblies nominally contains 894 moles of water and cylinders with seven of the large assemblies begin their storage with 625 moles of water.

2.2.1 Theoretical Quantity of Uranium Hydride

If it is assumed that the reaction in Equation 1 continues to completion and is significantly more rapid than Equation 2, calculation can show all of the uranium in a cylinder with seven of the shortest fuel assemblies (344 moles of U) is consumed in reacting the 894 moles of water. For a cylinder with seven of the longest fuel assemblies (689 moles of U) and 625 moles water, approximately 45% of the uranium, or 312 moles is consumed in reacting with all the water via Equation 1. However, if the hydrogen generated from Equation 1 were to immediately react with some of the uranium metal as in Equation 2, then the theoretical amount of uranium hydride could be as large as 395 moles. This assumes, however the highly unlikely sequence that (1) the hydrogen reacts with uranium as soon as it is generated and does not escape from the cylinder through the vent and (2), none of the hydride is itself oxidized by water as in Equation 3. No inleaking of water is assumed or required to complete the reaction to 395 moles of hydride.

Arguments made in Baker 1966 however, suggest that bulk quantities of uranium hydride are not formed by reaction of the hydrogen in the bulk gas, but rather it "is formed during the uranium water reaction, part reacting with water to form hydrogen and uranium dioxide and the rest being protected by the

coherent oxide formed." This suggests that hydride is an intermediate product and not a direct result of uranium and hydrogen. Also, if the hydrogen from Equation 1 were to collect and reach pressures of approximately 0.5 atmosphere the cylinder will vent any additional hydrogen to the basin water. If the vent is plugged, the additional hydrogen will vent out around the cylinder lid at pressures of 6 to 7 atmospheres.

The hypothesis that the uranium and hydrogen reacts to form 395 moles of uranium hydride is therefore not plausible and is highly unlikely to occur.

2.2.2 Maximum Quantity of Uranium Hydride

A more realistic scenario to determine a maximum quantity of uranium hydride may be found from the experimental data published by Baker et. al. (Baker, 1966) with conservatism added where it appears appropriate. Baker et al. reacted uranium metal with water and water vapor in carefully controlled conditions and through various analyses procedures determined the quantities of uranium hydride present in the primary uranium oxide reaction products. They also investigated the reaction rate of granular uranium hydride in water at room temperatures.

Baker 1966 reports that 2 to 9% UH_3 was found in the reaction products of uranium (mostly UO_2) reacting with moist atmospheres of 2 - 100% humidity. To be conservative in this report and analysis, the high end of the hydride reported by Baker et al. was chosen, that is 9%, and a value of 20% was arbitrarily selected. In the KW basin, the condition for the maximum credible quantity of reaction product to form is in the canister with some combination of fuel assemblies that have 490 moles of U and approximately 780 moles of H_2O . All the water is consumed in converting approximately 390 moles of uranium to 390 moles of UO_2 . Part of the hydrogen generated is assumed to react immediately forming uranium hydride from the remaining 100 moles of U. The excess hydrogen would escape the canister through the vent or around the lid seals. This assumes also the unlikely situation that the UH_3 formed does not react with the water as it is forming. Again, no in leakage of water into the cylinder is assumed.

Thus the maximum amount of hydride, if any, to be expected in the KW canisters is approximately 100 moles.

It was also reported by Baker 1966 that the reaction of uranium hydride and water at room temperature is rapid initially but slows in a few minutes and, that after two weeks, less than 20% of the hydride had reacted with water. To provide additional conservatism, it will be assumed here that 20% of the hydride reacts instantaneously. Therefore of the initial 100 moles of hydride present in a KW cylinder, less than 20% or 20 moles is expected to react with the incoming water.

There are 3.5 moles H_2 formed per mole of UH_3 reacting with water (Equation 3). A conservative choice representing possible quantities of H_2 resulting from opening a cylinder under water in KW Basin would be 70 moles or in volume at STP conditions 1568 liters or 55 ft^3 . This case will be considered the bounding event because of the ample conservatism assumed at each step of hydride formation and reaction with water.

These analyses, for both the maximum quantity (section 2.2.2) and the theoretical quantity (section 2.2.1) of uranium hydride, are based only on the geometry of the storage arrangements for the fuel elements. Thus the quantities of uranium hydride calculated for either case are not dependent on the length of time in storage.

3.0 POTENTIAL SEQUENCE OF EVENTS

This section describes the sequence of events for the two postulated accident conditions that are analyzed in this report. This includes the opening of a sealed cylinder containing several N-Reactor fuel elements in KW Basin, and raising and draining of a shipping cask, containing N-Reactor fuel elements, from the KW Basin.

3.1 In KW Basin

Figure 1 shows the potential sequence of events for N-Reactor fuel stored in sealed cylinders in the K-Basins. The path "No Corrosion" is taken

Figure 1. Potential Sequence of Events for N-Reactor Fuel in K-Basin.

when the fuel cladding remains intact protecting the uranium metal from water contact. However, as some of the stored fuel cladding is breached, there is the potential to form corrosion products of UO_2 and UH_3 plus hydrogen gas as discussed above. The proportion of UH_3 to UO_2 is shown to be small. Therefore, the path "Limited Hydride from Corrosion" is the most likely sequence for breached cladding. However, the case "Maximum Hydride from Corrosion" will be evaluated as a conservative sequence path.

The hydrogen evolved from the oxidation of uranium is released slowly and would be vented continuously from cylinders through a designed vent in the Mark II Fuel Encapsulation Canisters. This continuous release prevents the buildup of significant pressures and is the design basis path "Closed Can Vents Continuously." If, however, the vent becomes plugged, gas pressure can build. Pressure testing of the cylinders has shown that leakage occurs at the cylinder-to-cover lid sealing surface at internal pressures of 95 to 105 psig. This is consistent with analysis results (Becker, 1991). Therefore, with a plugged vent, pressure buildup due to hydrogen release will be relieved periodically, or more continuously if the seals did not reseal, and will be limited to about 100 psi ("Closed Can Vents in Burps") path.

In either case, a cylinder is opened underwater, the corrosion products from the uranium water reaction, which will include UH_3 , will become immersed in water. The hydride has the potential for reacting with the water, and a "Hydride Reaction" is probable. In experiments exposing pure uranium hydride powder to pure water vapor at room temperature, the hydride initially reacted rapidly but became slow within a few minutes. This releases the hydrogen very slowly and has no significant consequences.

The "Rapid Hydride Reaction" path would bubble hydrogen into the basin water over a period of several minutes to several hours. The hydrogen bubbles would emerge from the pool and mix with the air without significant quantities becoming flammable. The consequences, if any, are minimal but this event is enveloped by the pathway "Instantaneous Hydride Reaction." The consequences for this pathway are evaluated in Section 4.1 for the bounding case where 100 moles of UH_3 are formed (Section 2.2.2) and for the case of the theoretical quantity of 395 moles of UH_3 (Section 2.2.1).

An important point to be made in discussing the potential sequence of events in the KW-Basin is that the 395 moles of hydride calculated as the theoretical quantity of uranium hydride in section 2.2.1, is the upper limit of hydride that can form in the cylinder independent of how the hydride is assumed to be protected. One idea that has been presented is that the hydride is protected somehow from reacting with the water in the cylinder by a thick low density, non-porous, uncracked layer of uranium oxide. As discussed in section 2.1, the perfect protection of significant amounts of hydride from water in the cylinder is highly unlikely to incredible, given that the water must have access to the uranium surface in order to produce more hydrogen. Another suggested hydride protection idea is to assume hydride forms in some fuel assemblies (but not in the others in the cylinder) by hydrogen entering through an end of the element that is above the level of the water in the cylinder and proceeding to diffuse down through an ever lengthening path to an exposed uranium surface. This idea requires several improbable to incredible circumstances such as: (1) the low density hydride does not expand to cause breaks in the fuel element Zr-2 cladding allowing water to enter and react with the hydride, or push the upper layers of hydride up and out the top to fall and react with the water in the cylinder, (2) the hydrogen generated by the water-uranium reaction in certain fuel elements can escape those fuel elements without reacting with the uranium in them and reach the exposed uranium surface of the hydriding fuel elements through the existing and lengthening hydride column and react with the uranium before the hydrogen pressure exceeds that to escape through the vent or the somewhat greater pressure to escape around the cylinder-lid seal, and (3) that the reaction of the water with the uranium to form the hydrogen is somehow partitioned to occur only in approximately three-sevenths of the fuel assemblies and the hydrogen reaction with uranium occurs only in the remaining four-sevenths of the fuel assemblies.

In the KE-Basin where the fuel assemblies are stored in the open cylinders, the access of the water to the uranium, as well as to any uranium hydride formed at the uranium surfaces, is essentially unlimited. Thus the potential build-up of significant hydride in these fuel elements is far less than in KW-Basin and should be considered incredible.

3.2 Sequence in Shipping Cask

When the fuel element or assembly for characterization has been selected it will be placed in a shipping can full of basin water, then loaded into a cask under water. The cask is designed to drain when removed from the basin for shipment. The shipping can is designed to keep the fuel element covered with water. For the purposes of this analysis it is assumed the single element or assembly shipping container fails along the bottom weld and the water drains out. The likelihood of this occurring is extremely remote since the can will be hydraulically tested at 50 psi and inspected prior to being used in the facility. The scenario assumes removal of the cask from the basin drains both the cask cavity and single element can, causing the fuel to become dry.

In addition, it is postulated that an in-flow of air into the shipping cask can occur. Once dry there is a potential for residual hydride to react with air such that it will ignite and burn. The consequences of this event are evaluated in section 4.3.

4.0 EVALUATION OF EVENT CONSEQUENCES

4.1. Bounding case in KW Basin

The bounding case stems from the discussion in Section 2.2.2 with the sequence-of-events pathway in Figure 1.

- Maximum hydride from corrosion (100 moles)
- Closed can vents in burps
- Hydride reacts with water when the can is opened (20% of maximum)
- Instantaneous hydride reaction

The bounding case analysis for 20 moles of UH_3 reacting with water includes evaluation of the consequences of the highly unlikely burning of all the released hydrogen at the basin surface and the resulting pressure and temperatures, and the possibility of hydrogen detonation. The evaluation of consequences for the theoretical quantity of 395 moles (Section 2.2.1) is

included for comparison. The radiological doses released by the bounding case are compared relative to the Safety Evaluation of fuel stored in the K-Basins.

4.1.1. Hydrogen Burn and Pressure Increase

As the cylinder is opened, the residual gases will probably vent as a jet of discrete bubbles which will make their way to the surface with velocities of 1 to 1.5 ft/sec. The size-dependent bubble velocities cause them to arrive at the top at different times and locations which enhances mixing with air. In addition, water will flood inside the opened cylinder. This analysis assumes a rapid reaction with the hydride. All the hydrogen is assumed to be released suddenly as a single bubble which rises to the top and breaks the water surface. The release process causes mixing with air and dilution of the hydrogen. The low molecular weight of H_2 results in buoyancy effects and, along with turbulence, causes rapid mixing. Mixing studies of gas release events in waste tanks (Fox 1993) have shown that flammable mixtures of many thousands of cubic ft are diluted below the Lower Flammability Limit (LFL) before they reach the ventilation outlet at the top of the tank, 25 feet above the waste surface. It is reasonable to expect this sort of mixing will also occur in K-Basin and flammable mixtures will not persist. Therefore there would likely be no hydrogen burning and no consequences to the structure or personnel from the large amount of hydride reacting and the hydrogen released to the surface.

To further explore these highly unlikely cases and demonstrate the conservatism, the pressure and temperatures are calculated as if all hydrogen is burned. Hydrogen mixed with air is flammable in the concentration range of 4% to 75%. So, there is a short period of time after the bubbles break the surface when some portions of the released hydrogen mixture would be within this range and be combustible. We will assume an ignition source is present and examine the consequences of such an event.

When hydrogen combustion occurs in an open area, the flame front usually advances by a burning, or deflagration process, moving at tens of ft/sec velocity. The mixture behind the flame front is heated by the combustion energy and expands, compressing the surrounding air. The process is slow

enough that gas pressures, both inside and outside of the burn region, are the same. The largest building pressurization from combustion occurs when the hydrogen is mixed with the maximum amount of air but still remains flammable. However, the concentration limit for downward flame propagation is about 9% (Coward 1952). As hydrogen is diluted below about 8% in dry air, combustion completeness (fraction of hydrogen burned) decreases until at the LFL of about 4%, very little of the hydrogen is actually burned. However, to clearly demonstrate this is a bounding calculation, we will assume the hydrogen is diluted to a concentration of 4% and is all burned. The maximum building pressure is calculated using the plume burn model described in Fox 1993. However, these results may be visualized by the following description.

Starting with a bubble that initially contains 55 ft³ of hydrogen from the reaction of water with the 20 moles of hydride, the plume increases in size when mixing with air to 1,375 ft³ of gas with 4% hydrogen. If this were ignited, the deflagration would burn very slowly. The combustion energy produces a temperature increase to 620 K, causing a plume volume expansion of 1483 ft³. This expansion compresses the surrounding air and raises its pressure. The building pressure change may be approximated by the adiabatic compression formula.

$$\Delta P = -\gamma \frac{\Delta V}{V} P$$

$$= \frac{(1.4)(1,483)}{300,000} = 0.007 \text{ atm} \quad (4)$$

where:

- γ = Isentropic exponent for air, 1.4
- ΔV = Volume of air compression
- V = Volume of air in building, 300,000 ft³
- P = Pressure, 1 atm

This pressure is equal to 0.1 psig. This pressure would have no effect on the structure or wall panels of the building (Davis 1975).

These pressure calculations were performed for a series of hydrogen releases with the results shown in Figure 2. In addition, the lower scale on

Figure 2. K Basin Bounding Pressures.

the x-axis shows the amount of hydrogen produced when UH_3 is reacted with water. This facilitates examining margins based on the quantity of UH_3 formed and reacted.

These calculations are also performed for the theoretical quantity of UH_3 . If 395 moles of UH_3 were reacted instantaneously, this could produce 1380 mole of hydrogen or about 1100 ft^3 . If it is assumed all of this hydrogen burns, this could increase the building pressure to 1.8 psig which is equivalent to a water depth of four feet which is still harmless to a person. This pressure could blow some of the panels off the walls, but the building frame, superstructure, cranes etc. would remain intact (Davis 1975).

In both the bounding case and theoretical UH_3 case, the pressure gradient is very low. Therefore, there would be no danger from projectiles within the building. For the higher pressure of the theoretical UH_3 case there could be danger from panels blown off the building to personnel outside.

It should be reiterated these calculations carry the event beyond a highly unlikely event by introducing the maximum quantity of hydrogen, igniting the mixture before it can be diluted below the LFL, and unrealistically assuming that all the hydrogen will burn. These are incredible assumptions and are only done to demonstrate these pressures are still small.

4.1.2 Likelihood of Detonation

An occurrence of flammable mixtures which are rich in hydrogen usually result in questions about the possibility of detonation. This is discussed here to put that issue to rest. Detonations result in a shockwave which can produce high local pressures. The subject of hydrogen-air detonation was studied extensively by Sandia (Sherman 1988). They developed an approach which quantifies the likelihood of detonation. An ignition source is assumed present in this approach. Details are shown in Appendix A. The subject area is divided into "Mixture" classes, and "Geometry" classes. The mixture classes are defined by the percent mole fraction of hydrogen, class 1 having

the highest fraction of H_2 near stoichiometric and extremely detonable. Class 5 mixtures burn less vigorously and are highly unlikely to incur deflagration to detonation transitions.

The geometry classes also range from 1 to 5. Class 1 is for large geometries, has obstacles in path of unburned gases and is favorable to flame accelerations. Class 5 is for unfavorable geometries such as totally unconfined geometries and which are believed to represent the K-Basin system. A Results Table is created for use of the mixture and geometry classes and is shown as Table I. (See Appendix A for further discussions of mixture and geometry classes).

Table I. Dependence of Result Class on Mixture and Geometric Classes

Geometric Classes	Mixture Classes				
	1	2	3	4	5
1	1	1	2	3	4
2	1	2	3	4	5
3	2	3	3	4	5
4	3	4	4	5	5
5	4	5	5	5	5

Where:

Result class 1, Detonation is highly likely

Result class 2, Detonation is likely

Result class 3: Detonation may occur

Result class 4: Detonation is possible but unlikely

Result class 5: Detonation is highly unlikely to impossible

Using a class 5 geometry with a mixture class 1 shows that the highest result class is 4; i.e. Detonation is possible but unlikely. Given the mixture class is changing rapidly as the hydrogen mixes with air, detonation

should be considered highly unlikely to impossible event for potential K-Basin cylinder releases.

4.2 Radiological Doses Released

Accident doses relative to the maximum credible accident identified in WHC-SD-NR-TA-020 Rev. 0, Safety Evaluation of Fuel Encapsulation in the 105-KE Storage Basin (WHC-1), were calculated for cases which encompass potential events involving hydrided fuel. The following dose calculations were made for the theoretical quantity of UH_3 , 395 moles, and for the bounding maximum quantity of UH_3 , 20 moles. The maximum credible accident in the KE-Basin Safety Evaluation involves dropping of a cask containing three canisters, each with two barrels (cylinders) of seven fuel elements each, on the floor of the loadout area. It is further assumed that all 42 elements break in two pieces in such a way as to maximize the surface area. Heating occurs but melting does not. The accident resulted in the release of 244 gms of fuel, including contained fission products and transuranics for the time of interest. For this analysis of the water-uranium hydride reaction the maximum release would be that contained in one barrel of a canister, or in 0.1588 metric tons of fuel. This release is to the basin water, which then provides attenuation of the release to the air.

4.2.1 From Theoretical Quantity of UH_3

The relative dose for the water-uranium hydride reaction event to the current maximum credible accident is calculated as follows:

$$RD = \frac{\sum \frac{Ci(HE)_j}{DCG_j}}{\sum \frac{Ci(MCA)_j}{DCG_j}} \quad (5)$$

Where RD - Relative Dose Ratio Hydride Event to Maximum Credible Accident

$Ci(HE)_j$ - Curies release of a radionuclide for hydride events

$Ci(MCA)_j$ - Curies release of a radionuclide for Maximum Credible Accident

- DCG_j - Derived Concentration Guide, the concentration of a radionuclide in air under conditions of continuous exposure for one year by inhalation that results in an effective dose equivalent of 100 mrem (1 mSv). DCGs do not consider decay products when the parent radionuclide is the cause of the exposure

Table II provides the radioactive isotope concentrations in the fuel that were used for the MCA evaluation, the DCGs, and the evaluation of the relative dose ratio. The ratio has been calculated for the case where it is assumed that all of the fission products and transuranics are released to the water and then a decontamination factor of 10^4 (See Appendix D and Wassel 1985) is used for the water. This case shall be very conservative. The ratio for Cs only release to the water with the same decontamination factor is also given and is the more likely consequence.

The maximum offsite dose for the maximum credible accident was 0.29 Rem. Therefore the dose for the theoretical quantity hydride event, assuming all radioactive material is releasable through the water, would be 0.019 Rem at the site boundary. For Cs only this would be $1.5E-05$ Rem. The values can be evaluated using ratios depending on the number of fuel elements involved and the different release values. Thus the current Safety Evaluation bounds the potential release of radioactivity for the reaction of the theoretical quantity of UH_3 with water, and there is no significant problem past the site boundary.

4.2.2 From Bounding Quantity of UH_3

Calculations were performed for the dose from 20 moles of UH_3 , reacting with water. Estimates for the dose to an operator in the immediate basin area above a canister that is being opened assuming only the Cs becomes airborne, show the dose to the operator would be less than 1 mr/hr which should place no undue restrictions on operations.

Table II. Evaluation of Relative Dose Ratio Hydride Events vs. Maximum Credible Accident

Isotope	DCG Ci/mi	N Fuel Ci/MTU	Ci Release Cask Drop 244 GMS	Ci Release 7 Elements 0.1588 MT DF 10E+04	Relative Dose Cask Drop	Relative Dose 7 Element Event All Release	Relative Dose 7 Element Event Cs Release Only
	A	B	(Bx.000244)	(Bx1.588E-5)	(Bx.000244)/A	(Bx1.588E-5)/A	(Bx1.588E-5)/A
H-3	1.00E-07	2.63E+01	6.43E-03	4.18E-04	6.43E+04	4.18E+03	...
Kr-85	3.00E-06	4.81E+02	1.17E-01	7.64E-03	3.91E+04	2.55E+03	...
Sr-90	9.00E-12	5.80E+03	1.42E+00	9.21E-02	1.57E+11	1.02E+10	...
Y-90	1.00E-09	5.80E+03	1.42E+00	9.21E-02	1.42E+09	9.21E+07	...
Tc-99	2.00E-09	1.21E+00	2.95E-04	1.92E-05	1.48E+05	9.61E+03	...
Ru-106	3.00E-11	5.20E+02	1.27E-01	8.26E-03	4.23E+09	2.75E+08	...
Cd-113M	8.00E-12	2.32E+00	5.66E-04	3.68E-05	7.07E+07	4.60E+06	...
Te-125M	2.00E-09	3.00E+01	7.32E-03	4.76E-04	3.66E+06	2.38E+05	...
Sb-125	1.00E-09	1.20E+02	2.93E+02	1.91E+03	2.93E+07	1.91E+06	...
Cs-134	2.00E-10	1.30E+02	3.17E-02	2.06E-03	1.59E+08	1.03E+07	1.03E+07
Cs-137	4.00E-10	7.30E+03	1.78E+00	1.16E-01	4.45E+09	2.90E+08	2.90E+08
Ce-144	3.00E-11	2.80E+01	6.83E-03	4.45E-04	2.28E+08	1.48E+07	...
Pr-144	3.00E-07	2.80E+01	6.83E-03	4.45E-04	2.28E+04	1.48E+03	...

Table II. Evaluation of Relative Dose Ratio Hydride Events vs. Maximum Credible Accident (cont'd)

Pm-147	2.00E-03	2.00E+03	4.88E-01	3.18E-02	2.44E+02	1.59E+01	...
Sm-151	4.00E-10	8.70E+01	2.12E-02	1.38E-03	5.31E+07	3.45E+06	...
Eu-154	5.00E-11	8.80E+01	2.15E-02	1.40E-03	4.29E+08	2.79E+07	...
Eu-155	3.00E-10	3.40E+01	8.30E-03	5.40E-04	2.77E+07	1.80E+06	...
Pu-236	8.00E-14	2.20E-04	5.37E-08	3.49E-09	6.71E+05	4.37E+04	...
Pu-238	3.00E-14	4.80E+01	1.17E-02	7.62E-04	3.90E+11	2.54E+10	...
Pu-239	2.00E-14	1.10E+02	2.68E-02	1.75E-03	1.34E+12	8.73E+10	...
Pu-240	2.00E-14	5.80E+01	1.42E-02	9.21E-04	7.08E+11	4.61E+10	...
Pu-241	1.00E-12	4.40E+03	1.07E+00	6.99E+02	1.07E+12	6.99E+10	...
Pu-242	2.00E-14	2.10E-02	5.12E-06	3.33E-07	2.56E+08	1.67E+07	...
Am-241	2.00E-14	9.30E+01	2.27E-02	1.48E-03	1.13E+12	7.38E+10	...
Cm-244	4.00E-14	4.60E+00	1.12E-03	7.30E-05	2.81E+10	1.83E+09	...
SUMMARY							
Total Relative Dose (Curies released/DCG)					4.84E+12	3.15E+11	3.00E+08
Ratio of Doses from seven element disruptive event in basin to cask drop event						6.51E-02	6.19E-05
Note: Seven Element release assumes all radioactive material escapes from fuel in one barrel of canister and the water has a decontamination factor of 10E+04							

4.3 Bounding Case in Shipping Cask

The consequences for the event of a single assembly accidentally becoming dry in its shipping container while in the shipping cask, as described in section 3.2 were analyzed (Plys 1994). The details of the analyses are presented in Appendix C. (Note: The term "element" in Appendix C is intended to be the fuel assembly, that is an inner and outer element).

The analyses included four parts, (1) the potential for fuel ignition, (2) the extent of reaction under the conditions expected in the shipping container, (3) the fission product release, and (4) the attenuation of fission products.

Neither hydride burning nor bulk uranium burning are considered reasonable under the conditions in the shipping container. The analysis showed temperatures expected in the container from the decay power and the chemical reaction balanced by the system heat losses would not be high enough to cause ignition in the thin layer of uranium hydride unless it were presented as submicron particles. Hydride burning was nonetheless assumed in order to illustrate the consequences.

If ignition of the hydride did occur, the extent of long-term reaction is limited by the availability of air. The amount of air that could leak into the container through the bottom failure and out through the top vent was calculated. The steady state temperature resulting from the hydride/air reaction is calculated to be approximately 57°C.

The fuel temperature of 57°C, is well below that for any data available on fission product release. Using the assumption that 1% of the fission products in the assembly is released as a unit of the fuel is oxidized, calculations (Appendix C) show that approximately 4 milligrams per hour of fission products are released from the fuel and 0.03 milligrams are released from the casks per hour. The relative dose for this case is 7.3×10^{-6} or 2.1×10^{-5} rem.

5.0 CONCLUSIONS

Storage cylinders in KW are known to have some broken N reactor fuel elements in which the exposed uranium is reacting chemically with water in the cylinder. The products of these reactions are uranium oxide, hydrogen and potentially some amount of uranium hydride. Of particular concern is the case where most or all the original water in the sealed cylinders may have reacted with the uranium leaving uranium oxide and some unknown but small amount of uranium hydride. When these cylinders are opened under water to remove the fuel elements or assemblies the basin water will rush in and can react with the uranium hydride. Part of this report analyzes the most likely and highly unlikely sequences of events and presents the extent of radiological dose release from the uranium hydride and water reaction in the cylinder and the potential of burning the released hydrogen. A further analysis examines an incredible hydrogen burn event at the basin surface and predicts an inconsequential pressure surge. A second part analyzes a postulated accident sequence for a fuel assembly in a water filled shipping container in a cask as the cask is being raised from the K-Basin and drained of water.

Analysis for the bounding case, considering data and information from the literature, indicates that under conditions similar to those expected in the cylinders, only a small fraction of the uranium (2-9%) reacts to form the hydride. This analysis using a safety factor of more than 2, that is, assuming 20% of the corrosion product is UH_3 , showed the maximum UH_3 would be 100 moles. The literature also indicates that less than 20% or approximately 20 moles of the hydride will react rapidly with water to form hydrogen. Thus, in this most likely event the amount of hydrogen formed when the cylinder is opened would be less than 55 ft³. No burning of hydrogen is probable in this case because of rapid mixing with air, and no pressure build up occurs. However, if this amount of hydrogen were assumed to be ignited and burned, the peak pressure would be about 0.1 psig. No damage to the K-Basin structures will occur nor would there be injury to personnel. Analysis shows the radiological dose to operators at the basin surface in this case is less than 1 mr/hr, which will not place any undue restrictions on operators opening the canisters.

Analysis for the theoretical quantity of uranium hydride showed that 395 moles would be formed in a cylinder. This is the upper limit of hydride that can form in a cylinder, independent of how the hydride may be assumed to be protected. Ideas were discussed in this report, such as a thick non-porous layer of oxide protecting the hydride from reacting with water in the cylinder, or the special partitioning of the uranium-water reaction to some of the fuel assemblies to form hydrogen and the hydrogen escaping to enter the remaining fuel assemblies at the top to form an ever lengthening column uranium hydride. These ideas require so many improbable series and sequence of circumstances as to be highly unlikely to incredible to occur. If this amount of uranium hydride mixed immediately with water approximately 1100 ft³ of hydrogen would be released. When the hydrogen reaches the surface, mixing will suppress the gas from burning. Thus, there is still no hazard to personnel or the K Basin structure. If it is assumed that all of this hydrogen is burned (an incredible event), analysis shows the maximum pressure is about 1.8 psig. Although the pressure gradient is low at this pressure, some of the building panels would probably be blown off which would be a risk to personnel outside, but the structure remains intact. There could be risk from the burned plume temperature for personnel depending on where they are located in the basin building. Irradiation analysis shows the release of radioactivity to the site boundary is 0.019 Rem or 6.5×10^{-2} of that allowed by the basin Safety Evaluation.

Since the access of water to the uranium, as well as to any uranium hydride that may have formed at the uranium surface in the fuel assemblies stored in the KE-Basin, is essentially unlimited, the analyses show that the potential for significant quantities of hydride formation in KE-Basin fuel is far less than for the fuel assemblies in the KW-Basin, and should be considered incredible.

In addition since the analyses in the report are based only on the geometry of the storage arrangements for the fuel elements, the quantities of uranium hydride are not dependent on the length of time in storage.

Analysis of the postulated single assembly shipping container accident in the cask during shipping showed the potential for significant release of

fission products to be highly unlikely. If ignition should occur, the release of fission products from this single element will be less than that for the maximum credible accident with 42 elements identified for the 105 KE Basin Safety Evaluation (WHC-1) and will result in a relative dose of 5.5×10^{-6} or 1.6×10^{-5} rem.

Independent reviews were made or alternate methods were used to check the calculations in this report. Appendix E contains statements or checklists from the reviewers. All the calculated results were found to be correct and consistent by the reviewers.

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7.0 APPENDICES

7.1 Appendix A. Evaluation of Flammable Gas Releases

Hazard evaluation of flammable gas releases frequently lead to discussions of deflagrations versus detonations. A rational basis is needed to define when detonation is an improbably event because the consequences are usually quite severe. This memo is based heavily on (Sherman 1988) and may be used to provide a better basis for the definition.

7.1.1 Background

A detonation can occur for a hydrogen/air mixture by two ways: (1) A direct ignition by a powerful shock source i.e., about 1g of high explosive for a stoichiometric mixture. This is considered incredible for K Basin events and will be discarded. (2) Deflagration-to-Detonation Transition (DDT). This involves igniting the gas plume, producing a subsonic flame (deflagration), which propagates into the unburned combustible mixture. The flame accelerates to velocities which cause compression waves to form in front of the combustion wave. Shock waves may form and the burning process may transition to a detonation wave. Flame acceleration is dependent on (a) the sensitivity of the mixture and (b) geometric factors such as obstacles, scale, and the amount of expansion volume near the accelerating wave front. The sensitivity of the mixture is usually characterized by the equivalence ratio, ϕ , as defined by Equation A1.

$$\phi = \frac{f/a}{(f/a)_{stoic}} \quad A1$$

where f = fuel concentration

a = air or oxidizer concentration

For stoichiometric conditions, the equivalence ratio is unity. For fuel-lean mixtures it is less than one and for fuel-rich mixtures, it is greater than one.

7.1.2 Methodology

There is no theory that can predict flame acceleration to detonation for all mixture conditions and geometries. The methodology summarized in the following paragraphs is based on experimental data and years of research experience. (Sherman 1988)

The methodology is based on the following assumptions:

- (1) The likelihood of DDT can be expressed as a function of two variables:
 - (a) The "sensitivity" of the mixture as measured by the equivalence ratio.
 - (b) The "geometry" influence on flame acceleration during the deflagration propagation. This characterizes the space and includes obstacles and size considerations.

Based on the equivalence ratio, ϕ , mixtures are divided into five sensitivity classes:

- (1) mixtures near stoichiometric that are extremely detonable,
- (2) mixtures that are less likely to detonate,
- (3) mixtures that have been observed to undergo detonations in geometries that favor flame acceleration,
- (4) mixtures that have been observed to propagate a detonation, but a DDT has not been observed,
- (5) mixtures that are unlikely to undergo DDT.

The classification of mixture sensitive to detonation is shown in Table A1.

Table A1. Classification of Hydrogen-Air Mixtures at 20°C and 1-atm Pressure.

Mixture Class	Equivalence Ratio	Mole Fraction, %
1	$0.75 < \phi \leq 1.5$	24 to 38
2	$0.63 \leq \phi < 0.75, 1.5 \leq \phi \leq 2.2$	21 to 24 and 38 to 48
3	$0.42 \leq \phi < 0.63, 2.2 < \phi \leq 4.1$	15 to 21 and 48 to 63
4	$0.37 \leq \phi < 0.42, 4.1 < \phi \leq 5.6$	13.5 to 15 and 63 to 70
5	$\phi < 0.37, \phi > 5.6$	< 13.5 and > 70

The flame acceleration potential of a given region is classified into one of five geometric classes beginning with geometric class 1 being the most conducive to flame acceleration, to geometric class 5 being the least conducive. A description of these classes follows.

Geometric Class 1. Large geometries with obstacles in the path of the expanding unburned gasses. Partial confinement favors gas expansion past obstacles. A large tube with numerous obstacles and with ignition going from a closed end to an open end is an example. Class 1 geometries are the most favorable to large flame acceleration.

Geometric Class 2. Large geometries similar to class 1 but with some features that hinder flame acceleration. Examples would be a tube open on both ends or large amounts of volume with transverse expansion to the direction of the flame propagation.

Geometric Class 3. Geometries that yield moderate flame acceleration but are neutral to DDT. Examples are large tubes without obstacles and small tubes (several in. diameter) with obstacles.

Geometric Class 4. Geometries unfavorable to flame acceleration. Examples are large volumes with few obstacles and large amounts of venting transverse to the flame path, and small volumes without obstacles. DDT will not usually occur in a class 4 geometry.

Geometric Class 5. Geometries are so unfavorable to flame acceleration that not even large volumes of stoichiometric hydrogen/air mixtures are likely to detonate. Examples are a totally unconfined geometry at large scale or a small spherical geometry without obstacles and central ignition.

A results table (Table A2) gives the result class as a function of mixture and geometric classes. The entries in this table are based on the subjective judgment of the likelihood of transition to detonation based on investigator's opinions at the Sandia National Laboratories with many years of experience and laboratory experimentation in the field of detonation physics.

Table A2. Dependence of Result Class on Mixture and Geometric Classes

Geometric Classes	Mixture Classes				
	1	2	3	4	5
1	1	1	2	3	4
2	1	2	3	4	5
3	2	3	3	4	5
4	3	4	4	5	5
5	4	5	5	5	5

The entries in Table A2 can be interpreted as follows:

Result class 1: DDT is highly likely

Result class 2: DDT is likely

Result class 3: DDT may occur

Result class 4: DDT is possible but unlikely

Result class 5: DDT is highly unlikely to impossible

7.2 Appendix B. N Reactor Fuel Dimensions and Weights

Diameters and lengths for the Mark IA and Mark IV inner and outer fuel elements are given in Table B1.

Table B2 shows the uranium fuel weights as "factors" for the several types and lengths of the Mark IA and Mark IV fuel elements.

These tables are from WHC-NR-M-2, Volume 3, pages 1 and 2, dated May 1, 1989.

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Table B1. Diameters and Lengths for the Mark IA and Mark IV Inner and Outer Fuel Elements.

DIMENSION SCHEDULE			
Dimension	Model		
	Mark IA	Mark IV	
A	.250	.125	
B	.800	.500	
C	3.72	3.45	
D	3.00	5.00	
DIAMETERS			
Outer OD	2.391-2.416	2.410-2.435	
Outer ID	1.754-1.779	1.691-1.716	
Inner OD	1.237-1.256	1.267-1.286	
Inner ID	0.431-0.450	0.473-0.492	
LENGTHS			
Length Code	Model	Inner	Outer
M	Mark IA	20.82	20.88
T	Mark IA	19.52	19.58
F	Mark IA	14.85	14.91
E	Mark IV	26.04	26.10
S	Mark IV	24.50	24.56
A	Mark IV	23.14	23.20
C	Mark IV	17.34	17.40

Table B2. Uranium Fuel Weights for the Several Types and Lengths of the MARK IA and MARK IV Fuel Elements.

Fuel Description	Fuel Type	Fuel Code	Factor* wt lb	Enrichment wt% ²³⁵ U	Comment
21" Spike Outer		A12M	24.43	1.25	Most common spike fuel
21" Spike Inner		N09M	12.12	0.95	
21" Spike Assy.	MK IA	A12N09M	36.55		
19.5" Spike Outer		A12T	22.88	1.25	Rework spike length
19.5" Spike Inner		N09T	11.34	0.95	
19.5" Spike Assy.	MK IA	A12H09T	34.22		
15" Spike Outer		A12F	17.29	1.25	Rework spike length
15" Spike Inner		M09F	8.57	0.95	
15" Spike Assy.	MK IA	A12M09F	25.86		
26" Outer		B09E	35.22	0.95	Most common MK IV in central zone
26" Inner		X09E	16.50	0.95	
26" Assy.	MK IV	B09X09E	51.72	0.95	
24.5" Outer		B09S	33.09	0.95	Rework
24.5" Inner		X09S	15.52	0.95	
24.5" Assy.	MK IV	B09X09S	48.61	0.95	
22" Standard Outer		B09R	29.45	0.95	
22" Standard Inner		X09R	13.90	0.95	
22" Standard Assy.	MK IV	B09X09R	43.35	0.95	
23" Outer		B09A	31.23	0.95	Most common MK IV in fringe
23" Inner		X09A	14.64	0.95	
23" Assy.	MK IV	B09X09A	45.87	0.95	
17" Outer		B09C	23.13	0.95	
17" Inner		X09C	10.94	0.95	
17" Assy.	MK IV	B09X09C	34.07	0.95	
6" Outer	Standard for Enrichment Tester			0.71	
6" Outer	Standard for Enrichment Tester			0.95	
6" Outer	Standard for Enrichment Tester			1.25	

*See current copy of "Factor Weights for N Fuel Elements" issued by Accountability Organization for most recent values.

Table B2. Uranium Fuel Weights for the Several Types
and Lengths of the MARK IA and MARK IV Fuel Elements. (cont.)

Fuel Description	Fuel Type	Fuel Code	Factor* wt lb	Enrichment wt% ²³⁵ U	Comment
26" Natural Outer		B07E	35.22	0.71	Most common MK IVB fuel in the reactor
26" Natural Inner		X07E	16.50	0.71	Standard length natural fuel
26" Natural Assy.	MK IVB	B07X07E	51.72	0.71	
23" Outer		B07A	31.23	0.71	
23" Inner		X07A	14.64	0.71	
23" Assy.	MK IVB	B07X07A	45.87	0.71	
21" Outer		B15M	28.11	1.15	PT-N-557
21" Inner		X09M	13.10	0.90	
21" Assy.	MK IVC	B15X09M	41.21	1.085 Avg.	
20" Natural Outer		A07B	24.01	0.71	
20" Natural Inner		N07B	11.99	0.71	
20" Natural Assy.	MK IB	A07N07B	36.00	0.71	
23" Standard Outer		A09A	27.21	0.95	
23" Standard Inner		N09A	13.59	0.95	
23" Standard Assy.	MK IC	A09N09A	40.80	0.95	
19" Standard Outer		A09P	22.18	0.95	
19" Standard Inner		N09P	11.07	0.95	
19" Standard Assy.	MK IC	A09N09P	33.25	0.95	
17" Standard Outer		A09C	20.29	0.95	
17" Standard Inner		N09C	10.13	0.95	
17" Standard Assy.	MK IC	A09N09C	30.42	0.95	
12" Standard Outer		A09D	13.35	0.95	
12" Standard Inner		N09D	6.65	0.95	
12" Standard Assy.	MK IC	A09N09D	20.00	0.95	2 pieces are in the basin
26" Spike Outer		A12E	30.69	1.25	12 pieces are in the basin
26" Spike Inner		A09E	15.33	0.95	
26" Spike Assy.	MK IA	A12N09E	46.02		

*See current copy of "Factor Weights for N Fuel Elements" issued by Accountability Organization for most recent values.

7.3 Appendix C. Analysis for Single Element Canister Drain and Cask
RolloverAccidents

WHC-SD-SNF-SARR-001, REV. 0

Fauske & Associates, Inc.

DATE: 23 August 1994
TO: Dave Bergmann, Bruce Makenas @ Westinghouse Hanford Co.
FROM: Martin Plys, Sung Jin Lee, Mike Epstein *Mart*
TOPIC: Single Element Canister Drain and Cask Rollover Accidents

FAI has reanalyzed the single fuel element canister drainage accident and has additionally analyzed a cask rollover accident postulated by WHC. This memorandum documents our results and supersedes our previous memorandum [1]. Fundamental conclusions that remain unchanged and are common to these accidents are: (1) Fuel ignition is not expected, (2) The extent of oxidation and fission product release would in any event be limited to very low values by phenomena limiting the supply of air and water vapor to fuel.

Single Element Canister Drain Accident

FAI has reanalyzed the postulated single element canister drainage accident to determine potential consequences. The difference between this analysis and our previous one [1] is that water vapor is now allowed as a reactant for fuel (hydride) oxidation. Note that the fuel mass we used may be slightly different than the mass of an element transported, but our answers are not sensitive to this nor to minor variation in other parameters.

Our results are summarized below. The main conclusions are that (1) Fuel ignition is not expected to occur, (2) Even if fuel ignition is assumed the reaction rate is severely limited by oxygen or steam availability and fuel does not significantly heat up, (3) Fission product release from fuel under these conditions would be very low, and (4) Released fission products would preferably plate out in the canister and cask, so that an overall decontamination factor for 1 micron particles is over 100.

First, here is a brief description of the problem we considered. A single fuel element (assumed to weigh 50 lbs) is contained in a 4" diameter, 27" long, 1/4" thick stainless steel canister with a 1/16" diameter top vent; this canister is in turn contained within a 26.5" diameter, 54" tall metal (steel-lined lead) cask with a 1/4" diameter bottom drain. The canister is assumed to fail at the bottom to allow drainage of its water, ultimately out of the cask as well, and the cask top is assumed leaky.

We were to assume that fuel could chemically react and evaluate consequences; in addition we were to consider the realism of that assumption. The assumed reactions were between oxygen and water vapor (oxidants) and uranium hydride (fuel) to yield hydrogen. These reactions maximize the potential for energy release by maximizing the density difference between gases

in the cask (high density) and in the canister (low density) which in turn leads to the highest supply of oxidant. Our results yield temperatures too low for the hydrogen to burn anyway.

1. Fuel Ignition. We believe that ignition would not occur. The potential for ignition is determined by the existence of a steady balance between decay power, the chemical reaction rate at the canister temperature, and heat losses from the system. One must postulate a porous layer of uranium hydride (or metal) powder on the fuel surface in order for ignition to be even remotely possible. Decay power turns out to be negligible in this case for ignition theory. The chemical reaction rate is significantly influenced by the presence of humidity, and changes little in this case for humidity in excess of about 50%. The canister gas temperature in C required for fuel ignition is given here for several particle sizes and layer thicknesses at high humidity:

Particle Diameter	2 mm Layer	5 mm Layer
1 micron	35.7 C	25.9 C
2 micron	43.6 C	33.3 C
3.3 micron	49.7 C	38.8 C
10 micron	64.8 C	52.1 C
50 micron	93.6 C	75.9 C

Discussion at Hanford established that layers of 2mm maximum should be considered, and particle sizes of nominally 50 microns could exist but hydriding could cause smaller sizes. Thus for a 2mm layer submicron particles are required for ignition. The model equations for ignition theory have been validated by FAI and will be presented to WHC in a forthcoming report on the potential for fuel ignition during K basin accidents [2].

2. Extent of Reaction. There is little initial oxidant present in the canister, and thus long-term reaction of fuel is limited by exchange flows between the canister and cask. The canister interior volume is about 6 liters, holding about 0.055 moles O₂, while there are about 95 moles U, so less than 0.1% of the U can initially react. A reaction cannot take place until the fuel is dry because evaporation will keep the fuel temperatures low. Logically this also means that there is adequate time for drainage of water from all interior surfaces. In the longer term, air may flow into the canister from the cask via the canister failure, and flow out via the top vent.

Hand calculations and computer calculations were made and are in accord for this case. Figure 1 shows the steady-state flowrate between the canister and cask (about 3 mg/s), and Figure 2 shows the steady state temperatures achieved (about 330 K). There is a brief initial transient (practically all on the vertical axis) while initially present canister oxygen and water vapor are consumed. The flowrate is important because this provides the carrier gas for any fission products, and the temperature is important because it provides the potential for fission product release.

3. Fission Product Release. The fuel temperature, even with chemical reactions considered, is well below a value ever investigated for fission product release and virtually no release would be expected except for release of any trapped noble gases. At temperatures above 600 C, for which data exist, the releases are generally proportional to the time at temperature and thus are effectively proportional to the oxidation rate. We assumed 1% of the fission products contained in the fuel could be released as a unit mass is oxidized; this is probably high by two or more orders of magnitude. Over the 10,000 second calculation period, about 11.1 mg of fp were released (see the balance table in item 4 below) out of 49 g available, or a fraction of 0.00224, because about 0.51 kg of 22.7 kg total fuel were oxidized. You may divide numbers presented

below for deposition and release to the environment by 100 to normalize to a release fraction of 0.01%. At high temperatures, fission products are released as vapors which condense into tiny particles; at these low temperatures, we must hypothesize some kind of mechanical release of fuel grain fragments, for example, micron-sized hydride particles could fall off the fuel.

4. Fission Product Attenuation. An extremely lean aerosol is created which will not undergo much coagulation and can be modeled using Stoke's law for settling if the source particle size is known. Figure 3 shows the deposition history in the canister and cask, and the releases to the environment, assuming 1 micron size particles. The fission product balance is:

Location	Fission Product, mg
Deposited - canister	7.5
Deposited - cask	3.5
Released - cask	0.09
Released - fuel	11.1

where suspended aerosol is negligible in this balance. The decontamination factor DF for the canister is thus $(11.1 \text{ in}) / (3.6 \text{ out}) = 3$ and for the cask it is $3.6 / 0.09 = 40$; the overall DF is 120. These decontamination factors would be lower for smaller particles, but there is little basis for choosing particles that would be much smaller than the particles formed by hydriding.

Cask Rollover Accident

A cask rollover accident during shipping was postulated by WHC for this scenario. Our analysis leads to the same basic conclusions as for the cask drainage accident above, ie, fuel ignition is not expected and fission product releases would be quite small and physically limited.

The scenario analyzed features the same fuel cask as before, but laying on its side, with a 1 square inch opening on its top representing leakage (flow oriented horizontally now) and with its bottom drain plugged. A single element canister inside the cask has been punctured at the bottom (flow also now oriented horizontally) with an area of 0.376 square inches and it has been drained of water. Again we ask the questions, will non-negligible exothermic oxidation of the fuel occur, and even if it does, what are the possible consequences.

Note that a single canister inside the cask was assumed and multiple canisters modify the results as follows: (1) The conclusion that ignition should not occur holds firm, and (2) Simply multiply the fission product source by the number of canisters. This is allowable since the sedimentation rate rises in greater proportion than the suspended aerosol concentration using the detailed aerosol model; strict proportionality would be observed if single particle sizes were used (ie for a lean aerosol with negligible coagulation as used in the calculation above).

Four features of the analysis differ from the previous case. First, the horizontal openings of the single element canister and cask allow countercurrent gas exchange. Less dense gas inside the canister (or cask) moves out to the cask (or ambient) through the upper half of the horizontally-oriented flowpath and denser gas flows countercurrent via the bottom half. That is, there are no longer pairs of openings at the bottom and top of each volume allowing a chimney type flow. This mechanism of course is the only flow exchange mechanism for the cask. Second, the aerosol sedimentation areas are greater for both cask and canister due to the horizontal orientation. Third, we have specified fission product release as 0.1% of the oxidized material

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in order to be less conservative than in the previous case. Last, we have used two different aerosol models for reasons elucidated below.

1. Fuel Ignition. Fuel ignition is not expected for this accident for the same reasons discussed for the single element canister drain accident above.

2. Extent of Reaction. Even if chemical reactions of the fuel are assumed, the reaction rate is limited by the supply of gas due to exchange flow between the canister and cask. This flowrate is smaller than for the accident examined above because the limiting canister opening is the 1/16" vent hole and the elevation difference between the failure and vent hole is now smaller. The fuel element temperature is thus lower, about 312 K.

3. Fission Product Release. Less fission product is released than in the previous case because 0.1 % of the reacted fuel inventory was released (vs 1 %), and also because the canister exchange flow is lower; 0.36 mg out of 49 g were released.

4. Fission Product Attenuation. Two aerosol model approaches were employed. First, as in the previous problem, because no vaporization release was expected, the mechanical entrainment of 1 micron particles was assumed. Second, in order to see the results that a polydisperse model would yield, the MAAP fission product model was employed. Figures 4 and 5 and the following list show the fission product balance for two aerosol models.

Location	Fission Product, mg	
	1 Micron Particles	Polydisperse (MAAP)
Deposited -canister	<0.36	0.3
Deposited - cask	0.007	0.05
Released - cask	0.0001	0.007
Released - fuel	0.36	0.36
DF	3600.	51.

For the 1 micron particle case, significant fission product release only occurs during the initial transient consumption of oxidant gases within the canister. The DF is higher for this case than for the single element canister case because exchange flowrates are lower. The DF is lower for the polydisperse case because the average particle size is well below 1 micron, so that the sedimentation rate is smaller. Of course, such small particles can only be formed by coagulation of condensed vapors, since mechanically produced particles would be 1 micron or larger. Since the temperature achieved by the fuel is too low for vaporization of fission products, we may conclude that the DF to expect in such a case would be closer to that of the 1 micron case.

[1] Martin Plys, FAI Memorandum to David Bergmann and Bruce Makenas, Single Element Canister Drain Accident, 4 August 1994.

[2] Michael Epstein et al, K-Basin Severe Accident Analysis: Fuel Heatup and Ignition Potential, FAI/94-76, draft, to be presented to Westinghouse Hanford Company, August, 1994.

cc: H. Fauske
 S. Lee
 M. Epstein

Figure 1. Single Element Canister Accident

Canister-Cask Circulation Flow Rates

Figure 2. Single Element Canister Accident

Figure 3. Single Element Canister Accident.

Figure 4. Cask Rollover Accident, Monodisperse.

Figure 5. Cask Rollover Accident, Poly Disperse.

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7.4 Appendix D. Decontamination Factors

September 22, 1994

Pool Scrubbing of Fuel and Corrosion Product Particulate

This one-page summary was sent to Jim Wiborg in February 1994 as background and support during the hydride discussions with DNFSB back then. Since that time I have retrieved numbers for a "downcomer" injection mode in which one large bubble enters a pool and breaks up. The DF for a 1 micron particle when the bubble originates under 3 m of water subcooled 10 C and contains no steam initially is just under 10^{**6} . The DF is larger for larger particles, all of which are true for K Basin.

Pool scrubbing of fuel and corrosion product particulate will greatly attenuate any releases from a suddenly vented submerged canister. The degree of attenuation is described commonly by the decontamination factor, DF, which is the ratio of source material flowrate to observed material flowrate. The DF thus represents the factor by which a source is attenuated.

Research on DF's for application to nuclear reactor safety has been conducted since the 1960's. It is fair to say that our knowledge in this area is technically mature and widely accepted in regulatory venues.

Factors which influence the DF for a canister release are:

Particle Size - The most important factor. DF's are typically plotted as a function of particle size. Competing mechanisms involved at different ends of the particle size spectrum (small particles - diffusion and thermophoresis, large particles - inertial impaction and gravitational sedimentation) mean that there is usually a minimum in the DF curve between 0.1 and 1 micron. The DF can increase dramatically away from the minimum. For K-Basin, this means any particle bigger than 1 micron will never see air. Fine corrosion particulate is about micron size.

Pool depth - Important for shallow pools or situations where the DF is otherwise low; not important for 10 ft deep cold pools, i.e., we do not care much if the pool is 8 ft or 15 ft deep for K-Basin.

Carrier gas - In this case, hydrogen. DF's are smaller when the carrier is a nearly pure noncondensable, i.e., at low steam fractions.

Pool subcooling - Not important for gases with low steam fractions, and very important for gases with high steam fractions. For K-Basin, the degree of subcooling is not important since H₂ is the carrier.

Carrier gas temperature - More important for cases with significant steam fractions or shallow pools, not very important for K-Basin. A higher gas temperature implies early bubble growth due to evaporation, and later collapse as the newly-added steam in the rising, cooling bubble condenses.

Injection mode - Here at high pressure through a small orifice, which provides a large DF. The higher the pressure the better, since injected particles are removed by inertial impaction.

The DF for a one micron particle carried by hydrogen at 500 K through a large number of 0.5 inch orifices into a 4 m deep pool with 20 C subcooling is on the order of 10^{**8} (ten to the eight power). This is four orders of magnitude greater than a DF which can be reliably measured. It is calculated using well-known physical models which agree well with data in lower DF situations. A plot of DF versus particle size was provided on January 7 for this case.

A regulatory case is best built when insensitive to variation in the DF, and in the case of K-Basin there are several orders of magnitude of cushion, so that a reasonable person would agree that it is incredible for more than 0.01% or even 0.001% of the released material emerge from the pool.

7.5 Appendix E. Independent Verification of Calculations

7.5.1 Calculation Verification Checklist

Calculations of the potential quantities of uranium hydride and hydrogen as reported in Section 2.2 were checked by A. E. Bridges, WHC. A checklist is included.

7.5.2 Review Pedigree for Appendices C and D.

Calculations and analysis for the "Single Element Canister Drain...Accident," Appendix C and the "Decontamination Factors," Appendix D, both used in Sections 4.2 and 4.3 were checked and reviewed by the staff of Fauske and Associates. A letter is included. References 1 and 2 refer to contents of Appendices C and D respectively.

7.5.3 Independent Review of Hydrogen Gas Plume-Burn Calculation for K-Basins

Calculations and analysis for pressure increases and the potential for hydrogen burn or detonation presented in Section 4.1 and Appendix A were reviewed by M. P. Weis. A memo is included.

7.5.4 Independent Verification of Relative Dose Calculations Hydride Document.

Calculations and analysis for the radiological doses presented in Section 4.2 and 4.3 were prepared by R. H. Meichle and checked by E. N. Dodd, Jr. A memo is included.

7.5.1 Calculations Verification Checklist

Document Reviewed: WHC-SD-SNF-SARR-001, Section 2.2

Yes	No	Question
X		Were the inputs for the calculations correctly selected?
X		Are the assumptions necessary to perform the design calculations adequately described and reasonable?
X		Was an appropriate methodology used in performing the calculations?
X		Were the inputs correctly incorporated into the calculations?
X		Are the outputs of the calculations correct and reasonable?

Alvia E. Bridges
Alvia E. Bridges, Engineer
Nuclear Fuel Evaluations

8/31/94
Date

WHC-SD-SNF-SARR-001, REV. 0

DATE: 26 August 1994
TO: Jim Weber @ Westinghouse Hanford Co.
FROM: Martin Plys *Martin Plys*
TOPIC: Review Pedigree for Refs. [1] and [2]

References [1] and [2] received internal review at FAI prior to transmittal to WHC.

I acted as a manager and reviewer for the calculations in [1] and I assembled memos transmitted to WHC based on that information. Specifically, Sung Jin Lee performed computer calculations in [1] which were observed to be in accord with hand calculations by Mike Epstein. I reviewed further calculations to ensure continued accord.

I authored [2] and drew the DF value from information transmitted by Barbara Schlenger of FAI which was entirely generated under the FAI QA plan as part of the MAAP code development, and Barbara and I discussed the problem to ensure correct application of the DF data.

[1] M.G. Plys, S.J. Lee, and M. Epstein, FAI memorandum to D. Bergmann and B. Makenas, Westinghouse Hanford Co., Single Element Canister Drain and Cask Rollover Accidents, 23 August 1994.

[2] M.G. Plys, WHC cemail to J. Weber, Pool Aerosol DFs, 12 August 1994.

cc: H.K. Fauske

Westinghouse
Hanford Company

WHC-SD-SNF-SARR-001, REV. 0

Internal
Memo

From: Component Stress Analysis
Phone: 6-5446 H5-56
Date: September 14, 1994
Subject: INDEPENDENT REVIEW OF HYDROGEN GAS PLUME-BURN CALCULATION FOR
K-BASINS

CSA:MPW:ggb:94/7

To: G. L. Fox L5-01

cc: L. W. Bartholf H5-53
B. J. Makenas L5-01
M. R. Lindquist H5-57
C. J. Moore H5-57 *gm*
R. P. Omberg R3-85
J. B. Truitt H5-56 *ggb*
J. W. Weber L5-01
MPW File/LB

References:

1. Fox, G. L., et al. 1993, *Tank 241-SY-103 Hazard Assessment*, WHC-SD-WM-SAR-061, Rev. 0, Westinghouse Hanford Company, Richland, Washington.
2. Weis, M. P., and C. J. Moore, 1993, *Hydrogen Gas Mix Burn Analysis for the Grout Disposal Facility*, WHC-SD-WM-ER-162, Rev. 0, Westinghouse Hanford Company, Richland, Washington.
3. Cashdollar, K. L., et al., 1992, *Laboratory Flammability Studies of Mixtures of Hydrogen, Nitrous Oxide, and Air*, WHC-SD-WM-ES-219, Rev. 0, Westinghouse Hanford Company, Richland, Washington.
4. Sherman M. P. and M. Berman, 1987, "The Possibility of Local Detonations During Degraded-Core Accidents in the Bellefonte Nuclear Power Plant," *Nuclear Technology*, Vol. 81, Albuquerque, New Mexico.

This memo responds to your request for an independent review of the hydrogen-burn analysis in the draft report *Review of Consequences of Uranium Hydride Formation in N-Reactor Fuel Elements Stored in the K-Basins*. You performed the burn calculations using the plume-burn model as documented in Reference 1. The pressure as a function of released hydrogen is given in Figure 2 of the draft report. This review verifies the conservatism of those pressures and discusses the high improbability of a detonation for the given conditions.

This review uses an alternate calculation to verify the calculated pressures in the K-Basin plume-burn analysis. The alternate calculation

G. L. Fox
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September 14, 1994

CSA:MPW:ggb:93/7

(Attachment 1), implemented in Mathcad¹, conservatively predicts the peak pressure and temperature in a constant-volume burn with no loss of heat to the surroundings. This Mathcad worksheet will perform the calculation for any valid mixture of hydrogen, nitrous oxide, nitrogen, and oxygen. Thus, the worksheet can predict the results of a hydrogen/nitrous oxide burn, a hydrogen/oxygen burn, or a combination of the two. The worksheet has been reviewed and checked (Reference 2) and shown to be conservative in comparison to experimental results (Reference 3).

The Mathcad worksheet implements a single lumped-parameter model, which assumes uniform gas composition and properties throughout the volume. Attachment 2 provides a list of assumptions for the calculation. Essentially, the worksheet determines the potential chemical energy in the reactants and assumes this energy increases the kinetic energy (temperature) of the gas. Using the ideal gas law, it calculates the corresponding pressure response from the temperature of the gas. This worksheet ignores the lower flammability limit of the mixture; it conservatively determines the bulk temperature and pressure response based on the amount of potential chemical energy stored in the reactants. Table 2 presents the comparison between selected data points in Figure 2 of the draft report and results from the Mathcad worksheet.

Table 2. Comparison of Mathcad Calculation and Plume-Burn Results.

Hydrogen Release (ft ³)	Peak Pressure (Plume-burn) (lbf/in ² gauge)	Peak Pressure (Mathcad) (lbf/in ² gauge)
55	0.1	0.106
200	0.35	0.387
400	0.72	0.773
600	1.05	1.158
800	1.4	1.542
1000	1.71	1.925
1046	1.8	2.013

The alternate calculation in Mathcad shows good agreement to the results from the plume-burn analysis. The higher pressures from the single lumped-parameter model (Mathcad) does not indicate that the plume-burn analysis is not conservative. Rather, it's due to the difference in the two phenomena. The plume burn heats the local plume gases to a higher

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G. L. Fox
Page 3
September 14, 1994

CSA:MPW:ggb:93/7

temperature than the surrounding gases resulting in a lower pressure in the overall vapor space. The noticeable trend from Table 2 is that as the amount of released hydrogen increases, the percent difference in the two results increases. In summary, the Mathcad analysis is very conservative and due to the close agreement between this alternate calculation and the plume-burn calculation, the plume-burn calculation is shown to be conservative.

Finally, detonation is highly improbable due to the K-Basin large open-air-space geometry combined with a small hydrogen release (based on the Sandia report results in Reference 4).

M. P. Weis, Advanced Engineer
Component Stress Analysis

ggb

*
Attachments (2)

Attachment 1

Mathcad Worksheet (Hydrogen Release Volume = 600 ft³)

ANALYTICAL CALCULATIONS

Page 1 of 4Subject Alternate Calculation to Check Hydrogen Gas Plume-Burn Calculations for K-BasinsOriginator M. P. WeisDate 9/5/94Checker See Weis and Moore 1993

Date _____

The following calculations are performed to predict the peak pressure resulting from a hydrogen gas burn in a closed volume.

Volume

Convert temperature from F to K.

$$TK(TF) = \frac{TF - 459.67}{1.8}$$

V = 300000

(ft³)

Convert temperature from K to F.

$$TF(TK) = 1.8 \cdot TK - 459.67$$

Conversion factors

$$\text{atm} = 101325 \quad (\text{Pa} = \text{N/m}^2)$$

$$\text{ft} = 0.3048 \quad (\text{m})$$

$$\text{atm} = 14.7 \quad (\text{psi})$$

$$\text{gal} = 0.13367 \quad (\text{ft}^3)$$

Initial gas conditions, constants

Ti = 289

Ti = 289

(K) initial temp of gas in closed volume

P = 1

(atm) initial air pressure in closed volume

Tr = 289

Tr = 289

(K) Cv reference temperature

HRH2N2O = 77.37

(kcal/mole) heat of combustion for H2+N2O

HRH2O2 = 57.3

(kcal/mole) heat of combustion for H2+O2

R = 1.986

(cal/g-mole K) universal gas constant

R' = 8.314510

(J/g-mole K) universal gas constant

Gas constituent percentages in closed volume

$$\text{cmpH2} = \frac{600 \cdot \text{ft}^3}{300000 \cdot \text{ft}^3} \cdot 100$$

(%) H2 volume (mole) percent

cmpN2O = 0.0

(%) N2O volume (mole) percent

cmpAIR = 100.0 - cmpH2

(%) air volume (mole) percent

cmpN2 = 0.79 · cmpAIR

(%) N2 volume (mole) percent

cmpO2 = 0.21 · cmpAIR

(%) O2 volume (mole) percent

gmH2Oi = 0.0

(g-moles H2O) water (moles) in closed vol (0=>dry air)

ANALYTICAL CALCULATIONS

Page 2 of 7Subject Alternate Calculation to Check Hydrogen Gas Plume-Burn Calculations for K-BasinsOriginator M. P. Weis

Date

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Date

Calculate the total gram-moles in the free volume from ideal gas law $PV = nRT$ or $n = PV/(RT)$.

$$gm = P \cdot atm \cdot V \cdot \frac{R^3}{R \cdot T_i}$$

Initial Gas Conditions:

 $T_i = 289$ $P = 1$ $V = 300000$ $gm = 358218.699$ Define the average constant-volume specific heat (cal/g-mole-K) for constituent gasses over the temperature (K) range T_r to T , i.e.,

$$C_v = C_p - R$$

where the average constant-pressure specific heat (cal/g-mole-K) is given by

$$aver_C_p(T) = \frac{1}{T - T_r} \int_{T_r}^T C_p(T) dT$$

Hydrogen:

$$C_{vH_2}(T) = 6.424 - \frac{0.001039}{2} \cdot (T - T_r) - 7.8 \cdot \frac{10^{-3}}{3} \cdot T^2 - T \cdot T_r - T_r^2 - R$$

Nitrogen:

$$C_{vN_2}(T) = 6.529 - \frac{0.001488}{2} \cdot (T - T_r) - 2.271 \cdot \frac{10^{-7}}{3} \cdot T^2 - T \cdot T_r - T_r^2 - R$$

Nitrous oxide:

$$C_{vN_2O}(T) = 18.036 - 4.474 \cdot \frac{10^{-5}}{2} \cdot (T - T_r) - 2.0 \cdot 158.08 \cdot \frac{\sqrt{T} - \sqrt{T_r}}{T - T_r} - R$$

Oxygen:

$$C_{vO_2}(T) = 6.732 - \frac{0.001505}{2} \cdot (T - T_r) - 1.79 \cdot \frac{10^{-7}}{3} \cdot T^2 - T \cdot T_r - T_r^2 - R$$

Water:

$$C_{vH_2O}(T) = 6.97 - \frac{0.003464}{2} \cdot (T - T_r) - 4.833 \cdot \frac{10^{-7}}{3} \cdot T^2 - T \cdot T_r - T_r^2 - R$$

ANALYTICAL CALCULATIONS

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Calculate individual constituent gram-moles before burn.

$$\begin{aligned} \text{gmH2Oi} &= 0.0 & \text{gmH2i} &= \text{gm} \cdot \frac{\text{cmpH2}}{100.} & \text{gmN2Oi} &= \text{gm} \cdot \frac{\text{cmpN2O}}{100.} \\ \text{gmN2i} &= \text{gm} \cdot \frac{\text{cmpN2}}{100.} & \text{gmO2i} &= \text{gm} \cdot \frac{\text{cmpO2}}{100.} \end{aligned}$$

Calculate individual constituent gram-moles products after burn.

$$\begin{aligned} \text{gmH2a} &= \text{if}(\text{gmH2i} \geq \text{gmN2Oi}, \text{gmH2i} - \text{gmN2Oi}, 0.0) \\ \text{gmH2p} &= \text{if}(\text{gmH2a} \geq 2 \cdot \text{gmO2i}, (\text{gmH2a} - 2 \cdot \text{gmO2i}), 0) \\ \text{gmO2p} &= \text{if}(\text{gmH2a} \geq 2 \cdot \text{gmO2i}, 0.0, (\text{gmO2i} - 0.5 \cdot \text{gmH2a})) \\ \text{gmH2Op} &= \text{gmH2i} - \text{gmH2p} \\ \text{gmN2Op} &= \text{if}(\text{gmH2i} < \text{gmN2Oi}, \text{gmN2Oi} - \text{gmH2i}, 0.0) \\ \text{gmN2p} &= \text{if}(\text{gmH2i} < \text{gmN2Oi}, \text{gmN2i} - \text{gmH2i}, \text{gmN2i} - \text{gmN2Oi}) \end{aligned}$$

Sum mole products for initial and post burn.

$$\begin{aligned} \text{gmToti} &= \text{gmH2Oi} + \text{gmH2i} + \text{gmN2Oi} + \text{gmN2i} + \text{gmO2i} \\ \text{gmTotp} &= \text{gmH2Op} + \text{gmH2p} + \text{gmN2Op} + \text{gmN2p} + \text{gmO2p} \end{aligned}$$

Calculate total average constant-volume specific heat for product gas mix.

$$\begin{aligned} \text{CvTot}(T) &= \text{CvH2O}(T) \cdot \frac{\text{gmH2Op}}{\text{gmTotp}} + \text{CvH2}(T) \cdot \frac{\text{gmH2p}}{\text{gmTotp}} + \text{CvN2O}(T) \cdot \frac{\text{gmN2Op}}{\text{gmTotp}} \dots \\ &\quad + \text{CvN2}(T) \cdot \frac{\text{gmN2p}}{\text{gmTotp}} + \text{CvO2}(T) \cdot \frac{\text{gmO2p}}{\text{gmTotp}} \end{aligned}$$

Calculate heat of reaction.

$$\begin{aligned} \text{heat1} &= \text{HRH2N2O} \cdot \text{gmH2i} \cdot 1000. \\ \text{heat2a} &= \text{HRH2N2O} \cdot \text{gmN2Oi} \cdot 1000. \dots \\ &\quad + \text{if}(\text{gmH2a} \geq 2 \cdot \text{gmO2i}, 2 \cdot \text{gmO2i} \cdot \text{HRH2O2} \cdot 1000, \text{gmH2a} \cdot \text{HRH2O2} \cdot 1000) \\ \text{heat2b} &= \text{HRH2N2O} \cdot \text{gmN2Oi} \cdot 1000. \\ \text{heat2} &= \text{if}(\text{cmpO2} \leq 0.0, \text{heat2b}, \text{heat2a}) \\ \text{heat} &= \text{if}(\text{gmH2i} \leq \text{gmN2Oi}, \text{heat1}, \text{heat2}). \end{aligned}$$

ANALYTICAL CALCULATIONS

Page 4 of 4Subject Alternate Calculation to Check Hydrogen Gas Plume-Burn Calculations for K-BasinsOriginator M. P. WeisDate 7/15/94Checker See Weis and Moore 1993

Date _____

$$T_{\text{guess}} = 1000$$

Given

Calculate post-burn gas temperature (MathCAD solves the equation for T_{guess} , given the initial value above.)

$$T_{\text{guess}} = \frac{\text{heat}}{C_v \text{Tot}(T_{\text{guess}}) \cdot \text{gmTotp}} - T_i$$

$$T_g' = \text{Find}(T_{\text{guess}})$$

$$1 \cdot \text{cal} = 4.1868 \cdot \text{joule}$$

$$T_g' = 312.1$$

Calculate final delta temperature of gas in space after burn.

$$\delta T = \frac{\text{heat}}{C_v \text{Tot}(T_g') \cdot \text{gmTotp}}$$

Calculate final burn gas temperature.

$$T_p = \delta T - T_i$$

$$T_p = 312.1$$

$$T_{pF} = T_F(T_p)$$

Calculate peak gas pressure (psig) resulting from burn for initial volume of H₂ at initial dome pressure and temperature.

$$\text{pres} = \frac{\text{gmTotp} \cdot R' \cdot T_p \cdot \frac{\text{atm}'}{(V) \cdot \text{ft}^3 \cdot \text{atm}}}{\text{atm}'}$$

(atmospheres)

$$\text{pres}_{\text{psi}} = (\text{pres} - 1) \cdot \text{atm}' \quad (\text{psig})$$

Gram-mole amounts

$$\text{gmH2i} = 716.437$$

$$\text{gmH2p} = 0$$

$$\text{gmN2Oi} = 0$$

$$\text{gmN2Op} = 0$$

$$\text{gmN2i} = 282426.787$$

$$\text{gmN2p} = 282426.787$$

$$\text{gmO2i} = 75075.475$$

$$\text{gmO2p} = 74717.256$$

$$\text{gmH2Oi} = 0$$

$$\text{gmH2Op} = 716.437$$

$$\text{gmToti} = 358218.699$$

$$\text{gmTotp} = 357860.48$$

Results

$$\text{heat} = 4.14 \cdot 10^7 \quad (\text{cal})$$

$$\text{heat} \cdot 4.187 = 1.7338 \cdot 10^8 \quad (\text{J})$$

$$\delta T = 23.069 \quad (\text{K})$$

$$T_p = 312.1 \quad (\text{K})$$

$$T_{pF} = 102.1 \quad (\text{F})$$

$$T_{pC} = T_p - 273.15 \quad (\text{C})$$

$$T_{pC} = 38.919$$

$$\text{pres} = 1.0787 \quad (\text{atm absolute})$$

$$\text{pres}_{\text{psi}} = 1.158 \quad (\text{psi gauge})$$

$$T_i = 239 \quad (\text{K})$$

$$P = 1 \quad (\text{atm})$$

Average constant-volume specific heat values (cal/g-mole-K).

$$C_v \text{H2}(T_g') = 4.743$$

$$C_v \text{O2}(T_g') = 5.182$$

$$C_v \text{N2O}(T_g') = 6.916$$

$$C_v \text{H2O}(T_g') = 5.981$$

$$C_v \text{N2}(T_g') = 4.97$$

$$C_v \text{Tot}(T_g') = 5.016$$

Attachment 2

Assumptions in the Mathcad Calculation

- Assumption 1. The initial temperature of the gas mixture is 289 K.
Basis: This is the initial temperature in the plume-burn analysis.
- Assumption 2. The initial pressure of the gas mixture is 14.7 lbf/in².
Basis: This is the initial pressure in the plume-burn analysis.
- Assumption 3. Air is 21 percent oxygen and 79 percent nitrogen.
Basis: Air is roughly 78 percent nitrogen, 21 percent oxygen, and 1 percent argon.
- Assumption 4. The ideal gas law equation of state applies.
Basis: Although no gas is ideal, the law applies reasonably well under the conditions of pressure and temperature considered in this analysis. Considerably high pressures are required to cause deviation from the ideal gas law.
- Assumption 5. There is a perfect mix of gas.
Basis: This is conservative in that the assumption will increase predicted pressures and temperatures.
- Assumption 6. There is a complete, perfect burn.
Basis: This is conservative.
- Assumption 7. There are reactions that generate the maximum heats of reaction. For example, if there are both nitrous oxide and oxygen available to react with the available hydrogen, the hydrogen and nitrous oxide react first followed by the remaining hydrogen and the oxygen. The first reaction generates more heat per mole of hydrogen.
Basis: This is conservative.
- Assumption 8. All heats of reaction increase the internal energy of the gasses only; that is, there is no heat transferred to the surrounding container (adiabatic condition) and there is no work done on the container
Basis: This is conservative
- Assumption 9. The volume of gas is constant.
Basis: This assumes that the volume is closed (no venting), which is likely not the case for the K-Basins, but is conservative.
- Assumption 10. The model is a simplified lumped-parameter thermodynamic model with temperature-dependent specific heats. (In this model the entire volume of gas is assumed to have a uniform temperature and pressure distribution at a given instant of time.)
Basis: The lumped-parameter model is judged to be capable of capturing the bulk behavior of the gas mixture in a deflagration analysis.
- Assumption 11. The lower flammability limit of the gas mixture is ignored.
Basis: This allows a comparison to a plume-burn calculation.

**Westinghouse
Hanford Company**

**Internal
Memo**

From: Technical Safety
Phone: 372-1369 X3-77
Date: September 19, 1994
Subject: INDEPENDENT VERIFICATION OF RELATIVE DOSE CALCS HYDRIDE DOCUMENT

To: J. W. Weber L5-01

cc: C. L. Bennett X3-77
E. N. Dodd Jr X3-77
File/LB RHM

The attached tables are the bases for the estimation of accident doses for hydride events. The tables show the originator and checker.

R H Meichle

R. H. Meichle
Principal Engineer

Attachments 2

Relative Dose - Barrel of Canister vs. Maximum Credible Accident - Cask Drop

ISOTOPE	DCG Ci/ml	N FUEL Ci/MTU	Ci RELEASE CASK DROP 244 GMS	Ci RELEASE 7 ELEMENTS 0.1588 MT DF 1x10 ⁴	RELATIVE DOSE CASK DROP	RELATIVE DOSE 7 ELEM EVENT ALL RELEASE	RELATIVE DOSE 7 ELEM EVENT Cs RELEASE ONLY
	A	B	(Bx.000244)	(Bx1.588E-5)	(Bx.000244)/A	(Bx1.588E-5)/A	(Bx1.588E-5)/A
H-3	1.00E-07	2.63E+01	6.43E-03	4.18E-04	6.43E+04	4.18E+03	...
Kr-85	3.00E-06	4.81E+02	1.17E-01	7.64E-03	3.91E+04	2.55E+03	...
Sr-90	9.00E-12	5.80E+03	1.42E+00	9.21E-02	1.57E+11	1.02E+10	...
Y-90	1.00E-09	5.80E+03	1.42E+00	9.21E-02	1.42E+09	9.21E+07	...
Tc-99	2.00E-09	1.21E+00	2.95E-04	1.92E-05	1.48E+05	9.61E+03	...
Ru-106	3.00E-11	5.20E+02	1.27E-01	8.26E-03	4.23E+09	2.75E+08	...
Cd-113M	8.00E-12	2.32E+00	5.66E-04	3.68E-05	7.07E+07	4.60E+06	...
Te-125M	2.00E-09	3.00E+01	7.32E-03	4.76E-04	3.66E+06	2.38E+05	...
Sb-125	1.00E-09	1.20E+02	2.93E-02	1.91E-03	2.93E+07	1.91E+06	...
Cs-134	2.00E-10	1.30E+02	3.17E-02	2.06E-03	1.59E+08	1.03E+07	1.03E+07
Cs-137	4.00E-10	7.30E+03	1.78E+00	1.16E-01	4.45E+09	2.90E+08	2.90E+08
Ce-144	3.00E-11	2.80E+01	6.83E-03	4.45E-04	2.28E+08	1.48E+07	...
Pr-144	3.00E-07	2.80E+01	6.83E-03	4.45E-04	2.28E+04	1.48E+03	...
Pm-147	2.00E-03	2.00E+03	4.88E-01	3.18E-02	2.44E+02	1.59E+01	...
Sm-151	4.00E-10	8.70E+01	2.12E-02	1.38E-03	5.31E+07	3.45E+06	...
Eu-154	5.00E-11	8.80E+01	2.15E-02	1.40E-03	4.29E+08	2.79E+07	...
Eu-155	3.00E-10	3.40E+01	8.30E-03	5.40E-04	2.77E+07	1.80E+06	...
Pu-236	8.00E-14	2.20E-04	5.37E-08	3.49E-09	6.71E+05	4.37E+04	...
Pu-238	3.00E-14	4.80E+01	1.17E-02	7.62E-04	3.90E+11	2.54E+10	...
Pu-239	2.00E-14	1.10E+02	2.68E-02	1.75E-03	1.34E+12	8.73E+10	...
Pu-240	2.00E-14	5.80E+01	1.42E-02	9.21E-04	7.08E+11	4.61E+10	...
Pu-241	1.00E-12	4.40E+03	1.07E+00	6.99E-02	1.07E+12	6.99E+10	...
Pu-242	2.00E-14	2.10E-02	5.12E-06	3.33E-07	2.56E+08	1.67E+07	...
Am-241	2.00E-14	9.30E+01	2.27E-02	1.48E-03	1.13E+12	7.38E+10	...
Cm-242	7.00E-13	0.00	0.00	0.00	0.00	0.00	...
Cm-244	4.00E-14	4.60E+00	1.12E-03	7.30E-05	2.81E+10	1.83E+09	...
Total Relative Dose (Curies released/DCG)					4.84E+12	3.15E+11	3.00E+08
Ratio of Doses from seven element disruptive event in basin to cask drop event						6.51E-02	6.19E-05
Note: Seven Element release assumes all radioactive material escapes from fuel in one barrel of canister and the water has a decontamination factor of 1E+04							

Prepared by R.H. Meier
checked by [Signature]

Relative Dose - Single Assembly in Rupture Can in Cask vs. Cask Drop (Max. Credible)

ISOTOPE	CURIES PER MTU	CURIES PER ELEMENT	DOSE CONVERSION GUIDE	RELATIVE DOSE (1)	RELATIVE DOSE CASK DROP
	(Bi)	(Ci)	(Di)		
		[(50*Bi)/2204]		[(7.7E-07*Ci)/Di]	
H-3	2.63E+01	5.98E-01	1.00E-07	4.60E+00	6.43E+04
Kr-85	4.81E+02	1.09E+01	3.00E-06	2.80E+00	3.91E+04
Sr-90	5.80E+03	1.32E+02	9.00E-12	1.13E+07	1.57E+11
Y-90	5.80E+03	1.32E+02	1.00E-09	1.01E+05	1.42E+09
Tc-99	1.21E+00	2.75E-02	2.00E-09	1.06E+01	1.48E+05
Ru-106	5.20E+02	1.18E+01	3.00E-11	3.03E+05	4.23E+09
Cd-113M	2.32E+00	5.26E-02	8.00E-12	5.06E+03	7.07E+07
Sb-125	1.20E+02	2.72E+00	1.00E-09	2.10E+03	3.66E+06
Te-125M	3.00E+01	6.81E-01	2.00E-09	2.62E+02	2.93E+07
Cs-134	1.30E+02	2.95E+00	2.00E-10	1.14E+04	1.59E+08
Cs-137	7.30E+03	1.66E+02	4.00E-10	3.19E+05	4.45E+09
Ce-144	2.80E+01	6.35E-01	3.00E-11	1.63E+04	2.28E+08
Pr-144	2.80E+01	6.35E-01	3.00E-07	1.63E+00	2.28E+04
Pm-147	2.00E+03	4.54E+01	2.00E-03	1.75E-02	2.44E+02
Sm-151	8.70E+01	1.97E+00	4.00E-10	3.80E+03	5.31E+07
Eu-154	8.80E+01	2.00E+00	5.00E-11	3.07E+04	4.29E+08
Eu-155	3.40E+01	7.71E-01	3.00E-10	1.98E+03	2.77E+07
Pu-236	2.20E-04	4.99E-06	8.00E-14	4.80E+01	6.71E+05
Pu-238	4.80E+01	1.09E+00	3.00E-14	2.79E+07	3.90E+11
Pu-239	1.10E+02	2.50E+00	2.00E-14	9.61E+07	1.34E+12
Pu-240	5.80E+01	1.32E+00	2.00E-14	5.07E+07	7.08E+11
Pu-241	4.40E+03	9.98E+01	1.00E-12	7.69E+07	1.07E+12
Pu-242	2.10E-02	4.76E-04	2.00E-14	1.83E+04	2.56E+08
Am-241	9.30E+01	4.76E-04	2.00E-14	1.83E+04	1.13E+12
Cm-244	4.60E+00	1.04E-01	4.00E-14	2.01E+06	2.81E+10
			TOTALS	2.66E+08	4.84E+12
RELATIVE DOSE SINGLE ELEMENT CAN VS CASK DROP					0.0000548
(1) ASSUMES 0.175 KGS OF FUEL ELEMENT OXIDIZES, AND 1 % OF TRANSURANICS AND FPS ARE RELEASED AND THE DF FOR CANSITER AND CASK IS 100					

Prepared by R. W. Marcher 9/19/54
Checked by [Signature]

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