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HYDROGEN COMBUSTION IN AN MCO DURING INTERIM STORAGE (FAUSKE & ASSOCIATES REPORT 99-14)

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Abstract: Flammable conditions are not expected to develop in an MCO during interim storage. This report considers potential phenomena which, although not expected to occur, could lead to flammable conditions. For example, reactions of hydrogen with fuel over decades are postulated to lead to flammable atmospheric mixtures. For the extreme cases considered in this report, the highest attainable post-combustion pressure is about 13 atmospheres absolute, almost a factor of two and a half below the MCO design pressure of 31 atmospheres.

*Fauske & Associates, Inc.

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1.0 PURPOSE

The purpose of this report is to present a sensitivity analysis of hypothetical conditions beyond those anticipated for safety basis conditions for a Multi-Canister Overpack (MCO) loaded with spent nuclear fuel during interim storage which could lead to flammable gas compositions, to identify a suitable range of compositions and initial pressures, and to calculate corresponding hypothetical post-combustion conditions. Although flammable compositions are not expected according to references [Duncan and Plys, 1998b], initial conditions and phenomena required for flammable compositions to evolve are explored and a range of implied pre-combustion compositions and pressure are evaluated. Adiabatic, isochoric, complete combustion pressure and temperature are shown to conservatively define a post-combustion static pressure, and cases where incomplete combustion and non-adiabatic effects are important are identified.

This report, FAI/99-14, incorporates Hanford Spent Nuclear Fuel Project Review Comment Record dispositions based on FAI/98-113, which was a draft for review of scope and content, and it also includes an internal FAI review in compliance with project requirements.

2.0 SUMMARY

Flammable conditions are not expected to develop in an MCO during interim storage given the phenomena and MCO material inventory considered by [Duncan and Plys, 1998a and 1998b]. This report considers phenomena and initial conditions which could potentially lead to flammable conditions. For example, reactions of hydrogen with fuel over decades of storage imply that in select cases presented by [Duncan and Plys, 1998b], flammable atmospheres could potentially evolve, although the initial inventories of hydrogen and oxygen would be low, and the initial pressure would be low, so that post-combustion conditions would a priori expected to be within MCO design limits.

Flammability data are presented for gases which may be present in an MCO during interim storage, namely, H_2 - O_2 -He- H_2O mixtures, and a flammability criterion for oxygen concentration is presented which includes the effect of temperature (see equation (4-2)). The adiabatic, isochoric (constant volume), complete combustion state is conservative for prediction of post-combustion pressures because heat transfer, and in some cases incomplete combustion, would mitigate post-combustion conditions. A general chart (see Figure 5-2) is presented to obtain post-combustion conditions given pre-combustion values for MCO O_2 and H_2 concentrations and pressure.

Literature data for reactions of hydrogen with uranium exist predominantly for the case of clean, unoxidized metal surfaces and reveal reaction rates which are several orders of magnitude faster than oxidation. Hydrogen reactions with uranium are likely to occur during interim storage, but the rate cannot be quantified with present information, so a range of possible hydrogen inventories in an MCO must be considered here. Thus the key quantity of interest for combustion evaluation is the MCO oxygen inventory, because this controls the available chemical energy.

Worst-case oxygen inventories occur for the case of zero scrap baskets and K-West fuel with the high bounding aluminum hydroxide cladding film inventory, and with other water sources also at the high bounding values. Variation of oxygen inventory is presented (Figure 8-1) and the zero reaction area limit is selected for a bounding inventory. Pre- and post-combustion pressures are shown as a function of end-of-life (40 years interim storage) pre-combustion oxygen concentration for nominal (Figures 8-2 and 8-3) and bounding (Figures 8-4 and 8-5) backfill cases. The worst case occurs for the highest MCO power, about 530 W, for fuel with the bounding cladding film, because this has the highest oxygen inventory. Even in bounding cases considered here, the highest calculated post-combustion pressure is about 13 atmospheres absolute, about a factor of 2.4 below the MCO design pressure of 450 psig (31 atm) for the bounding helium backfill (Figure 8-5).

3.0 SNF PROJECT SOURCES

3.1 MCO Initial Conditions

MCOs are vacuum dried to remove free water and backfilled with helium at the Cold Vacuum Drying (CVD) stations, and are subsequently shipped to the Canister Storage Building (CSB) for interim dry storage. Quasi-steady state temperature and pressure are achieved within a matter of days at the CSB, and these are defined as initial conditions for analysis of the evolution of gas concentrations and pressure during interim storage.

Pertinent MCO design parameters are listed in Table 3-1 [Pajunen and Sederburg, 1998; and Sherrell, 1999], and the interim storage life listed is a definition from [Sellers, 1996]. Relatively quick attainment of quasi-steady temperature and pressure are demonstrated by [Duncan and Plys, 1998b], where a straightforward relationship between MCO temperature and power is developed:

$$T = T_{av} + \frac{Q}{U} \quad (3-1)$$

where T = MCO temperature at a given location, °C,

T_{av} = Vault ambient temperature, 12°C,

Q = MCO power, W, and

U = Heat transfer conductance to location, W/K.

Here the average annual temperature is given, and the impact of annual variations is considered later on reaction rates. Values for the conductance U determine the local temperature. In the cited work, conservative values implied lower temperatures, and hence, lower reaction rates. A conservative value of 12.4 W/K applies for scrap, a conservative value for fuel is 9.5

Table 3-1: MCO Design Parameters Considered.		
Parameter	Value	Comment
Free water inventory	≤ 200 g	Radiolysis source
Backfill gas	99.9% He	Sets nominal initial condition Sets bounding initial condition Sets nominal initial condition Sets bounding initial condition Mechanical Seal Welded Seal
Backfill temperature	25 to 35°C 0°C	
Backfill pressure	40 to 60 kPa gauge 85 kPa gauge	
Leakage test acceptance	$< 10^{-5}$ std cc/sec $< 10^{-7}$ std cc/sec	
Maximum internal pressure	450 psig	30 atm gauge limit
Interim storage duration	≤ 40 years	Calculation scope
Released noble gases and He	< 0.2 g-mole	Neglect

W/K, and an average value for fuel is 8.3 W/K. To calculate MCO pressure, the average fuel value is recommended here, although the impact of this choice on results will be small.

MCO water inventories are more elaborate to present because they depend upon the number of scrap baskets and because references provide a range of estimates. Detailed values are derived by [Duncan and Plys, 1998a] and used in [Duncan and Plys, 1998b] to develop water inventories that depend upon fuel damage area, based upon the fact that some water sources are directly proportional to the inventory of material associated with fuel damage area. Values used in the previous work are listed in Table 3-2. The line item contributors are kept separate because of their variation with area and because their location determines alpha and beta dose relative to fuel, and chemical form determines gamma dose relative to fuel.

Table 3-2: Parameters Determining MCO Water Inventory		
Parameter	Value or Range	
Reactive Area: Per Fuel Basket	0.016	m ² minimum
	0.0425	m ² average
	0.79	m ² maximum
Reactive Area: Per Scrap Basket	1	m ² minimum
	1.7	m ² average
	4.5	m ² maximum
Residual Free H ₂ O	66.7	g/m ² 200 g maximum
Adhering Particulate H ₂ O	50	g/m ² nominal 297 g max, 0 scrap
	100	g/m ² sensitivity 667 g max, 1 scrap 1,032 g max, 2 scrap
Canister Particulate H ₂ O	40	g nominal 240 g max, 0 scrap
		190 g max, 1 scrap
		140 g max, 2 scrap
Bounding H ₂ O from Al(OH) ₃	3.73	kg, 0 scrap
	3.52	kg, 1 scrap
	3.32	kg, 2 scrap
Bounding H ₂ O from UO ₄ 2H ₂ O	50	g

3.2 MCO Gas Composition Model

[Duncan and Plys, 1998b] present a model for the evolution of MCO gas composition which considers radiolysis sources of hydrogen and oxygen, depletion of water-bearing source materials, and consumption of oxygen via reactions with fuel. The model consists of a set of differential equations whose state variables are the numbers of moles of: (1) hydrogen gas, (2) oxygen gas, (3) free water, (4) water associated with the Al(OH)₃ cladding film, (5) water associated with Al(OH)₃ in canister particulate, and (6) water associated with UO₃2H₂O and UO₄2H₂O from adhering particulate, canister particulate, and cladding films. The model considers time variation of decay power which reduces the dose rate for radiolysis and also reduces the MCO temperature and hence reactions of oxygen, using an exponential fit:

$$\ln \frac{Q_i}{Q_{i0}} = -\lambda_i t \quad (3-2)$$

where Q_i = Decay power, W, from $i = \alpha, \beta, \gamma$, or total,

Q_{i0} = Initial value,

λ_i = Decay constant for decay power, yr^{-1} , and

t = Time, years.

Production of gases by radiolysis is based on a dose fraction relative to uranium and g values (molecules of gas produced per 100 ev absorbed by the matrix) listed in Tables 3-3 and 3-4, respectively. Free water is assumed to be present in cracks in the fuel, and receives all radiation forms. Cladding films do not receive alpha and beta radiation. Canister particulate receives a reduced alpha and beta dose fraction relative to fuel based on the fraction of fuel in the particulate. All water-bearing materials receive a reduced gamma dose relative to uranium because of a lower energy absorption coefficient for gamma radiation relative to uranium metal.

For convenience, average beginning-of-life g values for these materials are listed in Table 3-5. These are defined as:

$$\bar{g}_{pj} = \sum_{i=\alpha,\beta,\gamma} g_{pi} r_{ji} f_{qi}(t) \quad (3-3)$$

where $\bar{g}_{pj}$ = Average g value for product gas $p = \text{H}_2$ or O_2 from source material j , molecule/100 ev,

g_{pi} = g value for product gas p for radiation type $i = \alpha, \beta, \gamma$,

r_{ji} = Absorption fraction of radiation type i for material j relative to U metal, and

$f_{qi}(t)$ = Power fraction from equation (3-2).

Table 3-3: $g(H_2)$ and $g(O_2)$ Values, molecules/100 ev			
$g(H_2)$	Alpha	Beta	Gamma
H ₂ O - Liquid (1)	1.6 (2)	0.53	0.5 (3)
H ₂ O - Vapor	-	-	0.5 (1)
Al(OH) ₃	0.525 (5)	0.1575 (6)	1.2 (4)
UO ₃ ·2H ₂ O	0.165 (5)	0.05 (6)	1.2 (4)
UO ₃ ·H ₂ O	0.083 (5)	0.025 (6)	1.2 (4)
$g(O_2)$	Alpha	Beta	Gamma
H ₂ O - Liquid (7)	0.8	0.265	0.25
H ₂ O - Vapor	-	-	0.25 (7)
Al(OH) ₃	0.2625 (9)	0.07875 (10)	0.135 (8)
UO ₃ ·2H ₂ O	0.083 (9)	0.025 (10)	0.101 (8)
UO ₃ ·H ₂ O	0.041 (9)	0.013 (10)	0.055 (11)
(1) [Green, 1994] (2) 5.3 Mev (3) 100°C (4) [Pajunen, 1998] for $0.04 < x_w < 0.35$ (5) [Pajunen, 1998] $g = 1.5 x_w$ (6) [Pajunen, 1998] $g = 0.45 x_w$ (7) Assumed stoichiometric with $g(H_2)$ (8) [Pajunen, 1998] $g = 0.0861 + 0.139 x_w$ for $x_w > 0.1$ (9) [Pajunen, 1998] $g = 0.75 x_w$ (10) [Pajunen, 1998] $g = 0.225 x_w$ (11) [Pajunen, 1998] $g = x_w$ for $x_w < 0.1$ where x_w = water mass fraction.			

Table 3-4: Dose Reduction Parameters		
Al(OH) ₃ / U,	0.35	Gamma
UO ₃ ·2H ₂ O / U,	0.86	Gamma
H ₂ O / U,	0.38	Gamma
Alpha, Beta for Canister Particulate	1.0	Nominal water content
	0.2	Bounding water content
Alpha decay power constant	- 0.00463	yr ⁻¹ (1, 2)
Beta decay power constant	+ 0.0241	yr ⁻¹ (2)
Gamma decay power constant	+ 0.00242	yr ⁻¹ (2)
Overall decay power constant	+ 0.0149	yr ⁻¹ (2)
(1) Slight increase with time.		
(2) Values of λ in: $\ln(Q/Q_0) = -\lambda t$, where (Q/Q_0) is the power fraction at time t .		

Table 3-5:
Average Beginning-of-Storage $\bar{g}$ (H_2) and $\bar{g}$ (O_2) Values,
molecules / 100 ev ⁽¹⁾

	$\bar{g}$ (H_2)	$\bar{g}$ (O_2)
H ₂ O-Liquid ⁽²⁾	0.63	0.32
H ₂ O-Vapor ^(2, 3)	0.16	0.08
Al(OH) ₃ , clad ^(3, 4)	0.13	0.015
Al(OH) ₃ , partic. ⁽⁴⁾	0.31	0.10
UO ₃ ·2H ₂ O ⁽⁵⁾	0.38	0.056

(1) Power fractions: $\alpha = 0.1967$, $\beta = 0.4862$, $\gamma = 0.3171$, and g values from Table 3-3.
 (2) Gamma absorption relative to $U = 0.38$, Table 3-4.
 (3) Gamma absorption only.
 (4) Gamma absorption relative to $U = 0.35$, Table 3-4.
 (5) Gamma absorption relative to $U = 0.86$, Table 3-4.

Differential equations used by [Duncan and Plys, 1998b] are summarized as:

$$\frac{dn_j}{dt} = -\lambda_{oj} \bar{g}_{H2j} n_j \quad (3-4)$$

$$\frac{dn_{H2}}{dt} = -\sum_j \frac{1}{a_j} \frac{dn_j}{dt} \quad (3-5)$$

$$\frac{dn_{O2}}{dt} = R_{O2} - G_{O2} \quad (3-6)$$

$$\text{where } \lambda_{oj} = a_j C \left(\frac{Q}{M} \right)_o M_j$$

$$\lambda_j = \text{Decay constant, yr}^{-1},$$

$$n_j = \text{Number of moles of water from source compound } j,$$

$$a_j = \text{Moles compound } j \text{ depleted per mole H}_2\text{O decomposed,}$$

$$C = \text{Conversion constant, } 1.038 \times 10^{-7},$$

$$\left(\frac{Q}{M} \right)_o = \text{Initial Power per unit mass fuel, W/kgU,}$$

$$M_j = \text{Molecular weight compound } j,$$

$$R_{O_2} = \text{O}_2 \text{ source, mole 1 year, evaluated like equation (3-5) but using } g \text{ values for O}_2 \text{ production, and}$$

$$G_{O_2} = \text{O}_2 \text{ getter rate, mole/year.}$$

The oxygen getter (consumption) rate is found by applying the appropriate kinetic rate law, evaluated at one average scrap temperature and three fuel temperatures, and considering the reaction area at each location. The Ritchie Law for uranium reactions in moist air and relative humidity less than 75%:

$$\log_{10} R_{\text{moist}} = 13.808 - \frac{5769.6}{T} \quad (3-7)$$

where R = Weight gain, mg/cm²hr, and

T = Temperature, K.

Unless the dry air correlation of Trimble is greater:

$$\log_{10} R_{\text{dry}} = 7.19 - \frac{3732}{T} \quad (3-8)$$

which occurs below about 40°C.

A notable model assumption is that hydrogen does not react with fuel. As explained in the source document, there is no reliable technical basis for quantification of the rate of reaction between hydrogen and dirty, oxidized uranium surfaces. Qualitatively, there are indications based upon experience that such reactions will occur over sufficient time. The impact of such reactions is to reduce the inventory of hydrogen, and thereby increase the concentration of all other gases.

Also, reactions between oxygen and uranium hydride are not considered. This is chiefly because the amount of hydride is difficult to quantify. In part however, uranium hydride may form due to reactions between hydrogen and uranium metal, as discussed above. The impact of oxygen reactions with uranium hydride is potentially greater oxygen removal rates and greater hydrogen production rates relative to consideration of fuel reactions alone. Note that a small mass of uranium hydride may provide a lot of surface area due to its small particle size, but assignment of the proper surface area and inventory requires some justification.

Figure 3-1, taken from [Duncan and Plys, 1998b], presents worst case end-of-storage results obtained with the model as described. These are worst case because of the combination of high $\text{Al}(\text{OH})_3$ cladding film inventory, i.e., K-West fuel, zero scrap baskets, and other water sources at the high values. The maximum MCO power is 525 W for this case, so the highest oxygen concentration at 40 years is less than 4%, even when zero reactive area is considered. (A case with initial $\text{He} = 1.0$ atm to represent leakage was considered in the reference, but not shown here because leakage over 40 years would also remove oxygen.)

Figure 3-1: Zero Scrap Bounding High Water Case From [Duncan and Plys, 1998b].

Oxygen Percentage at 40 Years as a Function of MCO Power for Various Reactive Surface Areas. Zero Scrap, Bounding Case: 10.6 kg Al(OH)₃Clad Film, 100 g/m² Adher. Partic. H₂O, 240 g. Can. Partic. H₂O, 66.7 g/m² free H₂O

4.0 FLAMMABILITY LIMITS

Flammability limit diagrams are typically found in the literature for Fuel-Air-Inertant mixtures. The conditions of interest for the present MCO analysis are Hydrogen-Oxygen-Inertant mixtures, where the inertant gas is either nitrogen (from air), helium, water vapor, or a combination of the three gases. Air contains 20.8% oxygen and 79.2% nitrogen plus other gases (about 1% argon for example), and nitrogen is not normally present in an MCO. Therefore the issue for MCO application is how to employ the typically available data in a nitrogen-deficient environment.

Figures 4-1, 4-2, and 4-3, respectively, contain flammability limit diagrams for hydrogen in air with added nitrogen, helium, and water vapor inertants, respectively. The flammable region lies inside the curve. The nose of the curve is the inerting point, which establishes the amount of inertant guaranteed to prevent flammability for any fuel-air ratio, and it typically coincides with a stoichiometric fuel-air mixture. The lower portion of the curve is the Lean or Lower Flammability Limit (LFL), corresponding to hydrogen concentrations less than stoichiometric, and the upper portion of the curve is the Rich or Upper Flammability Limit (RFL), corresponding to hydrogen concentrations greater than stoichiometric, or put another way, corresponding to the minimum oxygen requirement for flammability. The axes of the diagram are the concentrations of the fuel and inertant components, so that the air concentration is simply 100 minus the sum; the diagonal border of Figure 4-1 represents the border of possible mixtures.

The diagram for nitrogen appears in [Zabetekis, 1965] and [Kuchta, 1985]. Extra nitrogen in air occurs when air is oxygen-deficient, for example, by design (addition of nitrogen) or after a combustion event which consumes some of the oxygen. The diagram for helium was developed based upon a data table in [Coward and Jones, 1952] reproduced in Table 4-1. The nitrogen and helium diagrams are based on a temperature of 25°C. The diagram for water vapor contains the data and curve fit of [Marshall, 1986], taken at temperatures above 100°C to prevent condensation. Increasing temperature expands the flammability limits, as discussed below.

Figure 4-1:
Limits of Flammability of Hydrogen-Air Mixtures With Added Nitrogen and Carbon Dioxide at 25°C and 1 atm. [Kuchta, 1985]

Figure 4-2: Hydrogen-Air-Helium Flammability Limits Per [Coward and Jones, 1952].

Figure 4-3: Hydrogen-Air-Steam Flammability Data and Curve Fit for [Marshall, 1986].

Table 4-1: Limits of Flammability of Mixtures of Hydrogen and Helium in Air, Upward Propagation of Flame in Tube 2" in Diameter and 6' in Length, Open at its Lower End [Coward and Jones, 1952].				
Fuel Plus Inertant Gas Mixture, %		Limits of Flammability, %		Minimum Oxygen Concentration, %
Hydrogen	Helium	Lower	Upper	
100.0	0	4.2	71.5	6.00
58.1	41.9	7.1	76.2	5.00
27.9	72.1	16.6	79.2	4.37
19.3	80.7	24.9	81.2	3.95
10.7	89.3	51.3	80.3	4.14
8.7	91.3	69.8	69.8	6.34

Note that for zero inertant, the y-intercepts of all three diagrams should be identical at the LFL and RFL, and take on values of 4% and 75%, respectively [Kuchta, 1985]. The RFL implies 5.2% O₂ and 19.8% N₂. The RFL of the H₂-Air-He diagram is in conflict with the RFL of the other diagrams, i.e., about 6% oxygen is demanded for flammability versus the well-established value of 5%, which suggests the possibility that the oxygen concentration for flammability is over-estimated by other points of the diagram too.

For the case of zero nitrogen, i.e., pure H₂-O₂ mixtures, the LFL and RFL are given as 4% and 95% H₂, respectively [Zabetekis, 1965]. When He replaces N₂ in air, the LFL and RFL are 7.72% and 75.7%, respectively. Note that the LFL is somewhat higher for He than N₂ as the inertant, but the RFL is, for practical purposes, the same for He and N₂, and implies 5% O₂ as the minimum required to support combustion.

It is possible to create generalized flammability limit diagrams for combinations of fuels and inertants as shown in Figure 4-4 [Plys, 1993]. However, this level of detail is only necessary when the LFL must be considered as well as the RFL. Because the present application is concerned with hydrogen-rich mixtures, a simplified approach may be taken to combine the information provided by the RFL curves of Figures 4-1 to 4-3.

A common feature of the RFL curves for inertants of interest is the 5% O₂ limit for low inertant concentrations. Both the N₂ and He RFL curves show deviations from the straight line of constant oxygen concentration, and as seen from Table 4-1 at minimum value of 4%, O₂ was found near the inerting point, for example. For 10% H₂O, Marshall's curve fit implies 4.8% H₂O. Typically the H₂O concentration in an MCO cannot far exceed 10%-20% because of saturation at the storage temperature, and most of the MCO gas is He due to the backfill. Therefore a conservative RFL curve has 4% oxygen.

Another prominent feature of the flammability limit curves is the position of the inerting point, or "nose". From Figure 4-1, coordinates of the nose for H₂-air-N₂ are about 4% H₂, 71% added N₂ (see [Kuchta, 1985, p. 32]), implying 5.2% O₂ and 19.8% N₂ in air, for a total of about 91% inertant gas. From Figure 4-2, coordinates of the nose for H₂-air-He are: 72% He, 8.6% H₂, 4.1% O₂, and 15.6% N₂, for a total of about 72 + 16 = 88% inertant gas. Less steam, about 55% in air, is required for inerting, but such high steam concentrations are not of current practical interest for an MCO. Thus a conservative criterion for inerting in an MCO is a total inertant concentration of 88%.

The flammability envelope expands with increasing temperature, as shown for hydrogen in air in Figure 4-5. Zabetekis proposed a formula known as the modified Burgess-Wheeler Law (after the original authors of such a correlation) for the RFL of hydrocarbons in air:

$$R(T) = R(25) + \frac{0.75}{\Delta H_c} (T - 25) \quad (4-1)$$

Figure 4-4: Generalized H_2 -CO-Air- H_2O - CO_2 - N_2 Flammability Limit Diagram.

The inertant contains equal mole fractions of N_2 and ($\text{CO}_2 + \text{H}_2\text{O}$), and separate curves are shown for three fuels: H_2 , CO, and $\text{H}_2 + \text{CO}$ combined at equal mole fraction.

[Plys, 1993].

Figure 4-5:
Influence of Temperature on Limits of Flammability of Hydrogen in Air
(Downward Propagation of Flame). [Coward and Jones, 1952].

where R = Rich Flammability Limit (RFL), %,
 ΔH_c = Heat of combustion, kcal/mole,
 T = Temperature, °C, and
 0.75 = Approximate heat capacity of air, cal/mole, x 100 to convert R to %.

The heat of combustion of hydrogen is 57.8 kcal/mole (241.8 kJ/mole). The modified Burgess-Wheeler Law implies that the flammability envelope expands to its maximum (100% H_2 at the zero inertant limit) at a temperature of 1,952°C. However, the auto-ignition temperature for hydrogen in air is closer to 700°C. From hydrogen data of Figure 4-5, a slope of $(10\% / 380\text{ K}) = 0.0263$ is derived, which is greater than $(0.75 / 57.8) = 0.013$. Thus for MCO application, since O_2 is 20.8% of the inertant for derivation of the Burgess-Wheeler Law, the O_2 concentration for flammability may be written:

$$O_2\% (T) = 4 - 0.00547 (T - 25) \quad (4-2)$$

This implies zero $O_2\%$ required at 756°C because 4% O_2 was taken as the intercept at 25°C, versus 5.2% implied by an RFL of 75% H_2 at 25°C. Equation (4-2) is in accord with measured temperature variation for flammability in the H_2 -air system and is conservative by use of 4% oxygen as a limiting value when He is present.

5.0 COMBUSTION MODEL

Conservative post-combustion static pressure may be calculated using the adiabatic, isochoric (constant volume), complete combustion (AICC) relationship:

$$U_p = U_r + \Delta H \quad (5-1)$$

where U = Internal energy, J,
 ΔH = Heat of reaction, J,
 p = Product gases, and
 r = Reactant gases.

Specifying the initial temperature as a reference state, $U_r = 0$, and the equation may be written

$$\sum_i n_{ip} [u_i(T_p) - u_i(T_r)] = \Delta H \quad (5-2)$$

where n_i = Number of moles of gas i , and
 u_i = Internal energy function of gas i (at low pressure).

The internal energy is merely the integral of the specific heat at constant volume, $c_v(T)$, and the caveat "at low pressure" is added to indicate that ideal gas behavior is assumed such that U does not also depend on specific volume. Table 5-1 contains reference values for $c_v(T)$ and Table 5-2 contains polynomial fits which may be integrated analytically to yield the internal energy.

The heat of combustion and number of product moles are found by determining whether H_2 or O_2 is the limiting reactant:

Table 5-1: Reference Heat Capacities at Constant Volume, J/mole/K
[Chase, et al., 1985]

T(K)	H ₂	He	N ₂	O ₂	H ₂ O
298.15	20.866	12.47	20.64	20.783	25.18
500	20.909	12.47	21.37	22.831	26.94
1,000	21.87	12.47	24.258	26.36	32.859
1,500	24.056	12.47	26.647	28.045	38.756
2,000	27.331	12.47	27.475	28.505	43.214

Table 5-2: Polynomial Fits to $c_v(T)$,

$c_v(T) = A + BT + CT^2 + DT^3 + ET^4$, Output Value in J/mole/K.

GAS	A	B	C	D	E
H ₂	21.136	-1.529×10^{-3}	1.978×10^{-6}	4.018×10^{-10}	-1.171×10^{-13}
He	12.47	0	0	0	0
N ₂	20.785	-3.871×10^{-3}	1.34×10^{-5}	-7.216×10^{-9}	1.16×10^{-12}
O ₂	17.045	0.014	-4.96×10^{-6}	1.375×10^{-10}	1.375×10^{-13}
H ₂ O	24.044	-7.883×10^{-5}	1.513×10^{-5}	-7.323×10^{-9}	1.087×10^{-12}

$$\Delta n_{H_2O} = \min(n_{H_2,r}, 2n_{O_2,r}) \quad (5-3a)$$

$$n_{He,p} = n_{He,r} \quad (5-3b)$$

$$n_{N_2,p} = n_{N_2,r} \quad (5-3c)$$

$$n_{H_2,p} = n_{H_2,r} - \Delta n_{H_2O} \quad (5-3d)$$

$$n_{O_2,p} = n_{O_2,r} - \frac{1}{2} \Delta n_{H_2O} \quad (5-3e)$$

$$n_{H_2O,p} = n_{H_2O,r} + \Delta n_{H_2O} \quad (5-3f)$$

$$\Delta H = 241.8 \times 10^3 \Delta n_{H_2O} \quad (5-4)$$

where 241.8 KJ/mole is the heat of combustion.

Figure 5-1 displays the AICC pressure and temperature as the initial hydrogen content is varied for H₂ in air (solid) and H₂ in a mixture of O₂ and He where the proportion of He to O₂ is the same as in air (dashed), i.e., as if the N₂ of air were replaced by He. Initial pressure is 1 atm and initial temperature is 298 K. Note that AICC pressure and temperature are higher with He than N₂ because of the somewhat lower heat capacity of the noble gas. Functions used to derive Figure 5-1 are contained in Appendix A to demonstrate validation of the technique for later application.

Post-combustion conditions in an MCO are different than shown in Figure 5-1 because the initial gas concentrations are different. Figure 5-2 presents a general chart which may be used to determine post-combustion conditions in an MCO. For given initial concentrations of H₂ and O₂ in He, Figure 5-2 provides the pressure ratio $P_{final} / P_{initial}$. Note that for H₂-rich conditions, the ratio is nearly constant, especially for low O₂ concentrations. Also, note that the value of the pressure ratio is strictly valid for an He backfill of 1.5 atm at 25°C, which sets the number of moles of He, and stored at 50°C. However, small departures from these initial conditions (± 0.2 atm He, $\pm 25^\circ\text{C}$) will not cause significant errors in the value of P_{final} .

Figure 5-1: Pressure and Temperature for H₂-Air and H₂-O₂-He Mixtures.AICC Pressure for H₂-Air and H₂-(21% O₂, 79% He) Mixtures, 25 C, 1atm Initial AICC Temperature for H₂-Air and H₂-(21% O₂, 79% He) Mixtures, 25 C, 1atm Initial

Figure 5-2:

**Pressure Ratio ($P_{\text{final}} / P_{\text{initial}}$) For Various Initial $\text{H}_2\%$ and $\text{O}_2\%$ in an MCO
Backfilled to 1.5 atm He at 25°C, and Stored at 50°C.**

Multiply plotted value by initial pressure to yield final pressure in atm. Some combinations of initial $\text{H}_2\%$ and $\text{O}_2\%$ on the plot are not considered possible.

Pressure Ratio ($P_{\text{final}} / P_{\text{initial}}$) for various initial $\text{H}_2\%$ and $\text{O}_2\%$ in an MCO backfilled to 1.5 atm He at 25 C, and stored at 50 C. Multiply plotted value by initial pressure to yield final pressure in atm. Some combinations of initial $\text{H}_2\%$ and $\text{O}_2\%$ on the plot are not considered possible.

6.0 HYDROGEN REACTIONS WITH URANIUM

Hydrogen can react with uranium metal to form uranium hydride,

at rates which are potentially significant for interim storage of spent nuclear fuel. The rate of reaction depends upon temperature and pressure, and is the subject of numerous investigations. A valuable source of rate data is given by [Bloch and Mintz, 1981]; the effect of oxidizing gases to inhibit hydriding is demonstrated by [Bloch, et al., 1989]; and a useful model for the kinetics is given by [Kirkpatrick and Condon, 1991].

The key issue for interim storage is that hydrogen reactions with uranium are at least temporarily inhibited in the presence of oxygen and water vapor, as shown by [McD Baker, et al., 1966] and [Bloch, et al., 1989] and discussed by [Duncan and Plys, 1998b]. That is, when water vapor is present, hydrogen is observed as a reaction product in proportions nearly in stoichiometry with an oxidation reaction alone. But given sufficient time, hydriding can commence. At present, there are insufficient data to identify the combination of temperature, gas concentrations, and dwell time required to initiate hydriding during interim storage, and there are insufficient data to quantify the subsequent rate of reaction for "dirty" uranium systems (hydriding experiments are typically conducted with clean polished metal, in contrast to the current damage state of N reactor fuel). [Bloch, et al., 1989] suggest that hydriding can commence after a dwell time on the order of hours when the hydrogen pressure is between 10 and 20 atmospheres (Figure 6-1), but this pressure range is an order of magnitude higher than pertinent for most interim storage applications.

The rate of hydriding is actually faster than the rate of oxidation in the temperature range of interest during interim storage. Figure 6-2, taken from [Kirkpatrick and Condon, 1991], contains hydriding data and a detailed model fit for a hydrogen pressure of 1 atmosphere. Note

Figure 6-1:
Fractional Hydriding α of U Metal Foil for O_2 Concentrations
from (< 10 to f 16,000) ppm [Bloch, et al., 1989].

Curves a through f represent increasing initial oxygen concentrations in a fixed gas volume.

Figure 6-2:
 Apparent Spall Front Velocity For a Hydrogen Pressure of 1.0 atm
 Showing Comparison Data With Calculations:
 • Data; and ■ Data; — — Spall Velocity Using Proposed Fits
 [Kirkpatrick and Condon, 1991].

that the rate of hydriding attains a maximum between 250°C and 300°C, and that it changes sign so that de-hydriding occurs at about 375°C. For interim storage application, de-hydriding is simply not possible because the equilibrium hydrogen pressure above the metal and hydride is very low. The Kirkpatrick and Condon model may be simplified for low temperature applications and applied to interim storage calculations, as follows:

$$V_s = \frac{1}{t_1} \sqrt{\frac{D_E}{s k_1 U_E}} \quad (6-1)$$

$$t_1 = \frac{-\ell n U_c}{k_1 C_o} \quad (6-2)$$

$$D_E = D \sqrt{\frac{N}{N - C_o}} \quad (6-3)$$

$$U_E = U_c^{1/2} \quad (6-4)$$

$$U_c = 0.989 \quad \text{for } T \leq 250^\circ\text{C} \quad (6-5)$$

$$s = 3 \quad \text{for } \text{UH}_3 \quad (6-6)$$

$$k_1 = 10.4 \exp\left(\frac{1,592}{T}\right) \quad (6-7)$$

$$D = 1.9 \times 10^{-6} \exp\left(\frac{5,820}{T}\right) \quad (6-8)$$

$$N = \exp\left(-2.362 - \frac{2,305}{T}\right) \quad (6-9)$$

$$C_o = \frac{N S}{N + S} \quad (6-10)$$

$$S = 4.183 \times 10^{-6} \exp\left(\frac{-894}{T}\right) \sqrt{P} \quad (6-11)$$

where V_s	=	Spallation velocity, m/s,
t_1	=	Time to first spallation, s,
D_E	=	Effective diffusion coefficient, m^2/s ,
D	=	Diffusion coefficient, m/s,
N	=	Maximum diffusing hydrogen mole fraction in uranium,
U_E	=	Effective mole fraction for spall,
U_c	=	Uranium mole fraction for spall,
k_1	=	Hydriding rate constant, 1/s,
C_0	=	Solubility of free hydrogen in uranium,
T	=	Temperature, K, and
P	=	Hydrogen pressure, Pa.

Figure 6-3 compares the simplified model to selected points from the detailed curve of Figure 6-2, and demonstrates that the simplified model is valid.

The reaction rate of hydrogen with clean uranium surfaces may be compared with the reaction rate of oxygen by casting the latter in terms of an oxide front velocity. Evaluating the Ritchie correlation at 50°C, yields:

$$w'' \approx 10^{-4} \text{ mg/cm}^2 \cdot \text{hr} \quad (6-12a)$$

$$\approx 3 \times 10^{-10} \text{ kg/m}^2 \cdot \text{s} \quad (6-12b)$$

Using $w'' = \frac{32}{238} \rho U$, yields:

$$U \approx 10^{-13} \text{ m/s} \approx 10^{-4} \text{ nm/s} \quad (6-13)$$

for a metal density of 19,000 kg/m^3 .

Figure 6-3:
Hydriding Rate (nm/2) of Clean Uranium in Hydrogen at 1 atm;

With de-hydriding neglected for low temperatures and hydrogen pressures above saturation.

Solid line is correlation of [Kirkpatrick and Condon, 1991].

Diamonds are values from published curve for validation.

This is five orders of magnitude lower than the hydriding rate of about 10 nm/s for 1 atmosphere hydrogen! In real systems with "dirty" uranium surfaces, either an oxide layer may substantially reduce the hydriding rate - which is contradicted by [Bloch, et al., 1989] - or else hydriding can, after a suitable dwell period, proceed far faster than oxidation.

However, typical industrial experience with storage of uranium reveals that some hydrogen is encountered in containers to which water was either accidentally or inadvertently admitted. For example, [Wood, et al., 1994] describes a hydrogen explosion upon opening a drum containing uranium metal and wood; which was the inadvertent moisture source. The drum contained hydrogen at somewhat sub-atmospheric pressure, whereas the rate law used above would suggest near complete hydrogen removal.

Relating this to interim storage, an example presented by [Duncan and Plys, 1998b] for an average power MCO with bounding water content results in production of about 22 moles hydrogen over 40 years. This hydrogen source can be consumed by a hydriding rate given by:

$$\dot{n}'' \text{ (mole / year)} \approx 3.15 \times 10^7 \frac{3}{2} \frac{\rho}{238} V_s \text{ (m/s)} \quad (6-14a)$$

$$\approx 3.78 \times 10^9 V_s \text{ (m/s)} \quad (6-14b)$$

Assigning $\dot{n}'' = 0.5 \text{ mole/m}^2/\text{year}$, (i.e., allowing 1 m² reaction area) and taking an average reaction temperature of 50°C, results in a steady-state hydrogen pressure of only 2.3 Pa to force equal rates of production and consumption.

The clear implication is that either: (a) the rate of hydriding of oxidized uranium surfaces is far lower than given by literature correlations for clean uranium surfaces, (b) hydriding of oxidized surfaces requires a minimum hydrogen pressure far greater than implied by the correlation for clean surfaces, or (c) both statements are partially true.

For interim storage application, the implication is that hydrogen should react with fuel, but not completely as otherwise predicted from literature correlations. For MCOs whose capacity to react oxygen exceeds the radiolytic production rate, this merely implies that the pressures predicted by [Duncan and Plys, 1998b] are conservative overestimates. For MCOs which can yield net oxygen production over the interim storage period, however, the oxygen concentrations of [Duncan and Plys, 1998b] are underestimated because less hydrogen would be present. Based on the industrial experience, the gas compositions are likely (but not certain) to still be hydrogen-rich. Because the extent of hydriding cannot be reliably predicted, the gas compositions cannot be specified and a range of potentially flammable mixtures needs to be considered. The post-combustion pressure is not sensitive to the amount of hydrogen gettering when the pre-combustion mixture is hydrogen-rich because the oxygen inventory limits energy release (see Figure 5-2).

7.0 SUMMARY OF TECHNICAL BASES AND ASSUMPTIONS

Technical bases for this work are:

1. Initial MCO material inventories are given by [Duncan and Plys, 1998a], as discussed in Section 3.1.
2. Initial MCO conditions are provided by [Pajunen and Sederburg, 1998; Sherrell, 1999; and Duncan and Plys, 1998b], as discussed in Section 3.2.
3. Flammability data provide a conservative criterion of 4% oxygen in an MCO for storage temperatures 25°C - 75°C (Section 4.0).
4. The maximum static post-combustion pressure in an MCO is given by an adiabatic, isochoric, complete combustion model (Section 5.0).
5. Slow reactions of hydrogen with uranium may occur when water vapor and oxygen are present (Section 6.0).

An assumption is:

1. Because the actual rate of hydrogen reactions with fuel cannot be quantified, the key feature of the [Duncan and Plys, 1998b] model to investigate is sensitivity to these reactions. Therefore the oxygen inventory predicted by this reference yields the bounding energy source for combustion, and the amount of hydrogen may be parametrically varied.

8.0 CALCULATIONS

8.1 MCO Atmosphere Sensitivity Cases

Worst-case end-of-life oxygen concentrations arise for MCOs with low reactive area for oxygen consumption and high inventories of water-bearing compounds as described in Section 3.2. Figure 8-1 provides the number of moles of oxygen for various small reactive areas and two different MCO powers, 530 W (the maximum for K-West fuel with the aluminum hydroxide cladding film) and 400 W (approximate average power), using the bounding MCO water content (note, this is independent of the backfill conditions). Cases shown are consistent with Figure 3-1 taken from [Duncan and Plys, 1998b] and simply include more detail at low reactive area. The calculation file appears in Appendix C. Any other case group from [Duncan and Plys, 1998b] would result in a lower oxygen inventory; there are no instances with one or two scrap baskets where combustion is an issue because the reactive area is a minimum of 1 m² and only a trivial or zero oxygen inventory is calculated.

Oxygen is the critical reactant gas for determination of the potential for flammability and for prediction of post-combustion conditions. As mentioned, the model used for prediction of MCO gas composition did not consider hydrogen reactions with fuel. However, experimental evidence suggests that some reaction of hydrogen may take place during the relatively long interim storage period. Thus, the number of moles of oxygen in Figure 8-1 essentially determines the worst-case post-combustion conditions for a given reactive area.

Clearly, there can be no hydrogen reactions with fuel when the reactive area is zero. When the reaction area is only 0.01 m², the number of moles of oxygen drops nearly in half for the 530 W case, and declines by about 10% in the 400 W case. The actual reactive area in an MCO is unknown and could be between 0 and 0.01 m², and the inventory of oxygen is clearly bounded by the value given for zero area. The inventory of hydrogen is variable between the amount calculated by the reference model with zero hydrogen reactions, and an amount less than the

Figure 8-1:
Oxygen at 40 Years for K-West Zero Scrap Bounding Water Content
as Function of Reactive Area (m^2), $Q = 530 \text{ W}$ and $Q = 400 \text{ W}$.

inventory of oxygen. However, it is a moot point to consider less hydrogen than in stoichiometry with the oxygen because this would provide the same post-combustion condition as some other rich hydrogen inventory greater than stoichiometry.

Thus, even though it is somewhat unrealistic, a bounding MCO atmosphere for consideration of combustion combines the zero-area oxygen inventory limit (because some finite area which negligibly reacts oxygen could be chosen) with a variable amount of hydrogen between an amount evaluated at zero hydrogen reaction with fuel to an amount in stoichiometric proportion with the oxygen (because the actual rate of reaction cannot be specified).

8.2 Post-Combustion Sensitivity Results

Figures 8-2 and 8-3 contain pre- and post-combustion pressure as a function of pre-combustion oxygen concentration for MCO atmospheres, as described above, given a nominal helium backfill. The only difference between these figures is that the scale has been expanded in the latter to illustrate the margin between MCO design pressure and the bounding post-combustion pressure. In these figures, lower curves represent pre-combustion conditions as a function of reactive area. A reactive area of zero corresponds to the highest oxygen concentration on the lower curves, and symbols represent oxygen concentration - pressure pairs at the reactive areas considered by Figure 8-1. Eventually, as reactive area increases, the oxygen concentration is reduced to zero by reactions with fuel; the MCO pressure however can increase because higher reactive areas provide more water source and hence more hydrogen from radiolysis.

The upper curves of Figures 8-2 and 8-3 show post-combustion pressure as the amount of hydrogen in the MCO is varied. The highest amount of hydrogen corresponds to the lowest pre-combustion oxygen concentration and yields the highest post-combustion pressure because the available energy is the same but the initial pressure is higher versus a case with less hydrogen. The lowest amount of hydrogen corresponds to the highest pre-combustion oxygen concentration. The highest post-combustion pressure is about 11.9 atm, and is a factor of 2.6 less than the design

Figure 8-2: Pressure vs. Oxygen Concentration for Zero Scrap, Nominal Backfill.

Pressure vs Oxygen Concentration for Zero Scrap, K-West bounding water inventory. Lower lines with symbols indicate MCO conditions for various reactive areas with no combustion. Upper lines with no symbols are for post-burn sensitivity cases with hydrogen getting to increase the O₂ concentration up to stoichiometry.

Combustion is impossible for O₂ < 4%. The worst case group is for A=0, zero reactive area, because this maximizes the number of moles of oxygen. The worst case is for the highest power, hence highest moles of oxygen. The highest post-burn pressure is 11.9 atm.

Figure 8-3:
Pressure vs. Oxygen Concentration for Zero Scrap Indicating MCO Design Pressure,
Nominal Backfill.

Pressure vs Oxygen Concentration for Zero Scrap, K-West bounding water inventory. Lower lines with symbols indicate MCO conditions for various reactive areas with no combustion. Upper lines with no symbols are for post-burn sensitivity cases with hydrogen getting to increase the O₂ concentration up to stoichiometry. The upper horizontal dashed line is the MCO design pressure 450 psig (31 atm absolute).

Combustion is impossible for O₂ < 4%. The worst case group is for A=0, zero reactive area, because this maximizes the number of moles of oxygen. The worst case is for the highest power, hence highest moles of oxygen. The highest post-burn pressure is 11.9 atm.

value (about 31 atm absolute). Note that in the 400 W case, combustion is not possible until enough hydrogen is consumed that nearly stoichiometric conditions are attained.

Clearly, a similar exercise using the oxygen molar inventory from a case with non-zero reactive area would yield lower pressure than indicated in Figures 8-2 and 8-3. For a reactive area of 0.01 m², the oxygen inventory in the 530 W case drops below the zero area inventory in the 400 W case, so its maximum post-combustion pressure would be below 8 atm.

The preceding calculation is repeated using a bounding initial helium backfill inventory in order to bound the final pressure, and results appear in Figures 8-4 and 8-5 which are analogous to Figures 8-2 and 8-3. The initial number of moles of helium is about 33% higher in this case (41 moles versus 30.3 moles), but the heat capacity of the helium is significant and the maximum plotted post-combustion pressure is 13 atm, only about 10% higher than the analogous nominal case. Note that because 4% O₂ is required, in this case combustion is barely possible.

8.3 Conclusions

A worst-case MCO from the point of view of flammability and combustion has a very low reactive area, so that little oxygen consumption occurs, but some consumption of hydrogen can occur, so as to allow the gas mixture to be flammable. Worst-case oxygen inventories are bounded by calculations for zero reactive area, though obviously some finite non-zero reaction area must be present for reaction of some hydrogen to proceed. Worst-case oxygen inventories occur for the case of zero scrap baskets and K-West fuel with the high bounding aluminum hydroxide cladding film inventory, and with other water sources also at the high bounding values. Even in such cases, the highest calculated post-combustion pressure is about a factor of 2.4 below the MCO design pressure of 450 psig.

Figure 8-4: Pressure vs. Oxygen Concentration for Zero Scrap, Bounding Backfill.

Pressure vs Oxygen Concentration for Zero Scrap, K-West bounding water inventory, and high helium backfill. Lower lines with symbols indicate MCO conditions for various reactive areas with no combustion. Upper lines with no symbols are for post-burn sensitivity cases with hydrogen getting to increase the O₂ concentration up to stoichiometry.

Combustion is impossible for O₂ < 4%. The worst case group is for A=0, zero reactive area, because this maximizes the number of moles of oxygen. The worst case is for the highest power, hence highest moles of oxygen. The highest post-burn pressure is 13 atm.

Figure 8-5:
Pressure vs. Oxygen Concentration for Zero Scrap Indicating MCO Design Pressure,
Bounding Backfill.

Pressure vs Oxygen Concentration for Zero Scrap, K-West bounding water inventory, and high helium backfill. Lower lines with symbols indicate MCO conditions for various reactive areas with no combustion. Upper lines with no symbols are for post-burn sensitivity cases with hydrogen gettering to increase the O₂ concentration up to stoichiometry. The upper horizontal dashed line is the MCO design pressure 450 psig (31 atm absolute).

Combustion is impossible for O₂ < 4%. The worst case group is for A=0, zero reactive area, because this maximizes the number of moles of oxygen. The worst case is for the highest power, hence highest moles of oxygen. The highest post-burn pressure is 13 atm.

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APPENDIX A
AICC MATHCAD MODEL

ADIABATIC, ISOCHORIC, COMPLETE COMBUSTION FUNCTION AND APPLICATION FOR HYDROGEN - AIR - HELIUM MIXTURES

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FOR: Hanford Spent Nuclear Fuel Project, contact Darrell Duncan 509-372-1013.

Contains Cv(T) Polynomial fit used by transient analysis program HANSF. This fit is based on AlChE data, converted to this format for ease of integration.

Expand for other inert gases simply by adding polynomial fits and extra indices in the functions.
For other fuels or oxidants, require rules for proportion of reactants consumed.

1.0 GAS SPECIFIC HEAT DATA: CV(T) POLYNOMIAL FIT.

Gases are entered in the order: H2, He, N2, O2, H2O from HANSF input GASPROP.DAT.
Values in J/g-mole/K!!! FW is the formula weight vector, assists to identify each gas.

$$CCV := \begin{bmatrix} 21.136 & -1.529 \cdot 10^{-3} & 1.978 \cdot 10^{-6} & 4.018 \cdot 10^{-10} & -1.171 \cdot 10^{-13} \\ 12.47 & 0 & 0 & 0 & 0 \\ 20.785 & -3.871 \cdot 10^{-3} & 1.34 \cdot 10^{-5} & -7.216 \cdot 10^{-9} & 1.16 \cdot 10^{-12} \\ 17.045 & 0.014 & -4.96 \cdot 10^{-6} & 1.375 \cdot 10^{-10} & 1.375 \cdot 10^{-13} \\ 24.044 & -7.883 \cdot 10^{-5} & 1.513 \cdot 10^{-5} & -7.323 \cdot 10^{-9} & 1.087 \cdot 10^{-12} \end{bmatrix} \quad FW := \begin{bmatrix} 2 \\ 4 \\ 28 \\ 32 \\ 18 \end{bmatrix}$$

Functions for Cv and Ug of a specific gas:

$$fCv(i, T) := CCV_{i,0} + CCV_{i,1} \cdot T + CCV_{i,2} \cdot T^2 + CCV_{i,3} \cdot T^3 + CCV_{i,4} \cdot T^4$$

$$fug(i, T) := T \left[CCV_{i,0} + T \left[\frac{1}{2} CCV_{i,1} + T \left[\frac{1}{3} CCV_{i,2} + T \left(\frac{1}{4} CCV_{i,3} + T \frac{1}{5} CCV_{i,4} \right) \right] \right] \right]$$

Function for energy of a gas with mole vector N at temperature T (without integration constant):

$$fUg(N, T) := \begin{cases} U \leftarrow 0 \\ \text{for } i \in 0..4 \\ U \leftarrow U + N_i \cdot fug(i, T) \\ U \end{cases}$$

Test energy function by evaluating at 300 and 301 K, difference numerically equals Cv:

$$N := (1 \ 1 \ 1 \ 1 \ 1)^T \quad fUg(N, 301) - fUg(N, 300) = 99.986$$

2.0 AICC Function input is mole vector (see order above) and initial Temperature.
Output is a vector with: post-burn mole vector, AICC temperature, AICC pressure.

$$\begin{aligned}
 \text{fAICC } N, T_o, V &:= \begin{cases} H_2 \leftarrow N_0 \\ O_2 \leftarrow N_3 \\ \Delta H_{2O} \leftarrow \text{if}(H_2 \leq 2 \cdot O_2, H_2, 2 \cdot O_2) \\ NP \leftarrow [H_2 - \Delta H_{2O} \quad N_1 \quad N_2 \quad O_2 - 0.5 \cdot \Delta H_{2O} \quad N_4 + \Delta H_{2O}]^T \\ Q \leftarrow \Delta H_{2O} \cdot 241.8 \cdot 10^3 \\ U_o \leftarrow fUg(N, T_o) \\ T \leftarrow T_o + Q \cdot (fUg(N, T_o + 1) - U_o)^{-1} \\ T_f \leftarrow \text{root}(fUg(NP, T) - U_o - Q, T) \\ n_f \leftarrow \sum NP \\ P_f \leftarrow n_f \cdot 8.314 \cdot T_f \cdot V^{-1} \\ TP \leftarrow [T_f \quad P_f]^T \\ f \leftarrow \text{stack}(NP, TP) \\ f \end{cases}
 \end{aligned}$$

Test by creating atmospheres with various amounts of H2 in air, then H2 in air with He replacing N2:

$$\begin{aligned}
 V &:= 1 \quad T_o := 298.15 \quad P_o := 1.013 \cdot 10^5 \quad n_o := \frac{P_o \cdot V}{8.314 \cdot T_o} \quad n_o = 40.866 \\
 i &:= 2..40 \quad H_2\%_i := 2 \cdot i \quad H_{2,i} := n_o \cdot \frac{H_2\%_i}{100} \quad O_{2,i} := 0.208 \cdot (n_o - H_{2,i}) \quad N_{2,i} := 0.792 \cdot (n_o - H_{2,i})
 \end{aligned}$$

H2 in Air:

$$\begin{aligned}
 N_{1,0,i} &:= H_{2,i} \quad N_{1,1,i} := 0 \quad N_{1,2,i} := N_{2,i} \quad N_{1,3,i} := O_{2,i} \quad N_{1,4,i} := 0 \\
 A1^{<i>} &:= \text{fAICC}(N1^{<i>}, T_o, V) \quad T_{air,i} := A1_{5,i} \quad P_{air,i} := A1_{6,i} \cdot P_o^{-1}
 \end{aligned}$$

Check Vs. values published by Kuchta, USBOM, 1985: 4%, 746 K, 8%, 1151 K, 12%, 1528 K:

$$\begin{aligned}
 H_2\%_2 &= 4 \quad H_2\%_8 = 8 \quad H_2\%_{12} = 12 \quad \text{Error less than 1\%, attributable to small } C_v \text{ differences.} \\
 T_{air,2} &= 749.17 \quad T_{air,4} = 1.16 \cdot 10^3 \quad T_{air,6} = 1.542 \cdot 10^3
 \end{aligned}$$

H2 combustion in O2+He mixtures where He has same proportion as N2 in air:

$$\begin{aligned}
 N_{1,0,i} &:= H_{2,i} \quad N_{1,1,i} := N_{2,i} \quad N_{1,2,i} := 0 \quad N_{1,3,i} := O_{2,i} \quad N_{1,4,i} := 0 \\
 A1^{<i>} &:= \text{fAICC}(N1^{<i>}, T_o, V) \quad T_{He,i} := A1_{5,i} \quad P_{He,i} := A1_{6,i} \cdot P_o^{-1}
 \end{aligned}$$

AICC Pressure for H₂-Air and H₂-(21% O₂, 79% He) Mixtures, 25 C, 1atm Initial

AICC Temperature for H₂-Air and H₂-(21% O₂, 79% He) Mixtures, 25 C, 1atm Initial

Post-Combustion conditions in an MCO: Initial 1.5 atm He, various initial H2 and O2 moles

$$V := 0.5 \quad T_o := 298.15 \quad P_o := 1.5 \cdot 10^5 \quad n_{he} := \frac{P_o \cdot V}{8.314 \cdot T_o} \quad n_{he} = 30.256$$

Vary initial H2 from 5% to 75% in steps of 5%: Vary initial O2 from 4% to 12% in steps of 2%:

$$i := 0..15 \quad H2\%_i := 5 \cdot (i + 1) \quad j := 0..4 \quad O2\%_j := 4 + 2 \cdot j$$

Solve for sum of H2 and O2 moles: $OH_{i,j} := 0.01 \cdot (H2\%_i + O2\%_j) \cdot n_{he} \cdot [1 - 0.01 \cdot (H2\%_i + O2\%_j)]^{-1}$

$$nH2_{i,j} := 0.01 \cdot H2\%_i \cdot (n_{he} + OH_{i,j}) \quad nO2_{i,j} := 0.01 \cdot O2\%_j \cdot (n_{he} + OH_{i,j})$$

Use 50 C as an average storage temperature for pre-combustion conditions:

$$P0_{i,j} := \frac{n_{he} + OH_{i,j}}{n_{he}} \cdot \frac{P_o}{10^5} \cdot \frac{323.15}{298.15} \quad P_{i,j} := 10^{-5} \cdot fAICC \cdot \begin{bmatrix} nH2_{i,j} \\ n_{he} \\ 0 \\ nO2_{i,j} \\ 0 \end{bmatrix} \cdot 323.15, V \quad R_{i,j} := \frac{P_{i,j}}{P0_{i,j}}$$

Pressure Ratio (P-final / P-initial) for various initial H₂% and O₂% in an MCO backfilled to 1.5 atm He at 25 C, and stored at 50 C. Multiply plotted value by initial pressure to yield final pressure in atm. Some combinations of initial H₂% and O₂% on the plot are not considered possible.

APPENDIX B
KIRKPATRICK - CONDON HYDRIDING MODEL

HYDRIDING OF URANIUM METAL

Kirkpatrick and Condon Hydriding model from J. Less Common Metals 172-174, 1991
 Limit of no dehydriding, temperatures below 300 C.

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 For: Hanford Spent Nuclear Fuel Project, Duke Engineering & Services Hanford, Darrel Duncan.

Hydriding constant (Eq. 7), 1/s

$$fk_1(T) := 10.4 \cdot \exp\left(\frac{1592}{T}\right)$$

Diffusion constant (Eq. 9), m²/s

$$fD(T) := 1.9 \cdot 10^{-6} \cdot \exp\left(\frac{-5820}{T}\right)$$

Saturation parameter (Eq. 12), mf

$$fN(T) := \exp\left(-2.362 - \frac{2305}{T}\right)$$

Solubility of H₂ in U (Eq. 10), mf
 where P is in Pa

$$fC_o(T, P) := \begin{cases} N \leftarrow fN(T) \\ E \leftarrow 4.183 \cdot 10^{-6} \cdot \exp\left(\frac{-894}{T}\right) \cdot \sqrt{P} \\ N \cdot E \\ N + E \end{cases}$$

Mole fraction U of spill material (Eq. 13)
 asymptotic value below 250 to 300 C,
 and generalized mole fraction for spill

$$U_C := 0.989 \quad U_E := \sqrt{U_C}$$

Stoichiometry factor for UH₃

$$s := 3$$

Generalized effective diffusivity (Eq. 16), m²/s

$$fD_E(T, P) := fD(T) \cdot \frac{fN(T)}{\sqrt{fN(T) - fC_o(T, P)}}$$

Time to spill (Eq. 15), s

$$ft_1(T, P) := \frac{-\ln(U_C)}{fk_1(T) \cdot fC_o(T, P)}$$

Spill front velocity (Eq. 14), m/s

$$fV_S(T, P) := \frac{1}{ft_1(T, P)} \cdot \frac{fD_E(T, P)}{\sqrt{s \cdot fk_1(T) \cdot U_E}}$$

To reproduce Fig. 1 of paper, set P=1 atm, loop from 25 C to 225 C, get V in nm/s:

$$T_k := 273.15 \quad P := 1.013 \cdot 10^5 \quad i := 0..20 \quad T_i := T_k + 25 + i \cdot 10 \quad T_{i1} := 1000 / T_i \cdot 10^3 \quad V_i := fV_S(T_i, P) \cdot 10^9$$

Datapoints from published curve: j:=0..3

$$TD := (50 \ 100 \ 150 \ 200)^T + T_k \quad LVD := (1.2 \ 1.8 \ 2.25 \ 2.6)^T \quad VD := \frac{1000}{LVD} \quad TDI := \frac{1000}{TD}$$

Values at 0.5 atm H₂ and 2 atm H₂:

$$V2_i := fV_S(T_i, 2 \cdot P) \cdot 10^9 \quad V05_i := fV_S(T_i, 0.5 \cdot P) \cdot 10^9$$

Hydriding rate (nm/s) of clean uranium in hydrogen at 1 atm, with de-hydriding neglected for low temperatures and hydrogen pressures above saturation. Solid line is correlation of Kirkpatrick and Condon, 1991, diamonds are values from published curve for validation.

Hydriding rate (nm/s) of clean uranium in hydrogen at 1 atm, with de-hydriding neglected for low temperatures and hydrogen pressures above saturation. Solid line is correlation of Kirkpatrick and Condon, 1991, diamonds are values from published curve for validation.

APPENDIX C
ZERO SCRAP COMBUSTION SENSITIVITY CASES

MCO O₂ AND PRESSURIZATION: RADIOLYSIS AND GETTERING OF O₂**ZERO SCRAP BASKET END-OF-LIFE CASES**

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DATE: October, 1998.

Calculation Technical Basis and Assumptions:

1. Decay power varies per HNF-SD-SNF-CN-006 Regulatory/Safety Design Basis; see below. Alpha, beta, and gamma fractions are applied for all total MCO powers. Absorption based on fuel mass of 6339 kg.
2. Water-bearing materials are: Al(OH)₃ cladding film, Canister particulate composed of (Al,Fe)(OH)₃, adhering particulate containing UO₃·2H₂O, and free water. Other sources are negligible for radiolysis.
3. g(O₂) and g(H₂) values from HNF-SD-SNF-CN-006; see below.
4. Gamma absorption by Al(OH)₃, UO₃·2H₂O, and H₂O relative to that by U based on 0.6 MeV gamma.
5. Al(OH)₃ cladding film radiolysis is by gamma dose alone; all other materials get alpha, beta, and gamma.
6. Canister particulate has alpha, beta dose/kg reduced by the U fraction; 20% for bounding case.
7. Uranium Oxide Hydrates are conservatively represented by UO₃·2H₂O.
8. No thermal decomposition of hydrates - residual H₂O evaporates first, system is saturated.
9. Fuel and scrap temperatures related to decay power as a function of time by conservative conductances.
10. No hydrogen gettering - only occurs when Oxygen is depleted. This allows the maximum pressure to be calculated, before substantial H₂ gettering.
11. Oxygen gettering by Ritchie's moist air correlation, since H₂O present, with a minimum limit of Trimble's dry air correlation.
12. MCO is backfilled to 1.5 atm He at 25 °C - normally. Neglect difference between atm and 10⁻⁵ Pascals.
12. Calculations may be conducted with bounding or best-estimate values.

Parameter	Bound	Best-Est.	
H ₂ O from UO ₃ ·2H ₂ O canister particulate	100 g H ₂ O / m ²	50 g H ₂ O / m ²	
Scrap reactive area / basket	4.5 m ²	1.7 m ²	
Fuel reactive area / basket	0.79 m ²	0.0425 m ²	
H ₂ O from UO ₃ ·2H ₂ O	1036 g two scrap		
	667 g one scrap		
	297 g no scrap		
H ₂ O from canister particulate	80% Al, 20% U hydrate	25% Al, 75% U hydrate	
	144 g two scrap	29 g two scrap	
	192 g one scrap	39 g one scrap	
	240 g no scrap	49 g no scrap	
water:	66.7 grams/m ² , 200 gram limit, all cases!		Free

**** Units: time in years, mass in grams, area in m², with appropriate conversions used.**

1.0 INPUT AND DERIVED VALUES**Constants**

Avogadro's number	$N_a := 6.022 \cdot 10^{23}$	Conversion factor J/100 ev	$J_{ev} := 1.6 \cdot 10^{-17}$
Seconds in a year	$Sec_y := 3600 \cdot 24 \cdot 365$	Ideal gas constant	$R_{gas} := 8.314$
Molecular weights of Al(OH)3, UO3.2H2O, H2O:		$M_{ah} := 78$	$M_{uh} := 322$ $M_w := 18$

MCO Backfill and Fuel Inventory

MCO volume, m^3, backfill temperature, K	$V_{mco} := 0.5$		
MCO backfill temperature, K, and Pressure, atm:	$T_{bf} := 298$	$P_{bf} := 1.5$	
Helium backfill moles:	$n_{he} := P_{bf} \cdot 10^5 \cdot V_{mco} \cdot (R_{gas} \cdot T_{bf})^{-1}$		$n_{he} := 30.27$
Fuel Mass (grams):	$M_f := 6.339 \cdot 10^6$		

MCO Water Inventory Values: See HNF-1523 and HNF-1527

UO3.xH2O water mass per unit area gram/m^2	$\mu := 50$	!! BEST-ESTIMATE 50, BOUND 100 !!	
Max g H2O from UO3.xH2O Adhering Partic.	$UH_{max} := 1036$	!! 0 scrap: 297 g; 1 scrap: 667 g !!	
Max g of Al(OH)3 Clad Film:	$AL_{max} := 10650$		
Free H2O, g, bounding value:	$FW_{max} := 200$		
Amount of water from UO4.2H2O if no AL(OH), g	$m_{u04} := 52$		

MCO Power - Temperature Relations:

Heat transfer conductances: Scrap, Low T. fuel,	$U_{sc} := 12.4$	$U_{fl} := 9.5$	$U_{fa} := 8.7$	$U_{fh} := 8.2$
Avg. T fuel, High T. fuel, W/K:		$N_{fl} := \frac{18}{54}$	$N_{fa} := \frac{30}{54}$	$N_{th} := \frac{6}{54}$
Fraction of assemblies per fuel group, low to high:				
Conservative annual average vault T and half-amplitude		$T_{av} := 12 + 3$	$dT_{av} := 12$	
Hanford avg. is 12, High is 26, Low is -3; Vault is 6 C higher,				

g(H2) and g(O2) Values from HNF-SD-SNF-CN-006:

Rad type	g(H2)	g(O2)
alpha	$1.5 \cdot x$	$0.75 \cdot x$
beta	$0.45 \cdot x$	$0.225 \cdot x$
gamma	1.2 for $0.04 < x < 0.35$	x for $x < 0.1$, else $0.0861 + 0.139 \cdot x$

g(H2) value for Al(OH)3, molec/100 ev	$g_{haa} := 0.525$	$g_{ha\beta} := 0.1575$	$g_{ha\gamma} := 1.2$
g(O2) value for Al(OH)3, molec/100 ev	$g_{oaa} := 0.2625$	$g_{oa\beta} := 0.07875$	$g_{oa\gamma} := 0.135$
g(H2) values for UO3 hydrates, molec/100 ev	$g_{hua} := 0.165$	$g_{hu\beta} := 0.05$	$g_{hu\gamma} := 1.2$
g(O2) values for UO3 hydrates, molec/100 ev	$g_{oua} := 0.083$	$g_{ou\beta} := 0.025$	$g_{ou\gamma} := 0.101$
g(H2) values for free H2O, molec/100 ev	$g_{hwa} := 1.6$	$g_{hw\beta} := 0.53$	$g_{hw\gamma} := 0.5$
g(O2) values for free H2O, molec/100 ev	$g_{owa} := 0.8$	$g_{ow\beta} := 0.265$	$g_{ow\gamma} := 0.25$
Relative gamma absorption for Al, U, H2O:	$rQ_{a\gamma} := 0.35$	$rQ_{u\gamma} := 0.86$	$rQ_{w\gamma} := 0.38$

Decay Power Variation with Time: HNF-SD-SNF-CN-006 Regulatory/Safety Design Basis

source	1995	2040	lamda	tau	Where lamda in 1/year and tau in year
alpha	26.3	32	-4.36e-3	-159	Alpha increases as fraction with time
beta	65	22	+2.41e-2	28.8	
gamma	42.4	14.3	+2.42e-2	28.7	Note decay power in W/MT here
TOTAL	133.7	68.3	1.49e-2	46.4	

Initial power fractions; Each independently decayed with time.

$$fQ_{\alpha 0} := \frac{26.3}{133.7} \quad fQ_{\beta 0} := \frac{65}{133.7} \quad fQ_{\gamma 0} := \frac{42.4}{133.7}$$

Decay rates for alpha,beta,gamma, and total power based on 1995 to 2040 changes. Note alpha power increases slightly, so rate is negative.

$$\lambda_{\alpha} := \frac{-1}{45} \cdot \ln \left(\frac{32}{26.3} \right) \quad \lambda_{\alpha} = -4.36 \cdot 10^{-3}$$

$$\lambda_{\beta} := \frac{-1}{45} \cdot \ln \left(\frac{22}{65} \right) \quad \lambda_{\beta} = 0.02$$

$$\lambda_q := \frac{-1}{45} \cdot \ln \left(\frac{68.3}{133.7} \right) \quad \lambda_q = 0.01$$

$$\lambda_{\gamma} := \frac{-1}{45} \cdot \ln \left(\frac{14.3}{42.4} \right) \quad \lambda_{\gamma} = 0.02$$

****** CASES FOR ZERO SCRAP BASKETS ******

$$AL_{\max} := 10650$$

$$UH_{\max} := 297$$

2.1 TIME-DEPENDENT POWER FRACTIONS: Multiply by initial power to get power(time) for each mode:

$$fQ_{\alpha}(t) := fQ_{\alpha 0} \cdot \exp(-\lambda_{\alpha} \cdot t) \quad fQ_{\beta}(t) := fQ_{\beta 0} \cdot \exp(-\lambda_{\beta} \cdot t) \quad fQ_{\gamma}(t) := fQ_{\gamma 0} \cdot \exp(-\lambda_{\gamma} \cdot t)$$

Example for use of alpha power: $fQ_{\alpha}(45) = 0.24 \quad 32 \cdot (32 + 22 + 14.3)^{-1} \cdot \exp(-\lambda_{\alpha} \cdot 45) = 0.24$

2.2 FUNCTIONS FOR DECAY CONSTANTS AND EXAMPLES

Decay constant for free H2O radiolysis: WH=H2 yield, WO=O2 yield

$$\lambda_{wo} := M_f^{-1} \cdot M_w (\text{Jev} \cdot \text{Na})^{-1} \cdot \text{Secy}$$

$$fg_{wh}(t) := g_{hw\beta} \cdot fQ_{\alpha}(t) + g_{hw\beta} \cdot fQ_{\beta}(t) + g_{hw\gamma} \cdot fQ_{\gamma}(t) \quad fg_{wh}(0) = 0.63$$

$$fg_{wo}(t) := g_{ow\alpha} \cdot fQ_{\alpha}(t) + g_{ow\beta} \cdot fQ_{\beta}(t) + g_{ow\gamma} \cdot fQ_{\gamma}(t) \quad fg_{wo}(0) = 0.32$$

$$fl_{wh}(Q, t) := \lambda_{wo} \cdot Q \cdot fg_{wh}(t) \quad fl_{wh}(396, 0) = 2.33 \cdot 10^{-3}$$

$$fl_{wo}(Q, t) := \lambda_{wo} \cdot Q \cdot fg_{wo}(t) \quad fl_{wo}(396, 0) = 1.16 \cdot 10^{-3}$$

Water fraction at 40 years, average power MCO: $\exp \left(- \int_0^{40} fl_{wh}(400, t) dt \right) = 0.92$

Decay constant for Al(OH)3 radiolysis: AC=Cladding Film

$$\lambda_{ao} := \left[M_f^{-1} \cdot M_{ah} \cdot (\text{Jev} \cdot \text{Na})^{-1} \cdot \text{Secy} \right]$$

$$fg_{ach}(t) := g_{hay} \cdot rQ_{ay} \cdot fQ_{\gamma}(t)$$

$$fg_{ach}(0) = 0.13$$

$$fg_{aco}(t) := g_{oay} \cdot rQ_{ay} \cdot fQ_{\gamma}(t)$$

$$fg_{aco}(0) = 0.01$$

$$fl_{ach}(Q, t) := \lambda_{ao} \cdot Q \cdot fg_{ach}(t)$$

$$fl_{ach}(396, 0) = 2.12 \cdot 10^{-3}$$

$$fl_{aco}(Q, t) := \lambda_{ao} \cdot Q \cdot fg_{aco}(t)$$

$$fl_{aco}(396, 0) = 2.39 \cdot 10^{-4}$$

$$\text{Al clad fraction at 40 years, average power MCO: } \exp \left(- \int_0^{40} \frac{2}{3} fl_{ach}(400, t) dt \right) = 0.96$$

Decay constant for Al(OH)3 radiolysis: AP=Al in Adhering Particulate

$$fg_{aph}(f_u, t) := f_u \cdot (g_{haa} \cdot fQ_{\alpha}(t) + g_{hap} \cdot fQ_{\beta}(t)) + g_{hay} \cdot rQ_{ay} \cdot fQ_{\gamma}(t)$$

$$fg_{aph}(0.2, 0) = 0.17$$

$$fg_{apo}(f_u, t) := f_u \cdot (g_{oaa} \cdot fQ_{\alpha}(t) + g_{oap} \cdot fQ_{\beta}(t)) + g_{oay} \cdot rQ_{ay} \cdot fQ_{\gamma}(t)$$

$$fg_{apo}(0.2, 0) = 0.03$$

$$fl_{aph}(Q, f_u, t) := \lambda_{ao} \cdot Q \cdot fg_{aph}(f_u, t)$$

$$fl_{aph}(396, 0.2, 0) = 2.7 \cdot 10^{-3}$$

$$fl_{apo}(Q, f_u, t) := \lambda_{ao} \cdot Q \cdot fg_{apo}(f_u, t)$$

$$fl_{apo}(396, 0.2, 0) = 5.26 \cdot 10^{-4}$$

$$\text{Al Adhering Partic. fraction at 40 years, average power MCO: } \exp \left(- \int_0^{40} fl_{aph}(400, 0.2, t) dt \right) = 0.93$$

Decay constant for UO3.2H2O radiolysis

$$\lambda_{uo} := \left[M_f^{-1} \cdot M_{uh} \cdot (\text{Jev} \cdot \text{Na})^{-1} \cdot \text{Secy} \right]$$

$$fg_{uh}(t) := g_{hua} \cdot fQ_{\alpha}(t) + g_{hup} \cdot fQ_{\beta}(t) + g_{huy} \cdot rQ_{uy} \cdot fQ_{\gamma}(t)$$

$$fg_{uh}(0) = 0.38$$

$$fg_{uo}(t) := g_{oua} \cdot fQ_{\alpha}(t) + g_{oup} \cdot fQ_{\beta}(t) + g_{ouy} \cdot rQ_{uy} \cdot fQ_{\gamma}(t)$$

$$fg_{uo}(0) = 0.06$$

$$fl_{uh}(Q, t) := \lambda_{uo} \cdot Q \cdot fg_{uh}(t)$$

$$fl_{uh}(396, 0) = 0.03$$

$$fl_{uo}(Q, t) := \lambda_{uo} \cdot Q \cdot fg_{uo}(t)$$

$$fl_{uo}(396, 0) = 3.69 \cdot 10^{-3}$$

$$\text{U Hydrates fraction at 40 years, average power MCO: } \exp \left(- \int_0^{40} \frac{1}{2} fl_{uh}(400, t) dt \right) = 0.71$$

2.3 FUNCTIONS FOR U GETTERING RATE AND WATER VAPOR PRESSURE

$$\text{Water vapor pressure: } fP_{\text{sat}}(T) := e^{\frac{25.339 - \frac{5154.7}{T}}{}} \quad fP_{\text{sat}}(323) = 1.19 \cdot 10^4 \quad 50 \text{ C OK}$$

Ritchie correlation for U-H₂O-O₂, below 100% RH, below 100 C, agrees best with data BUT goes below dry air correlation at about 37 C - so switch to McGillivray dry air. Ritchie units of mg/cm²/hr, converted to grams O₂ per m² per year.; McGillivray units of kg/m²/s similarly converted.

$$K_{\text{rit}}(T) := 10^{13.8808 - 5769.6 \cdot T^{-1}} \cdot 10^{-8766} \quad \text{Ritchie} \quad K_{\text{trim}}(T) := 10^{7.19 - 3732 \cdot T^{-1}} \cdot 10^{-8766} \quad \text{Trimble}$$

$$T_{\text{cor}} := (5769.6 - 3732) \cdot (13.8808 - 7.19)^{-1} \quad T_{\text{cor}} = 304.54 \quad \text{Switch correlations here, 31 C}$$

Moist Air Getter Function 100% RH:

$$fK_o(323) \cdot 0.1 \cdot (8766)^{-1} = 1.04 \cdot 10^{-4}$$

$$fK_o(T) := \text{if}(T \geq T_{\text{cor}}, K_{\text{rit}}(T), K_{\text{trim}}(T))$$

OK @ 50 C in mg/cm²/hr

Shows no discontinuity

$$fK_o(323) \cdot 10^{-3} \cdot (3.15 \cdot 10^7)^{-1} = 2.9 \cdot 10^{-10}$$

OK @ 50 C in kg/m²/s

$$fK_o(T_{\text{cor}} + 0.01) \cdot 10^{-3} \cdot (3.15 \cdot 10^7)^{-1} = 2.4 \cdot 10^{-11}$$

$$fK_o(T_{\text{cor}} - 0.01) \cdot 10^{-3} \cdot (3.15 \cdot 10^7)^{-1} = 2.4 \cdot 10^{-11}$$

Gettering of Water vapor when Oxygen-Free:

$$fK_w(T) := \begin{cases} P_{\text{st}} \cdot 10^{-3} \cdot fP_{\text{sat}}(T) \\ K \leftarrow P_{\text{st}}^{0.5} \cdot 10^{4.33 - 2144 \cdot T^{-1}} \\ K \leftarrow K \cdot 10^{-8766} \end{cases}$$

$$fK_w(323) = 1.49 \cdot 10^3$$

$$fK_o(323) = 9.14$$

$$\frac{1486}{9.14} = 162.58$$

2.4 RELATIONSHIP BETWEEN MCO POWER AND GAS TEMPERATURE

Conservative relationships based on 733 W MCO, zero scrap case for fuel and one scrap case for scrap. Vault gas-tube dT=28 C, Fuel tube-MCO gap dT=39 C, Scrap gap dT=27 C. Inside MCO, fuel dT's are 12.5, 20, and 26 C; scrap dT is 4 C. Function yields scrap and low to high fuel T's in that order:

$$fT_{\text{get}}(Q_o, t) := Q_o \cdot e^{-\lambda \cdot q \cdot t} \left[\frac{1}{U_{\text{sc}}} \frac{1}{U_{\text{fl}}} \frac{1}{U_{\text{fa}}} \frac{1}{U_{\text{fh}}} \right]^T + T_{\text{av}}$$

$$fT_{\text{get}}(400, 0)^T = [47.26 \quad 57.11 \quad 60.98 \quad 63.78]$$

$$fT_{\text{get}}(770, 0)^T = [77.1 \quad 96.05 \quad 103.51 \quad 108.9]$$

2.5 ACCOUNT FOR ANNUAL TEMPERATURE VARIATION BY INTEGRAL AVERAGE FOR A YEAR

Create an interpolation table over the temperature range of interest, then define a new rate law function which automatically incorporates the average annual enhancement factor. Input T in Kelvins!

$$fT_a(T, t) := T + dT_{av} \sin(2\pi \cdot t)$$

$$fE(T) := fK_0(T)^{-1} \cdot \int_0^1 fK_0 \cdot fT_a(T, t) \cdot dt$$

$$j := 0..60 \quad T_{sj} := 283 + 2 \cdot j$$

$$E_j := fE(T_{sj})$$

$$fE(T) := \text{linterp}(T_{sj}, E_j, T)$$

$$fK_1(T) := fE(T) \cdot fK_0(T)$$

$$\text{Values at low, medium, high T: } fE(288) = 1.38$$

$$fE(333) = 1.54$$

$$fE(383) = 1.29$$

2.6 FUNCTIONS TO SET UP INITIAL CONDITIONS

User specifies:

- (1) Q = MCO Initial power, W;
- (2) As = Scrap reactive area, m²;
- (3) Af = Fuel reactive area, m²;
- (4) ma = Al(OH)3 film mass, g;
- (5) mwcp = Canister particulate water mass, g;
- (6) fUcp = U fraction of can. partic. for alpha,beta
- (7) fwUcp: U water fraction of can. particulate;
- (8) mu: Mass/area water from UO3.2H2O;
- (9) mfw: Free water mass per area, g/m².

State vector V assigned based on these inputs:

Actual state variables are:

- (0) nac= Al(OH)3 cladding film water moles
 - (1) nap=Al(OH)3 can particulate water moles
 - (2) nu=UO3.2H2O water moles
 - (3) nw=free H2O moles
 - (4) nh2=H2 + H2O vapor moles
 - (5) no2=O2 moles
- Parameters are:
- (6) Q = Power,
 - (7) AS = Scrap area,
 - (8) AF = Fuel Area,
 - (9) fucp = U fraction of canister particulate

Other assumptions of note:

- (1) Initial water vapor mass determined by scrap T;
- (2) Residual free water prevents hydrate thermal decomposition.

Initial steam from free water, assumed sufficient; free water not depleted; scrap T (index 0) used:

$$f n_{st}(Q) := \begin{cases} T_0 \leftarrow fT_{get}(Q, 0)_0 + 273 \\ \rho_{sat}(T_0) \cdot V_{mco} \cdot (R_{gas} \cdot T_0)^{-1} \end{cases}$$

Function for water moles of UO3.2HO plus UO4.2H2O given m = kg/m² from UO3.2H2O, A=fuel reactive area, and adding UO4 contribution in proportion the fraction not covered with Al(OH)3, given its mass ma.

$$f n_{wu}(\mu, A_s, A_f, m_{wcp}, fw_{ucp}, m_a) := \begin{cases} m_{ap} \leftarrow \mu \cdot (A_s + A_f) \\ m_{ap} \leftarrow \text{if}(m_{ap} > UH_{max}, UH_{max}, m_{ap}) \\ m_{clad} \leftarrow m_{uo4} \cdot (1 - m_a \cdot AL_{max}^{-1}) \\ m_{clad} \leftarrow \text{if}(m_a > AL_{max}, 0, m_{clad}) \\ m_{cp} \leftarrow m_{wcp} \cdot fw_{ucp} \\ n \leftarrow (m_{ap} + m_{clad} + m_{cp}) \cdot M_w^{-1} \end{cases}$$

$$f n_{fw}(m_{fw}, A_s, A_f) := \begin{cases} m \leftarrow m_{fw} \cdot (A_s + A_f) \\ n \leftarrow \text{if}(m > FW_{max}, FW_{max}, m) \cdot M_w^{-1} \end{cases}$$

$$fV(Q, A_s, A_f, m_a, m_{wcp}, f_{ucp}, fw_{ucp}, \mu, m_{fw_j}) := \begin{bmatrix} 1.5 \cdot m_a \cdot M_{ah}^{-1} \\ m_{wcp} \cdot 1 - fw_{ucp} \cdot M_w^{-1} \\ fn_{wu} \cdot \mu \cdot A_s \cdot A_f \cdot m_{wcp} \cdot fw_{ucp} \cdot m_a \\ fn_{fw} \cdot m_{fw} \cdot A_s \cdot A_f \\ fn_{st}(Q) \\ 10^{-5} \cdot n_{he} \\ Q \\ A_s \\ A_f \\ f_{ucp} \end{bmatrix}$$

Test for bounding conditions, one scrap basket:

$$fV(733, 4.5, 3.16, 10050, 192, 0.1, 0.1, 100, 30)^T = \begin{bmatrix} 193.27 & 9.6 & 17.73 & 11.11 & 6.22 & 3.03 \cdot 10^{-4} & 733 \end{bmatrix}$$

2.7 FUNCTIONS FOR H2, O2 SOURCE AND SINK; R=Radiolysis Source, G=Getter

Current O2 model assumes O2 getting phase from beginning of transient.
Current H2 model assumes no getting.

$$fR_{O2}(Q, t, n_{ac}, n_{ap}, n_u, n_w, f_{ucp}) := \dot{n}_{aco}(Q, t) \cdot n_{ac} + \dot{n}_{apo}(Q, f_{ucp}, t) \cdot n_{ap} + \dot{n}_{uo}(Q, t) \cdot n_u + \dot{n}_{wo}(Q, t) \cdot n_w$$

$$fGO2(Q, t, A_s, A_f) := \begin{cases} T_{get} \leftarrow fTget(Q, t) + 273 \\ GS \leftarrow A_s \cdot fK_1(T_{get_0}) \\ GF \leftarrow A_f \cdot (N_{fl} \cdot fK_1(T_{get_1}) + N_{fa} \cdot fK_1(T_{get_2}) + N_{fh} \cdot fK_1(T_{get_3})) \\ (GS + GF) \cdot 32^{-1} \end{cases}$$

3.0 RATES OF CHANGE OF RADIOLYSIS SOURCES & PRODUCTS

Need a trick because Mathcad demands a function F whose arguments are t, Y where t is time and Y is a vector of state variables. Output of F is a vector dY/dt. Trick: dY/dt = 0 for constant terms needed.

State variables thus include parameters expected to vary from case to case. Coding first assigns scrutable names to the state vector; see comment below. Coding for readability, not compactness.

$$\begin{aligned}
 dYdt(t, Y) = & \begin{cases} n_{ac} \leftarrow Y_0 \\ n_{ap} \leftarrow Y_1 \\ n_u \leftarrow Y_2 \\ n_w \leftarrow Y_3 \\ n_{h2} \leftarrow Y_4 \\ Y_5 \leftarrow \text{if}[Y_5, 0, 0, Y_5] \\ n_{o2} \leftarrow Y_5 \\ Q \leftarrow Y_6 \\ A_s \leftarrow Y_7 \\ A_f \leftarrow Y_8 \\ f_{ucp} \leftarrow Y_9 \\ dn_{ac} \leftarrow \frac{-2}{3} \cdot \dot{n}_{ach}(Q, t) \cdot n_{ac} \\ dn_{ap} \leftarrow \frac{-2}{3} \cdot \dot{n}_{aph}(Q, f_{ucp}, t) \cdot n_{ap} \\ dn_u \leftarrow \frac{-1}{2} \cdot \dot{n}_{uh}(Q, t) \cdot n_u \\ dn_w \leftarrow \dot{n}_{wh}(Q, t) \cdot n_w \\ \text{sorH2} \leftarrow -(1.5 \cdot dn_{ac} + 1.5 \cdot dn_{ap} + 2 \cdot dn_u + dn_w) \\ \text{sorO2} \leftarrow \text{fR}_{O2}(Q, t, n_{ac}, n_{ap}, n_u, n_w, f_{ucp}) \\ \text{sinkO2} \leftarrow \text{fGO2}(Q, t, A_s, A_f) \\ \text{net} \leftarrow \text{sorO2} - \text{sinkO2} \\ dO2dt \leftarrow \begin{cases} \text{net} & \text{if } (n_{O2} > 0) + (\text{net} > 0) \\ 0 & \text{otherwise} \end{cases} \\ dY \leftarrow [dn_{ac} \quad dn_{ap} \quad dn_u \quad dn_w \quad \text{sorH2} \quad dO2dt \quad 0 \quad 0 \quad 0 \quad 0]^T \\ dY \end{cases}
 \end{aligned}$$

First, assign scrutable names to elements of Y:

Actual state variables are:

nac= Al(OH)₃ cladding film water moles

n_{ap}=Al(OH)₃ can particulate water moles

n_u=UO₃.2H₂O water moles

n_w=free H₂O moles

n_{h2}=H₂ + H₂O vapor moles

n_{o2}=O₂ moles

Parameters are:

Q = Power,

A_S = Scrap area,

A_F = Fuel Area,

f_{ucp} = U frac. of can particulate

Make O₂ moles > 0 for numerical purposes.

Net rate includes sink when there is O₂ present, or at least when the rate is positive (net rate is zero when no O₂ and sink exceeds source).

Function to get End-of-Life values after integration of a single case:

$$\text{fEOL}(Q, A_s, A_f, m_a, m_{wcp}, f_{ucp}, f_{w_{ucp}}, \mu, m_{fw}, t_{\text{end}}) := \begin{cases} Y \leftarrow fV(Q, A_s, A_f, m_a, m_{wcp}, f_{ucp}, f_{w_{ucp}}, \mu, m_{fw}) \\ Z \leftarrow \text{rkadapt}(Y, 0, t_{\text{end}}, 0.001, dYdt, 1000, 0.0001) \\ L \leftarrow \text{rows}(Z) - 1 \\ \text{EOL} \leftarrow [Z_{L,5} \quad Z_{L,6}]^T \end{cases}$$

4.0 COMBUSTION FUNCTIONS

4.1 GAS SPECIFIC HEAT DATA: CV(T) POLYNOMIAL FIT.: Gases are entered in the order: H2, He, N2, O2, H2O from HANSF input GASPROP.DAT. Values in J/g-mole/K!!! FW is the formula weight vector.

$$CCV := \begin{bmatrix} 21.136 & -1.529 \cdot 10^{-3} & 1.978 \cdot 10^{-6} & 4.018 \cdot 10^{-10} & -1.171 \cdot 10^{-13} \\ 12.47 & 0 & 0 & 0 & 0 \\ 20.785 & -3.871 \cdot 10^{-3} & 1.34 \cdot 10^{-5} & -7.216 \cdot 10^{-9} & 1.16 \cdot 10^{-12} \\ 17.045 & 0.014 & -4.96 \cdot 10^{-6} & 1.375 \cdot 10^{-10} & 1.375 \cdot 10^{-13} \\ 24.044 & -7.883 \cdot 10^{-5} & 1.513 \cdot 10^{-5} & -7.323 \cdot 10^{-9} & 1.087 \cdot 10^{-12} \end{bmatrix} \quad FW := \begin{bmatrix} 2 \\ 4 \\ 28 \\ 32 \\ 18 \end{bmatrix}$$

Functions for Cv and Ug of a specific gas:

$$fCv(i, T) := CCV_{i,0} + CCV_{i,1} \cdot T + CCV_{i,2} \cdot T^2 + CCV_{i,3} \cdot T^3 + CCV_{i,4} \cdot T^4$$

$$fug(i, T) := T \left[CCV_{i,0} + T \left[\frac{1}{2} CCV_{i,1} + T \left[\frac{1}{3} CCV_{i,2} + T \left[\frac{1}{4} CCV_{i,3} + T \cdot \frac{1}{5} CCV_{i,4} \right] \right] \right] \right]$$

Function for energy of a gas with mole vector N at temperature T (without integration constant):

$$fUg(N, T) := \begin{cases} U \leftarrow 0 \\ \text{for } i \in 0..4 \\ U \leftarrow U + N_i \cdot fug(i, T) \end{cases} U$$

2.0 AICC Function input is mole vector (see order above) and initial Temperature. Output is a vector with: post-burn mole vector, AICC temperature, AICC pressure.

$$fAICC(N, T_o, V) := \begin{cases} H2 \leftarrow N_0 \\ O2 \leftarrow N_3 \\ \Delta H2O \leftarrow \text{if}(H2 \leq 2 \cdot O2, H2, 2 \cdot O2) \\ NP \leftarrow [H2 - \Delta H2O \quad N_1 \quad N_2 \quad O2 - 0.5 \cdot \Delta H2O \quad N_4 + \Delta H2O]^T \\ Q \leftarrow \Delta H2O \cdot 241.8 \cdot 10^3 \\ U_o \leftarrow fUg(N, T_o) \\ T \leftarrow T_o + Q \cdot (fUg(N, T_o + 1) - U_o)^{-1} \\ T_f \leftarrow \text{root}(fUg(NP, T) - U_o - Q, T) \\ n_f \leftarrow \sum NP \\ P_f \leftarrow n_f \cdot 8.314 \cdot T_f \cdot V^{-1} \\ TP \leftarrow [T_f \quad P_f]^T \\ f \leftarrow \text{stack}(NP, TP) \end{cases} f$$

5.1 K-West Bounding Case & High Power: High Al(OH)₃, High Canister+Adhering Particulate**5.1A Define highest K-West Power, 530 W, and Investigate Fuel area up to 4 m²:**

$$a := 1..10 \quad A_a := \text{if}(a \geq 7, a - 6, \text{if}(a > 1, (a - 1) \cdot 0.05, 0.01)) \quad A_0 := 0 \quad a := 0..10$$

Zero Scrap:	$A_s := 0$	Bounding Can. partic:	$m_{wcp} := 240$
Bounding Al(OH) ₃ :	$m_a := 10650$	Bounding Can. partic U:	$f_{ucp} := 0.2$
Bounding Adher. Partic:	$\mu := 100$	Can. water frac. from U:	$fw_{ucp} := 0.08$
Free water g/m ² :	$m_{fw} := 66.7$	MCO Power	$Q_0 := 530$

$$\begin{bmatrix} nh2_a \\ no2_a \end{bmatrix} := \text{fEOL}(Q_0, A_s, A_a, m_a, m_{wcp}, f_{ucp}, fw_{ucp}, \mu, m_{fw}, 40)$$

$$ntot_a := n_{he} + no2_a + nh2_a \quad O2\%_a := no2_a \cdot (ntot_a)^{-1} \quad O2\%_a := \text{if}(O2\%_a > 0, 100 \cdot O2\%_a, 0)$$

$$PA_a := ntot_a \cdot R_{gas} \cdot (fTget(Q_0, 40)_0 + 273) \cdot V_{mco}^{-1} \cdot 10^{-5} \quad TA_a := fTget(Q_0, 40)_2 \quad NO2A_a := O2\%_a \cdot 0.01 \cdot ntot_a$$

For A = 0, vary moles of H₂ from value with no getter until stoichiometric, and get post-combustion pressure.

$$n_{st} := fn_{st}(Q_0) \quad \delta nh2 := 0.1 \cdot (nh2_0 - n_{st} - 2 \cdot no2_0) \quad n_{st} = 3.13 \quad no2_0 = 2.03 \quad nh2_0 = 19.69$$

$$i := 0..10 \quad n1H2_i := nh2_0 - n_{st} - i \cdot \delta nh2 \quad O2\%_i := 100 \cdot no2_0 \cdot (n_{he} + n_{st} + no2_0 + n1H2_i)^{-1}$$

$$N1_{0,i} := n1H2_i \quad N1_{1,i} := n_{he} \quad N1_{2,i} := 0 \quad N1_{3,i} := no2_0 \quad N1_{4,i} := n_{st} \quad Tk := T_0 + 273$$

$$A1^{<i>} := fAICC(N1^{<i>}, Tk, V_{mco}) \quad P1_i := A1_{6,i} \cdot 101325^{-1} \quad T_0 = 48.53 \quad Tk = 321.53 \quad P1_0 = 11.89$$

$$\mathbf{5.2 \text{ } Q=400 \text{ W:}} \quad Q_0 := 400 \quad \begin{bmatrix} nh2_a \\ no2_a \end{bmatrix} := \text{fEOL}(Q_0, A_s, A_a, m_a, m_{wcp}, f_{ucp}, fw_{ucp}, \mu, m_{fw}, 40)$$

$$ntot_a := n_{he} + no2_a + nh2_a \quad O2B\%_a := no2_a \cdot (ntot_a)^{-1} \quad O2B\%_a := \text{if}(O2B\%_a > 0, 100 \cdot O2B\%_a, 0)$$

$$PB_a := ntot_a \cdot R_{gas} \cdot (fTget(Q_0, 40)_0 + 273) \cdot V_{mco}^{-1} \cdot 10^{-5} \quad TB_a := fTget(Q_0, 40)_2 \quad NO2B_a := O2B\%_a \cdot 0.01 \cdot ntot_a$$

$$n_{st} := fn_{st}(Q_0) \quad \delta nh2 := 0.1 \cdot (nh2_0 - n_{st} - 2 \cdot no2_0) \quad n_{st} = 1.94 \quad no2_0 = 1.55 \quad nh2_0 = 14.54$$

$$i := 0..10 \quad n1H2_i := nh2_0 - n_{st} - i \cdot \delta nh2 \quad O2\%_i := 100 \cdot no2_0 \cdot (n_{he} + n_{st} + no2_0 + n1H2_i)^{-1}$$

$$N1_{0,i} := n1H2_i \quad N1_{1,i} := n_{he} \quad N1_{2,i} := 0 \quad N1_{3,i} := no2_0 \quad N1_{4,i} := n_{st} \quad Tk := T_0 + 273$$

$$A1^{<i>} := fAICC(N1^{<i>}, Tk, V_{mco}) \quad P2_i := A1_{6,i} \cdot 101325^{-1}$$

Number of moles of O₂ at 40 years as function of reactive area and power:

$$A^T =$$

0	0.01	0.05	0.1	0.15	0.2	0.25	1	2	3
---	------	------	-----	------	-----	------	---	---	---

$$Q=400 \text{ W} \quad \text{NO}_2 B^T =$$

1.55	1.34	0.57	0.16	0.03	0	0	0	0	0
------	------	------	------	------	---	---	---	---	---

$$Q=530 \text{ W} \quad \text{NO}_2 A^T =$$

2.03	1.15	0.11	0	0	0	0	0	0	0
------	------	------	---	---	---	---	---	---	---

Pressure (no H₂ gettering) at 40 years as function of reactive area and power:

$$A^T =$$

0	0.01	0.05	0.1	0.15	0.2	0.25	1	2	3
---	------	------	-----	------	-----	------	---	---	---

$$Q=400 \text{ W} \quad \text{PB}^T =$$

2.36	2.35	2.32	2.3	2.31	2.31	2.32	2.46	2.64
------	------	------	-----	------	------	------	------	------

$$Q=530 \text{ W} \quad \text{PA}^T =$$

2.69	2.65	2.61	2.61	2.62	2.63	2.65	2.82	3.05
------	------	------	------	------	------	------	------	------

Moles Oxygen at 40 years for K-West Zero-Scrap Bounding Water Content as function of Reactive Area (M²), Q=530 W and Q=400 W

Pressure vs Oxygen Concentration for Zero Scrap, K-West bounding water inventory. Lower lines with symbols indicate MCO conditions for various reactive areas with no combustion. Upper lines with no symbols are for post-burn sensitivity cases with hydrogen gettingter to increase the O₂ concentration up to stoichiometry.

Combustion is impossible for O₂ < 4%. The worst case group is for A=0, zero reactive area, because this maximizes the number of moles of oxygen. The worst case is for the highest power, hence highest moles of oxygen. The highest post-burn pressure is 11.9 atm.

$$k := 0.6 \quad PL_k := 31 \quad O2L_k := k$$

Pressure vs Oxygen Concentration for Zero Scrap, K-West bounding water inventory. Lower lines with symbols indicate MCO conditions for various reactive areas with no combustion. Upper lines with no symbols are for post-burn sensitivity cases with hydrogen gettingter to increase the O₂ concentration up to stoichiometry. The upper horizontal dashed line is the MCO design pressure 450 psig (31 atm absolute).

Combustion is impossible for O₂ < 4%. The worst case group is for A=0, zero reactive area, because this maximizes the number of moles of oxygen. The worst case is for the highest power, hence highest moles of oxygen. The highest post-burn pressure is 11.9 atm.

MCO O₂ AND PRESSURIZATION: RADIOLYSIS AND GETTERING OF O₂ AND COMBUSTION**ZERO SCRAP BASKET END-OF-LIFE HIGH HELIUM CASE**

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FOR: Hanford Spent Nuclear Fuel Project - Duke Engineering & Services Hanford - Richland, WA

Contact: Darrell Duncan 509-372-1013.

DATE: October, 1998.

Calculation Technical Basis and Assumptions:

1. Decay power varies per HNF-SD-SNF-CN-006 Regulatory/Safety Design Basis; see below. Alpha, beta, and gamma fractions are applied for all total MCO powers. Absorption based on fuel mass of 6339 kg.
2. Water-bearing materials are: Al(OH)₃ cladding film, Canister particulate composed of (Al,Fe)(OH)₃, adhering particulate containing UO₃·2H₂O, and free water. Other sources are negligible for radiolysis.
3. g(O₂) and g(H₂) values from HNF-SD-SNF-CN-006; see below.
4. Gamma absorption by Al(OH)₃, UO₃·2H₂O, and H₂O relative to that by U based on 0.6 MeV gamma.
5. Al(OH)₃ cladding film radiolysis is by gamma dose alone; all other materials get alpha, beta, and gamma.
6. Canister particulate has alpha, beta dose/kg reduced by the U fraction; 20% for bounding case.
7. Uranium Oxide Hydrates are conservatively represented by UO₃·2H₂O.
8. No thermal decomposition of hydrates - residual H₂O evaporates first, system is saturated.
9. Fuel and scrap temperatures related to decay power as a function of time by conservative conductances.
10. No hydrogen gettering - only occurs when Oxygen is depleted. This allows the maximum pressure to be calculated, before substantial H₂ gettering.
11. Oxygen gettering by Ritchie's moist air correlation, since H₂O present, with a minimum limit of Trimble's dry air correlation.
12. MCO is backfilled to 1.5 atm He at 25 C - normally. Neglect difference between atm and 10**5 Pascals.

12. Calculations may be conducted with bounding or best-estimate values.

Parameter	Bound	Best-Est.
H ₂ O from UO ₃ ·2H ₂ O canister particulate	100 g H ₂ O / m ²	50 g H ₂ O / m ²
Scrap reactive area / basket	4.5 m ²	1.7 m ²
Fuel reactive area / basket	0.79 m ²	0.0425 m ²
H ₂ O from UO ₃ ·2H ₂ O	1036 g two scrap	
	667 g one scrap	
	297 g no scrap	
H ₂ O from canister particulate	80% Al, 20% U hydrate	25% Al, 75% U hydrate
	144 g two scrap	29 g two scrap
	192 g one scrap	39 g one scrap
	240 g no scrap	49 g no scrap

water: 66.7 grams/m², 200 gram limit, all cases!

Free

**** Units: time in years, mass in grams, area in m², with appropriate conversions used.**

1.0 INPUT AND DERIVED VALUES**Constants**

Avogadro's number	$N_a := 6.022 \cdot 10^{23}$	Conversion factor J/100 ev	$J_{ev} := 1.6 \cdot 10^{-17}$
Seconds in a year	$Sec_y := 3600 \cdot 24 \cdot 365$	Ideal gas constant	$R_{gas} := 8.314$
Molecular weights of Al(OH)3, UO3.2H2O, H2O:		$M_{ah} := 78$	$M_{uh} := 322$ $M_w := 18$

MCO Backfill and Fuel Inventory HIGH HELIUM BACKFILL

MCO volume, m ³ , backfill temperature, K	$V_{mco} := 0.5$		
MCO backfill temperature, K, and Pressure, atm:	$T_{bf} := 273$	$P_{bf} := 1.86$	
Helium backfill moles:	$n_{he} := P_{bf} \cdot 10^5 \cdot V_{mco} \cdot (R_{gas} \cdot T_{bf})^{-1}$		$n_{he} := 40.97$
Fuel Mass (grams):	$M_f := 6.339 \cdot 10^6$		

MCO Water Inventory Values: See HNF-1523 and HNF-1527

UO3.xH2O water mass per unit area gram/m ²	$\mu := 50$	!! BEST-ESTIMATE 50, BOUND 100 !!	
Max g H2O from UO3.xH2O Adhering Partic.	$UH_{max} := 1036$	!! 0 scrap: 297 g; 1 scrap: 667 g !!	
Max g of Al(OH)3 Clad Film:	$AL_{max} := 10650$		
Free H2O, g, bounding value:	$FW_{max} := 200$		
Amount of water from UO4.2H2O if no AL(OH). g	$m_{uo4} := 52$		

MCO-Power - Temperature Relations:

Heat transfer conductances: Scrap, Low T. fuel,	$U_{sc} := 12.4$	$U_{fl} := 9.5$	$U_{fa} := 8.7$	$U_{fh} := 8.2$
Avg. T fuel, High T. fuel, W/K:				
Fraction of assemblies per fuel group, low to high:		$N_{fl} := \frac{18}{54}$	$N_{fa} := \frac{30}{54}$	$N_{fh} := \frac{6}{54}$
Conservative annual average vault T and half-amplitude Hanford avg. is 12, High is 26, Low is -3; Vault is 6 C higher,		$T_{av} := 12 + 3$	$dT_{av} := 12$	

g(H2) and g(O2) Values from HNF-SD-SNF-CN-006:

Rad type	g(H2)	g(O2)
alpha	$1.5 \cdot x$	$0.75 \cdot x$
beta	$0.45 \cdot x$	$0.225 \cdot x$
gamma	1.2 for $0.04 < x < 0.35$	x for $x < 0.1$, else $0.0861 + 0.139 \cdot x$

g(H2) value for Al(OH)3, molec/100 eV	$g_{haa} := 0.525$	$g_{hap} := 0.1575$	$g_{hay} := 1.2$
g(O2) value for Al(OH)3, molec/100 eV	$g_{oaa} := 0.2625$	$g_{oap} := 0.07875$	$g_{oay} := 0.135$
g(H2) values for UO3 hydrates, molec/100 ev	$g_{hua} := 0.165$	$g_{hup} := 0.05$	$g_{huy} := 1.2$
g(O2) values for UO3 hydrates, molec/100 ev	$g_{oua} := 0.083$	$g_{oup} := 0.025$	$g_{ouy} := 0.101$
g(H2) values for free H2O, molec/100 ev	$g_{hwa} := 1.6$	$g_{hwp} := 0.53$	$g_{hwy} := 0.5$
g(O2) values for free H2O, molec/100 ev	$g_{owa} := 0.8$	$g_{owp} := 0.265$	$g_{owy} := 0.25$
Relative gamma absorption for Al, U, H2O:	$rQ_{ay} := 0.35$	$rQ_{uy} := 0.86$	$rQ_{wy} := 0.38$

Decay Power Variation with Time: HNF-SD-SNF-CN-006 Regulatory/Safety Design Basis

source	1995	2040	lamda	tau	Where lamda in 1/year and tau in year
alpha	26.3	32	-4.36e-3	-159	Alpha increases as fraction with time
beta	65	22	+2.41e-2	28.8	
gamma	42.4	14.3	+2.42e-2	28.7	Note decay power in W/MT here
TOTAL	133.7	68.3	1.49e-2	46.4	

Initial power fractions; Each independently decayed with time.

$$fQ_{\alpha 0} := \frac{26.3}{133.7} \quad fQ_{\beta 0} := \frac{65}{133.7} \quad fQ_{\gamma 0} := \frac{42.4}{133.7}$$

Decay rates for alpha,beta,gamma, and total power based on 1995 to 2040 changes. Note alpha power increases slightly, so rate is negative.

$$\lambda_{\alpha} := \frac{-1}{45} \ln \left(\frac{32}{26.3} \right) \quad \lambda_{\alpha} = -4.36 \cdot 10^{-3}$$

$$\lambda_{\beta} := \frac{-1}{45} \ln \left(\frac{22}{65} \right) \quad \lambda_{\beta} = 0.02$$

$$\lambda_{\gamma} := \frac{-1}{45} \ln \left(\frac{14.3}{42.4} \right) \quad \lambda_{\gamma} = 0.02$$

$$\lambda_{\gamma} := \frac{-1}{45} \ln \left(\frac{14.3}{42.4} \right) \quad \lambda_{\gamma} = 0.02$$

****** CASES FOR ZERO SCRAP BASKETS ******

$$AL_{\max} := 10650$$

$$UH_{\max} := 297$$

2.1 TIME-DEPENDENT POWER FRACTIONS: Multiply by initial power to get power(time) for each mode:

$$fQ_{\alpha}(t) := fQ_{\alpha 0} \cdot \exp(-\lambda_{\alpha} \cdot t) \quad fQ_{\beta}(t) := fQ_{\beta 0} \cdot \exp(-\lambda_{\beta} \cdot t) \quad fQ_{\gamma}(t) := fQ_{\gamma 0} \cdot \exp(-\lambda_{\gamma} \cdot t)$$

$$\text{Example for use of alpha power:} \quad fQ_{\alpha}(45) = 0.24 \quad 32 \cdot (32 + 22 + 14.3)^{-1} \cdot \exp(-\lambda_{\alpha} \cdot 45) = 0.24$$

2.2 FUNCTIONS FOR DECAY CONSTANTS AND EXAMPLES

Decay constant for free H2O radiolysis: WH=H2 yield, WO=O2 yield

$$\lambda_{wo} := M_f^{-1} \cdot M_w (\text{Jev} \cdot \text{Na})^{-1} \cdot \text{Secy}$$

$$fg_{wh}(t) := g_{hwa} \cdot fQ_{\alpha}(t) + g_{hw\beta} \cdot fQ_{\beta}(t) + g_{hw\gamma} \cdot fQ_{\gamma}(t) \quad fg_{wh}(0) = 0.63$$

$$fg_{wo}(t) := g_{owa} \cdot fQ_{\alpha}(t) + g_{ow\beta} \cdot fQ_{\beta}(t) + g_{ow\gamma} \cdot fQ_{\gamma}(t) \quad fg_{wo}(0) = 0.32$$

$$fl_{wh}(Q, t) := \lambda_{wo} \cdot Q \cdot fg_{wh}(t) \quad fl_{wh}(396, 0) = 2.33 \cdot 10^{-3}$$

$$fl_{wo}(Q, t) := \lambda_{wo} \cdot Q \cdot fg_{wo}(t) \quad fl_{wo}(396, 0) = 1.16 \cdot 10^{-3}$$

$$\text{Water fraction at 40 years, average power MCO:} \quad \exp \left(- \int_0^{40} fl_{wh}(400, t) dt \right) = 0.92$$

Decay constant for Al(OH)3 radiolysis: AC=Cladding Film

$$\lambda_{ao} := [M_f^{-1} \cdot M_{ah} \cdot (\text{Jev} \cdot \text{Na})^{-1} \cdot \text{Secy}]$$

$$fg_{ach}(t) := g_{hay} \cdot rQ_{ay} \cdot fQ_{\gamma}(t)$$

$$fg_{ach}(0) = 0.13$$

$$fg_{aco}(t) := g_{oay} \cdot rQ_{ay} \cdot fQ_{\gamma}(t)$$

$$fg_{aco}(0) = 0.01$$

$$fl_{ach}(Q, t) := \lambda_{ao} \cdot Q \cdot fg_{ach}(t)$$

$$fl_{ach}(396, 0) = 2.12 \cdot 10^{-3}$$

$$fl_{aco}(Q, t) := \lambda_{ao} \cdot Q \cdot fg_{aco}(t)$$

$$fl_{aco}(396, 0) = 2.39 \cdot 10^{-4}$$

$$\text{Al clad fraction at 40 years, average power MCO: } \exp\left(-\int_0^{40} \frac{2}{3} \cdot fl_{ach}(400, t) dt\right) = 0.96$$

Decay constant for Al(OH)3 radiolysis: AP=Al in Adhering Particulate

$$fg_{aph}(f_u, t) := f_u \cdot (g_{haa} \cdot fQ_{\alpha}(t) + g_{ha\beta} \cdot fQ_{\beta}(t)) + g_{hay} \cdot rQ_{ay} \cdot fQ_{\gamma}(t)$$

$$fg_{aph}(0.2, 0) = 0.17$$

$$fg_{apo}(f_u, t) := f_u \cdot (g_{oaa} \cdot fQ_{\alpha}(t) + g_{oa\beta} \cdot fQ_{\beta}(t)) + g_{oay} \cdot rQ_{ay} \cdot fQ_{\gamma}(t)$$

$$fg_{apo}(0.2, 0) = 0.03$$

$$fl_{aph}(Q, f_u, t) := \lambda_{ao} \cdot Q \cdot fg_{aph}(f_u, t)$$

$$fl_{aph}(396, 0.2, 0) = 2.7 \cdot 10^{-3}$$

$$fl_{apo}(Q, f_u, t) := \lambda_{ao} \cdot Q \cdot fg_{apo}(f_u, t)$$

$$fl_{apo}(396, 0.2, 0) = 5.26 \cdot 10^{-4}$$

$$\text{Al Adhering Partic. fraction at 40 years, average power MCO: } \exp\left(-\int_0^{40} fl_{aph}(400, 0.2, t) dt\right) = 0.93$$

Decay constant for UO3.2H2O radiolysis

$$\lambda_{uo} := [M_f^{-1} \cdot M_{uh} \cdot (\text{Jev} \cdot \text{Na})^{-1} \cdot \text{Secy}]$$

$$fg_{uh}(t) := g_{hua} \cdot fQ_{\alpha}(t) + g_{hu\beta} \cdot fQ_{\beta}(t) + g_{huy} \cdot rQ_{uy} \cdot fQ_{\gamma}(t)$$

$$fg_{uh}(0) = 0.38$$

$$fg_{uo}(t) := g_{oua} \cdot fQ_{\alpha}(t) + g_{ou\beta} \cdot fQ_{\beta}(t) + g_{ouy} \cdot rQ_{uy} \cdot fQ_{\gamma}(t)$$

$$fg_{uo}(0) = 0.06$$

$$fl_{uh}(Q, t) := \lambda_{uo} \cdot Q \cdot fg_{uh}(t)$$

$$fl_{uh}(396, 0) = 0.03$$

$$fl_{uo}(Q, t) := \lambda_{uo} \cdot Q \cdot fg_{uo}(t)$$

$$fl_{uo}(396, 0) = 3.69 \cdot 10^{-3}$$

$$\text{U Hydrates fraction at 40 years, average power MCO: } \exp\left(-\int_0^{40} \frac{1}{2} \cdot fl_{uh}(400, t) dt\right) = 0.71$$

2.3 FUNCTIONS FOR U GETTERING RATE AND WATER VAPOR PRESSURE

$$\text{Water vapor pressure: } fP_{\text{sat}}(T) := e^{\frac{25.339 - \frac{5154.7}{T}}{}} \quad fP_{\text{sat}}(323) = 1.19 \cdot 10^4 \quad 50 \text{ C OK}$$

Ritchie correlation for U-H₂O-O₂, below 100% RH, below 100 C, agrees best with data BUT goes below dry air correlation at about 37 C - so switch to McGillivray dry air. Ritchie units of mg/cm²/hr, converted to grams O₂ per m² per year.; McGillivray units of kg/m²/s similarly converted.

$$K_{\text{rit}}(T) := 10^{13.8808 - 5769.6 \cdot T^{-1}} \cdot 10^{-8766} \quad \text{Ritchie} \quad K_{\text{trim}}(T) := 10^{7.19 - 3732 \cdot T^{-1}} \cdot 10^{-8766} \quad \text{Trimble}$$

$$T_{\text{cor}} := (5769.6 - 3732) \cdot (13.8808 - 7.19)^{-1} \quad T_{\text{cor}} = 304.54 \quad \text{Switch correlations here, 31 C}$$

Moist Air Getter Function 100% RH:

$$fK_{\text{O}}(323) \cdot 0.1 \cdot (8766)^{-1} = 1.04 \cdot 10^{-4} \quad fK_{\text{O}}(T) := \text{if}(T \geq T_{\text{cor}}, K_{\text{rit}}(T), K_{\text{trim}}(T))$$

$$fK_{\text{O}}(323) \cdot 10^{-3} \cdot (3.15 \cdot 10^7)^{-1} = 2.9 \cdot 10^{-10} \quad \text{OK @ 50 C in mg/cm}^2/\text{hr} \quad \text{Shows no discontinuity}$$

$$fK_{\text{O}}(323) \cdot 10^{-3} \cdot (3.15 \cdot 10^7)^{-1} = 2.9 \cdot 10^{-10} \quad \text{OK @ 50 C in kg/m}^2/\text{s}$$

$$fK_{\text{O}}(T_{\text{cor}} + 0.01) \cdot 10^{-3} \cdot (3.15 \cdot 10^7)^{-1} = 2.4 \cdot 10^{-11} \quad fK_{\text{O}}(T_{\text{cor}} - 0.01) \cdot 10^{-3} \cdot (3.15 \cdot 10^7)^{-1} = 2.4 \cdot 10^{-11}$$

Gettering of Water vapor when Oxygen-Free:

$$fK_{\text{W}}(T) := \begin{cases} P_{\text{st}} \leftarrow 10^{-3} \cdot fP_{\text{sat}}(T) & fK_{\text{W}}(323) = 1.49 \cdot 10^3 \\ K \leftarrow P_{\text{st}}^{0.5} \cdot 10^{4.33 - 2144 \cdot T^{-1}} & fK_{\text{O}}(323) = 9.14 \\ K \leftarrow K \cdot 10^{-8766} & \frac{1486}{9.14} = 162.58 \end{cases}$$

2.4 RELATIONSHIP BETWEEN MCO POWER AND GAS TEMPERATURE

Conservative relationships based on 733 W MCO, zero scrap case for fuel and one scrap case for scrap. Vault gas-tube dT=28 C, Fuel tube-MCO gap dT=39 C, Scrap gap dT=27 C. Inside MCO, fuel dT's are 12.5, 20, and 26 C; scrap dT is 4 C. Function yields scrap and low to high fuel T's in that order:

$$fT_{\text{get}}(Q_{\text{O}}, t) := Q_{\text{O}} \cdot e^{-\lambda \cdot q \cdot t} \cdot \left[\frac{1}{U_{\text{sc}}} \frac{1}{U_{\text{fl}}} \frac{1}{U_{\text{fa}}} \frac{1}{U_{\text{fh}}} \right]^T + T_{\text{av}}$$

$$fT_{\text{get}}(400, 0)^T = [47.26 \quad 57.11 \quad 60.98 \quad 63.78] \quad fT_{\text{get}}(770, 0)^T = [77.1 \quad 96.05 \quad 103.51 \quad 108.9]$$

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2.5 ACCOUNT FOR ANNUAL TEMPERATURE VARIATION BY INTEGRAL AVERAGE FOR A YEAR

Create an interpolation table over the temperature range of interest, then define a new rate law function which automatically incorporates the average annual enhancement factor. Input T in Kelvins!

$$fT_a(T, t) := T + dT_{av} \sin(2\pi \cdot t)$$

$$fE(T) := fK_o(T)^{-1} \cdot \int_0^1 fK_o(fT_a(T, t)) \, dt$$

$$j := 0..60 \quad T_{s_j} := 283 + 2 \cdot j$$

$$E_j := fE(T_{s_j})$$

$$fE(T) := \text{interp}(T_{s_j}, E_j, T)$$

$$fK_1(T) := fE(T) \cdot fK_o(T)$$

$$\text{Values at low, medium, high T: } fE(288) = 1.38$$

$$fE(333) = 1.54$$

$$fE(383) = 1.29$$

2.6 FUNCTIONS TO SET UP INITIAL CONDITONS

User specifies:

- (1) Q = MCO Initial power, W;
- (2) As = Scrap reactive area, m²;
- (3) Af = Fuel reactive area, m²;
- (4) ma = Al(OH)3 film mass, g;
- (5) mwcp = Canister particulate water mass, g;
- (6) fUcp = U fraction of can. partic. for alpha,beta
- (7) fwUcp: U water fraction of can. particulate;
- (8) mu: Mass/area water from UO3.2H2O;
- (9) mfw: Free water mass per area, g/m².

State vector V assigned based on these inputs:

Actual state variables are:

- (0) nac= Al(OH)3 cladding film water moles
- (1) nap=Al(OH)3 can particulate water moles
- (2) nu=UO3.2H2O water moles
- (3) nw=free H2O moles
- (4) nh2=H2 + H2O vapor moles
- (5) no2=O2 moles

Parameters are:

- (6) Q = Power,
- (7) AS = Scrap area,
- (8) AF = Fuel Area,
- (9) fucp= U fraction of canister particulate

Other assumptions of note:

- (1) Initial water vapor mass determined by scrap T;
- (2) Residual free water prevents hydrate thermal decomposition.

Initial steam from free water, assumed sufficient; free water not depleted; scrap T (index 0) used:

$$f n_{st}(Q) := \begin{cases} T_o \leftarrow fT_{get}(Q, 0)_0 + 273 \\ fP_{sat}(T_o) \cdot V_{mco} \cdot (R_{gas} \cdot T_o)^{-1} \end{cases}$$

Function for water moles of UO3.2HO plus UO4.2H2O given m = kg/m² from UO3.2H2O, A=fuel reactive area, and adding UO4 contribution in proportion the fraction not covered with Al(OH)3, given its mass ma.

$$f n_{wU}(\mu, A_s, A_f, m_{wcp}, f w_{ucp}, m_a) := \begin{cases} m_{ap} \leftarrow \mu \cdot (A_s + A_f) \\ m_{ap} \leftarrow \text{if}(m_{ap} > UH_{max}, UH_{max}, m_{ap}) \\ m_{clad} \leftarrow m_{uO4} \cdot (1 - m_a \cdot AL_{max}^{-1}) \\ m_{clad} \leftarrow \text{if}(m_a > AL_{max}, 0, m_{clad}) \\ m_{cp} \leftarrow m_{wcp} \cdot f w_{ucp} \\ n \leftarrow (m_{ap} + m_{clad} + m_{cp}) \cdot M_w^{-1} \end{cases}$$

$$f n_{fw}(m_{fw}, A_s, A_f) := \begin{cases} m \leftarrow m_{fw} \cdot (A_s + A_f) \\ n \leftarrow \text{if}(m > FW_{max}, FW_{max}, m) \cdot M_w^{-1} \end{cases}$$

$$fV(Q, A_s, A_f, m_a, m_{wcp}, f_{ucp}, f_{wucp}, \mu, m_{fw}) := \begin{bmatrix} 1.5 \cdot m_a \cdot M_{ah}^{-1} \\ m_{wcp} \cdot (1 - f_{wucp}) \cdot M_w^{-1} \\ f_{wucp} \cdot \mu \cdot A_s \cdot A_f \cdot m_{wcp} \cdot f_{wucp} \cdot m_a \\ f_{fw} \cdot m_{fw} \cdot A_s \cdot A_f \\ f_{st}(Q) \\ 10^{-5} \cdot n_{he} \\ Q \\ A_s \\ A_f \\ f_{ucp} \end{bmatrix}$$

Test for bounding conditions, one scrap basket:

$$fV(733, 4.5, 3.16, 10050, 192, 0.1, 0.1, 100, 30)^T = \begin{bmatrix} 193.27 & 9.6 & 17.73 & 11.11 & 6.22 & 4.1 \cdot 10^{-4} & 733 & 4.5 \end{bmatrix}$$

2.7 FUNCTIONS FOR H2, O2 SOURCE AND SINK; R=Radiolysis Source, G=Getter

Current O2 model assumes O2 gettering phase from beginning of transient.

Current H2 model assumes no gettering.

$$fR_{O2}(Q, t, n_{ac}, n_{ap}, n_u, n_w, f_{ucp}) := f_{aco}(Q, t) \cdot n_{ac} + f_{apo}(Q, f_{ucp}, t) \cdot n_{ap} + f_{uo}(Q, t) \cdot n_u + f_{wo}(Q, t) \cdot n_w$$

$$fGO2(Q, t, A_s, A_f) := \begin{cases} T_{get} \leftarrow fT_{get}(Q, t) + 273 \\ GS \leftarrow A_s \cdot fK_1(T_{get_0}) \\ GF \leftarrow A_f \cdot (N_{fl} \cdot fK_1(T_{get_1}) + N_{fa} \cdot fK_1(T_{get_2}) + N_{fh} \cdot fK_1(T_{get_3})) \\ (GS + GF) \cdot 32^{-1} \end{cases}$$

3.0 RATES OF CHANGE OF RADIOLYSIS SOURCES & PRODUCTS

Need a trick because Mathcad demands a function F whose arguments are t,Y where t is time and Y is a vector of state variables. Output of F is a vector dY/dt. Trick: dY/dt = 0 for constant terms needed.

State variables thus include parameters expected to vary from case to case. Coding first assigns scrutable names to the state vector; see comment below. Coding for readability, not compactness.

$$dYdt(t, Y) :=$$

$$n_{ac} \leftarrow Y_0$$

$$n_{ap} \leftarrow Y_1$$

$$n_u \leftarrow Y_2$$

$$n_w \leftarrow Y_3$$

$$n_{h2} \leftarrow Y_4$$

$$Y_5 \leftarrow \text{if} [Y_5 < 0, 0, Y_5]$$

$$n_{o2} \leftarrow Y_5$$

$$Q \leftarrow Y_6$$

$$A_s \leftarrow Y_7$$

$$A_f \leftarrow Y_8$$

$$f_{ucp} \leftarrow Y_9$$

$$dn_{ac} \leftarrow \frac{-2}{3} \cdot \dot{n}_{ach}(Q, t) \cdot n_{ac}$$

$$dn_{ap} \leftarrow \frac{-2}{3} \cdot \dot{n}_{aph}(Q, f_{ucp}, t) \cdot n_{ap}$$

$$dn_u \leftarrow \frac{-1}{2} \cdot \dot{n}_{uh}(Q, t) \cdot n_u$$

$$dn_w \leftarrow \dot{n}_{wh}(Q, t) \cdot n_w$$

$$\text{sorH2} \leftarrow (1.5 \cdot dn_{ac} + 1.5 \cdot dn_{ap} + 2 \cdot dn_u + dn_w)$$

$$\text{sorO2} \leftarrow fR_{O2}(Q, t, n_{ac}, n_{ap}, n_u, n_w, f_{ucp})$$

$$\text{sinkO2} \leftarrow fGO2(Q, t, A_s, A_f)$$

$$\text{net} \leftarrow \text{sorO2} - \text{sinkO2}$$

$$dO2dt \leftarrow \begin{cases} \text{net} & \text{if } (n_{o2} > 0) + (\text{net} > 0) \\ 0 & \text{otherwise} \end{cases}$$

$$dY \leftarrow [dn_{ac} \quad dn_{ap} \quad dn_u \quad dn_w \quad \text{sorH2} \quad dO2dt \quad 0 \quad 0 \quad 0]^T$$

$$dY$$

First, assign scrutable names to elements of Y:

Actual state variables are:

n_{ac} = Al(OH)3 cladding film water moles

n_{ap} = Al(OH)3 can particulate water moles

n_u = UO3.2H2O water moles

n_w = free H2O moles

n_{h2} = H2 + H2O vapor moles

n_{o2} = O2 moles

Parameters are:

Q = Power,

A_s = Scrap area,

A_f = Fuel Area,

f_{ucp} = U frac. of can particulate

Make O2 moles > 0 for numerical purposes.

Net rate includes sink when there is O2 present, or at least when the rate is positive (net rate is zero when no O2 and sink exceeds source).

Function to get End-of-Life values after integration of a single case:

$$fEOL(Q, A_s, A_f, m_a, m_{wcp}, f_{ucp}, f_w, m_{ucp}, m_{fw}, t_{end}) := \begin{cases} Y \leftarrow fV(Q, A_s, A_f, m_a, m_{wcp}, f_{ucp}, f_w, m_{ucp}, m_{fw}) \\ Z \leftarrow \text{rkadapt}(Y, 0, t_{end}, 0.001, dYdt, 1000, 0.0001) \\ L \leftarrow \text{rows}(Z) - 1 \\ EOL \leftarrow [Z_{L,5} \quad Z_{L,6}]^T \end{cases}$$

4.0 COMBUSTION FUNCTIONS

4.1 GAS SPECIFIC HEAT DATA: CV(T) POLYNOMIAL FIT.: Gases are entered in the order: H2, He, N2, O2, H2O from HANSF input GASPROP.DAT. Values in J/g-mole/K!!! FW is the formula weight vector.

$$CCV := \begin{bmatrix} 21.136 & -1.529 \cdot 10^{-3} & 1.978 \cdot 10^{-6} & 4.018 \cdot 10^{-10} & -1.171 \cdot 10^{-13} \\ 12.47 & 0 & 0 & 0 & 0 \\ 20.785 & -3.871 \cdot 10^{-3} & 1.34 \cdot 10^{-5} & -7.216 \cdot 10^{-9} & 1.16 \cdot 10^{-12} \\ 17.045 & 0.014 & -4.96 \cdot 10^{-6} & 1.375 \cdot 10^{-10} & 1.375 \cdot 10^{-13} \\ 24.044 & -7.883 \cdot 10^{-5} & 1.513 \cdot 10^{-5} & -7.323 \cdot 10^{-9} & 1.087 \cdot 10^{-12} \end{bmatrix} \quad FW := \begin{bmatrix} 2 \\ 4 \\ 28 \\ 32 \\ 18 \end{bmatrix}$$

Functions for Cv and Ug of a specific gas:

$$fCv(i, T) := CCV_{i,0} + CCV_{i,1} \cdot T + CCV_{i,2} \cdot T^2 + CCV_{i,3} \cdot T^3 + CCV_{i,4} \cdot T^4$$

$$fug(i, T) := T \cdot \left[CCV_{i,0} + T \cdot \left[\frac{1}{2} \cdot CCV_{i,1} + T \cdot \left[\frac{1}{3} \cdot CCV_{i,2} + T \cdot \left[\frac{1}{4} \cdot CCV_{i,3} + T \cdot \frac{1}{5} \cdot CCV_{i,4} \right] \right] \right] \right] \right]$$

Function for energy of a gas with mole vector N at temperature T (without integration constant):

$$fUg(N, T) := \begin{cases} U \leftarrow 0 \\ \text{for } i \in 0..4 \\ U \leftarrow U + N_i \cdot fug(i, T) \end{cases} U$$

2.0 AICC Function input is mole vector (see order above) and initial Temperature, Output is a vector with: post-burn mole vector, AICC temperature, AICC pressure.

$$fAICC(N, T_o, V) := \begin{cases} H2 \leftarrow N_0 \\ O2 \leftarrow N_3 \\ \Delta H2O \leftarrow \text{if}(H2 \leq 2 \cdot O2, H2, 2 \cdot O2) \\ NP \leftarrow [H2 - \Delta H2O \quad N_1 \quad N_2 \quad O2 - 0.5 \cdot \Delta H2O \quad N_4 + \Delta H2O]^T \\ Q \leftarrow \Delta H2O \cdot 241.8 \cdot 10^3 \\ U_o \leftarrow fUg(N, T_o) \\ T \leftarrow T_o + Q \cdot (fUg(N, T_o + 1) - U_o)^{-1} \\ T_f \leftarrow \text{root}(fUg(NP, T) - U_o - Q, T) \\ n_f \leftarrow \sum NP \\ P_f \leftarrow n_f \cdot 8.314 \cdot T_f \cdot V^{-1} \\ TP \leftarrow [T_f \quad P_f]^T \\ f \leftarrow \text{stack}(NP, TP) \\ f \end{cases}$$

5.1 K-West Bounding Case & High Power: High Al(OH)3, High Canister-Adhering Particulate

5.1A Define highest K-West Power, 530 W, and Investigate Fuel area up to 4 m²:

$$a := 1..10 \quad A_a := \text{if}(a \geq 7, a - 6, \text{if}(a > 1, (a - 1) \cdot 0.05, 0.01)) \quad A_0 := 0 \quad a := 0..10$$

Zero Scrap:	$A_s := 0$	Bounding Can. partic:	$m_{wcp} := 240$
Bounding Al(OH)3:	$m_a := 10650$	Bounding Can. partic U:	$f_{ucp} := 0.2$
Bounding Adher. Partic:	$\mu := 100$	Can. water frac. from U:	$fw_{ucp} := 0.08$
Free water g/m ² :	$m_{fw} := 66.7$	MCO Power	$Q_0 := 530$

$$\begin{bmatrix} nh2_a \\ no2_a \end{bmatrix} := fEOL(Q_0, A_s, A_a, m_a, m_{wcp}, f_{ucp}, fw_{ucp}, \mu, m_{fw}, 40)$$

$$ntot_a := n_{he} + no2_a + nh2_a \quad O2\%_a := no2_a \cdot (ntot_a)^{-1} \quad O2\%_a := \text{if}(O2\%_a > 0, 100 \cdot O2\%_a, 0)$$

$$PA_a := ntot_a \cdot R_{gas} \cdot (fTget(Q_0, 40)_0 + 273) \cdot V_{mco}^{-1} \cdot 10^{-5} \quad T_a := fTget(Q_0, 40)_2 \quad NO2A_a := O2\%_a \cdot 0.01 \cdot ntot_a$$

For A = 0, vary moles of H2 from value with no getter until stoichiometric, and get post-combustion pressure.

$$n_{st} := fn_{st}(Q_0) \quad \delta nh2 := 0.1 \cdot (nh2_0 - n_{st} - 2 \cdot no2_0) \quad n_{st} = 3.13 \quad no2_0 = 2.03 \quad nh2_0 = 19.69$$

$$i := 0..10 \quad n1H2_i := nh2_0 - n_{st} - i \cdot \delta nh2 \quad O2\%_i := 100 \cdot no2_0 \cdot (n_{he} + n_{st} + no2_0 + n1H2_i)^{-1}$$

$$N1_{0,i} := n1H2_i \quad N1_{1,i} := n_{he} \quad N1_{2,i} := 0 \quad N1_{3,i} := no2_0 \quad N1_{4,i} := n_{st} \quad Tk := T_0 + 273$$

$$Al^{<i>} := fAICC(N1^{<i>}, Tk, V_{mco}) \quad P1_i := A1_{6,i} \cdot 101325^{-1} \quad T_0 = 48.53 \quad Tk = 321.53 \quad P1_0 = 13.04$$

5.2 Q=400 W:

$$Q_0 := 400 \quad \begin{bmatrix} nh2_a \\ no2_a \end{bmatrix} := fEOL(Q_0, A_s, A_a, m_a, m_{wcp}, f_{ucp}, fw_{ucp}, \mu, m_{fw}, 40)$$

$$ntot_a := n_{he} + no2_a + nh2_a \quad O2B\%_a := no2_a \cdot (ntot_a)^{-1} \quad O2B\%_a := \text{if}(O2B\%_a > 0, 100 \cdot O2B\%_a, 0)$$

$$PB_a := ntot_a \cdot R_{gas} \cdot (fTget(Q_0, 40)_0 + 273) \cdot V_{mco}^{-1} \cdot 10^{-5} \quad TB_a := fTget(Q_0, 40)_2 \quad NO2B_a := O2B\%_a \cdot 0.01 \cdot ntot_a$$

$$n_{st} := fn_{st}(Q_0) \quad \delta nh2 := 0.1 \cdot (nh2_0 - n_{st} - 2 \cdot no2_0) \quad n_{st} = 1.94 \quad no2_0 = 1.55 \quad nh2_0 = 14.54$$

$$i := 0..10 \quad n1H2_i := nh2_0 - n_{st} - i \cdot \delta nh2 \quad O2\%_i := 100 \cdot no2_0 \cdot (n_{he} + n_{st} + no2_0 + n1H2_i)^{-1}$$

$$N1_{0,i} := n1H2_i \quad N1_{1,i} := n_{he} \quad N1_{2,i} := 0 \quad N1_{3,i} := no2_0 \quad N1_{4,i} := n_{st} \quad Tk := T_0 + 273$$

$$Al^{<i>} := fAICC(N1^{<i>}, Tk, V_{mco}) \quad P2_i := A1_{6,i} \cdot 101325^{-1}$$

Number of moles of O₂ at 40 years as function of reactive area and power:

$$A^T =$$

0	0.01	0.05	0.1	0.15	0.2	0.25	1	2	3
---	------	------	-----	------	-----	------	---	---	---

$$Q=400 \text{ W} \quad \text{NO}_2\text{B}^T =$$

1.55	1.34	0.57	0.16	0.03	0	0	0	0	0
------	------	------	------	------	---	---	---	---	---

$$Q=530 \text{ W} \quad \text{NO}_2\text{A}^T =$$

2.03	1.15	0.11	0	0	0	0	0	0	0
------	------	------	---	---	---	---	---	---	---

Pressure (no H₂ gettering) at 40 years as function of reactive area and power:

$$A^T =$$

0	0.01	0.05	0.1	0.15	0.2	0.25	1	2	3
---	------	------	-----	------	-----	------	---	---	---

$$Q=400 \text{ W} \quad \text{PB}^T =$$

2.9	2.89	2.86	2.85	2.85	2.86	2.87	3	3.18
-----	------	------	------	------	------	------	---	------

$$Q=530 \text{ W} \quad \text{PA}^T =$$

3.25	3.2	3.16	3.17	3.18	3.19	3.2	3.37	3.6
------	-----	------	------	------	------	-----	------	-----

Moles Oxygen at 40 years for K-West Zero-Scrap Bounding Water Content as function of Reactive Area (M²), Q=530 W and Q=400 W

Pressure vs Oxygen Concentration for Zero Scrap, K-West bounding water inventory, and high helium backfill. Lower lines with symbols indicate MCO conditions for various reactive areas with no combustion. Upper lines with no symbols are for post-burn sensitivity cases with hydrogen gettering to increase the O₂ concentration up to stoichiometry.

Combustion is impossible for O₂ < 4%. The worst case group is for A=0, zero reactive area, because this maximizes the number of moles of oxygen. The worst case is for the highest power, hence highest moles of oxygen. The highest post-burn pressure is 13 atm.

$$k := 0..6 \quad PL_k := 31 \quad O2L_k := k$$

Pressure vs Oxygen Concentration for Zero Scrap, K-West bounding water inventory, and high helium backfill. Lower lines with symbols indicate MCO conditions for various reactive areas with no combustion. Upper lines with no symbols are for post-burn sensitivity cases with hydrogen gettering to increase the O₂ concentration up to stoichiometry. The upper horizontal dashed line is the MCO design pressure 450 psig (31 atm absolute).

Combustion is impossible for O₂ < 4%. The worst case group is for A=0, zero reactive area, because this maximizes the number of moles of oxygen. The worst case is for the highest power, hence highest moles of oxygen. The highest post-burn pressure is 13 atm.

APPENDIX D
QUALITY ASSURANCE DOCUMENTS

Included here are:

1. Calculation Note Cover Sheet
2. Calculation Note Methodology Checklist.

FAUSKE & ASSOCIATES, INC.
CALCULATION NOTE COVER SHEET

SECTION TO BE COMPLETED BY AUTHOR(S):

Page <u>i to D-3</u>	
Calc-Note Number <u>FAI/99-14</u>	Revision Number <u>1</u>
Title <u>Hydrogen Combustion in an MCO During Interim Storage</u>	
Project <u>Hanford Spent Nuclear Fuel Project</u>	Project No. or Shop Order <u>DESH01</u>
Purpose: Find hypothetical post-combustion MCO pressure.	
Results Summary: Maximum 13 atm static value a factor of 2.4 below design value 31 atm.	
References of Resulting Reports, Letters, or Memoranda (Optional)	
Author(s): Name (Print or Type)	Signature Completion Date
<u>Martin G. Plys</u>	<u><i>M. Plys</i></u> <u>2/9/99</u>

SECTION TO BE COMPLETED BY VERIFIER(S):

Verifier(s): Name (Print or Type)	Signature	Completion Date
<u>Boro Malinovic</u>	<u><i>Boro Malinovic</i></u>	<u>2/9/99</u>
Method of Verification: Design Review _____, Independent Review or Alternate Calculations ☒ _____, Testing _____		
Other (specify) _____		

SECTION TO BE COMPLETED BY MANAGER:

Responsible Manager: Name (Print or Type)	Signature	Approval Date
<u>Martin G. Plys</u>	<u><i>M. Plys</i></u>	<u>2/9/99</u>

CALC NOTE NUMBER FAI/99-14 REV. 1 PAGE i to D-3

CALCULATION NOTE METHODOLOGY CHECKLIST

CHECKLIST TO BE COMPLETED BY AUTHOR(S)

(CIRCLE APPROPRIATE RESPONSE)

1. Is the subject and/or the purpose of the design analysis clearly stated? YES • NO
2. Are the required inputs and their sources provided? YES • NO • N/A
3. Are the assumptions clearly identified and justified? YES • NO • N/A
4. Are the methods and units clearly identified? YES • NO • N/A
5. Have the limits of applicability been identified? YES • NO • N/A
(Is the analysis for a 3 or 4 loop plant or for a single application.)
6. Are the results of literature searches, if conducted, or other background data provided? YES • NO • N/A
7. Are all the pages sequentially numbered and identified by the calculation note number? YES • NO
8. Is the project or shop order clearly identified? YES • NO
9. Has the required computer calculation information been provided? YES • NO • N/A
10. Were the computer codes used under configuration control? YES • NO • N/A
11. Were the computer code(s) used applicable for modeling the physical and/or computational problems identified? YES • NO • N/A
(Is the correct computer code being used for the intended purpose.)
12. Are the results and conclusions clearly stated? YES • NO
13. Are Open Items properly identified YES • NO • N/A
14. Were approved Design Control practices followed without exception? YES • NO • N/A
(Approved Design Control practices refers to guidance documents within NSD that state how the work is to be performed, such as how to perform a LOCA analysis.)
15. Have all related contract requirements been met? YES • NO • N/A

NOTE: If NO to any of the above, Page Number containing justification _____

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		EDT No. 625804			
		ECN No.			

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