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Analysis of Plume Energy Associate Spent Fuel Pool Storage Accident
R.O. Gauntt 7/13/2000

Fuel and Canister Dimensions ************************************

$r_{o\_clad} := 6.135mm$ $r_{fuel} := \frac{0.410}{2} \cdot in$

$r_{i\_clad} := 5.322mm$ $can\_perimeter := 4 \cdot 5.215 \cdot in$

$assembly\_length := 4.1m$ $\Delta t_{canister} := 0.12 \cdot in$

Fuel Properties ************************************

$\rho_{Zr} := 6500 \frac{kg}{m^3}$ $Cp_{UO2} := 370 \cdot \frac{joule}{kg \cdot K}$

$\rho_{UO2} := 0.95 \cdot 10.96 \cdot \frac{gm}{cm^3}$

$\rho_{ZrO2} := 5.6 \cdot \frac{gm}{cm^3}$

$MW_{Zr} := 91.2 \frac{gm}{mol}$ $MW_{N2} := 28 \cdot \frac{gm}{mol}$

$MW_{ZrO2} := 123.2 \cdot \frac{gm}{mol}$

$MW_{O2} := 32 \cdot \frac{gm}{mol}$

Fuel Assembly Properties ************************************

$mass_{clad} := 64\pi \cdot \left(r_{o\_clad}{}^2 - r_{i\_clad}{}^2\right) \cdot assembly\_length \cdot \rho_{Zr}$

$mass_{canister} := assembly\_length \cdot can\_perimeter \cdot \Delta t_{canister} \cdot \rho_{Zr}$

$mass_{fuel} := 62 \cdot \pi \cdot r_{fuel}{}^2 \cdot assembly\_length \cdot \rho_{UO2}$

$mass_{canister} = 43.039\,kg$

$mass_{clad} = 49.91\,kg$

$mass_{fuel} = 225.442\,kg$

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Enthalpy (Internal Energy) of Zircaloy, UO_2 and ZrO_2 **
Properties from MATPRO

UO_2 Internal Energy **

$K_1 := 296.7 \cdot K^{-1}$

$K_2 := 2.43 \cdot 10^{-2} \cdot K^{-2}$

$K_3 := 8.745 \cdot 10^{7}$

$\theta := 535.285 \cdot K$

$E_D := 1.577 \cdot 10^{5} \cdot \frac{joule}{mol}$

$R := 8.3143 \cdot \frac{joule}{mol \cdot K}$

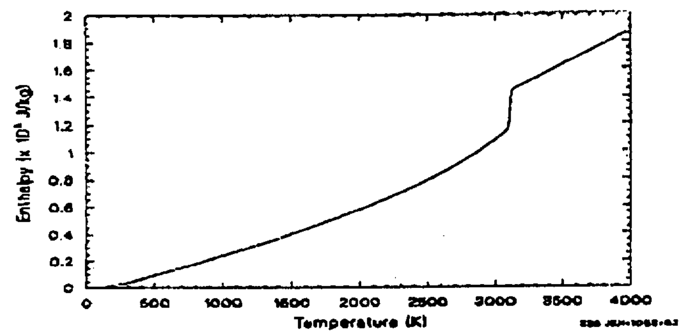
$\Delta H_{f\_UO2} := 2.74 \cdot 10^{5} \cdot \frac{joule}{kg}$

$Cp_{l\_UO2} := 503 \cdot \frac{joule}{kg \cdot K}$

$$H_{solid\_UO2}(T) := \left[\frac{K_1 \cdot \theta}{\left(e^{\frac{\theta}{T}} - 1 \right)} + \frac{K_2 \cdot T^2}{2} + K_3 \cdot e^{\left(\frac{-E_D}{R \cdot T} \right)} \right] \cdot \frac{joule}{kg}$$

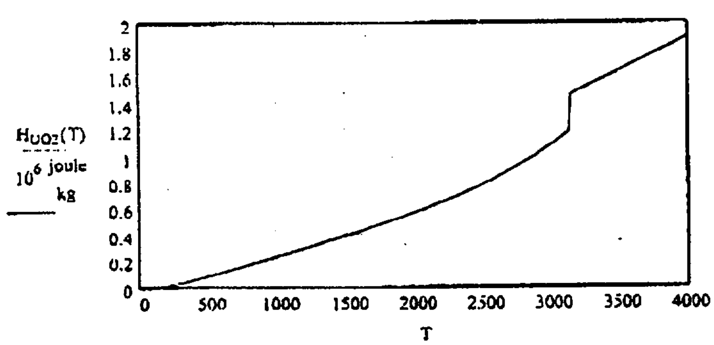
$$H_{UO2}(T) := \Phi(3138K - T) \cdot H_{solid\_UO2}(T) + \Phi(T - 3138K) \cdot \left[H_{solid\_UO2}(3138K) + \Delta H_{f\_UO2} + (T - 3138K) \cdot Cp_{l\_UO2} \right]$$

$T := 0K, 10K .. 4000K$



MATPRO Data

Figure 2-3. Enthalpy of UO_2 as a function of temperature to 4,000 K.



Curve Fit to MATPRO

Zircaloy Oxide Internal Energy

$$H_{300} := 1.194 \cdot 10^{4}$$

$$H_1(T) := \left[565 \cdot \frac{T}{K} + 3.055 \cdot 10^{-2} \cdot \left(\frac{T}{K}\right)^2 + 1.14 \cdot 10^{7} \cdot \left(\frac{K}{T}\right) - 2.102495 \cdot 10^{5} + H_{300}\right] \cdot \frac{joule}{kg}$$

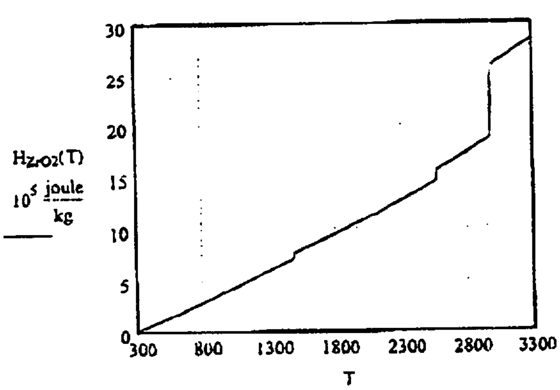
$$H_2(T) := \left[604.5 \cdot \left(\frac{T}{K}\right) - 1.46 \cdot 10^{5} + H_{300}\right] \cdot \frac{joule}{kg}$$

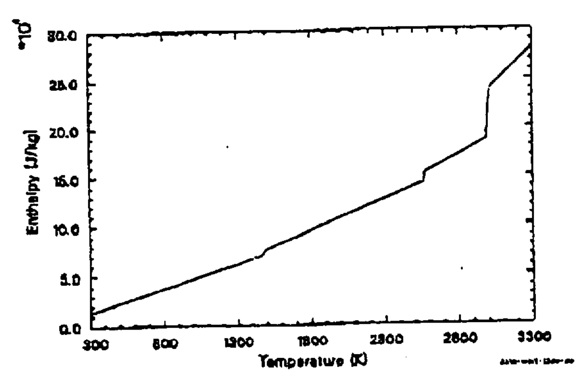
$$H_3(T) := \left[171.7 \cdot \left(\frac{T}{K}\right) + 0.1082 \cdot \left(\frac{T}{K}\right)^2 + 2.868 \cdot 10^{5} + H_{300}\right] \cdot \frac{joule}{kg}$$

$$H_4(T) := \left[171.7 \cdot \left(\frac{T}{K}\right) + 0.1082 \cdot \left(\frac{T}{K}\right)^2 + 3.888 \cdot 10^{5} + H_{300}\right] \cdot \frac{joule}{kg}$$

$$H_5(T) := \left[815.0 \cdot \left(\frac{T}{K}\right) + 1.39 \cdot 10^{5} + H_{300}\right] \cdot \frac{joule}{kg}$$

$$H_{ZrO2}(T) := \begin{cases} H_1(T) & \text{if } [(T > 273.0K) \wedge (T < 1478.0K)] \\ H_2(T) & \text{if } [(T > 1478.01K) \wedge (T < 2000.0K)] \\ H_3(T) & \text{if } [(T \geq 2000.0K) \wedge (T < 2558.0K)] \\ H_4(T) & \text{if } [(T \geq 2558.0K) \wedge (T < 2973.0K)] \\ H_5(T) & \text{if } [(T \geq 2973.01K) \wedge (T < 4100.0K)] \\ 0.0 \frac{joule}{kg} & \text{otherwise} \end{cases}$$





igure 5-3. Zircaloy oxide enthalpy as a function of temperature.

Enthalpy of Zr **

$$Hzr_1(T) := \frac{(2.6-0)\cdot 10^5 \frac{joule}{kg}}{(1100-300)K}\cdot(T-300K)$$

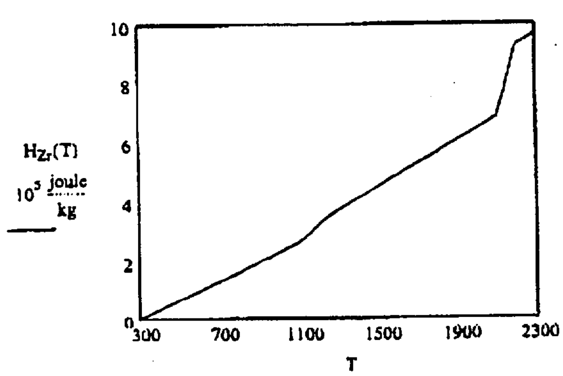
$$Hzr_2(T) := \frac{(3.5-2.6)\cdot 10^5 \frac{joule}{kg}}{(1250-1100)K}\cdot(T-1100K) + Hzr_1(1100K)$$

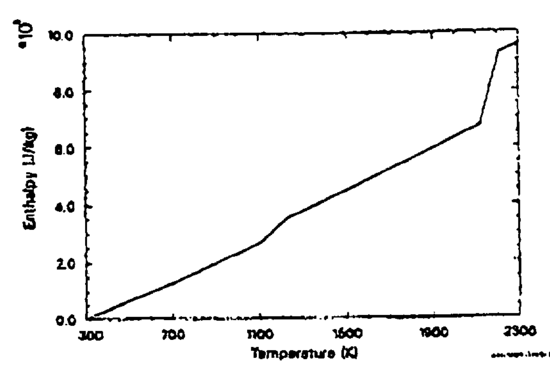
$$Hzr_3(T) := \frac{(6.75-3.5)\cdot 10^5 \frac{joule}{kg}}{(2100-1250)K}\cdot(T-1250K) + Hzr_2(1250K)$$

$$Hzr_4(T) := \frac{(9.25-6.75)\cdot 10^5 \frac{joule}{kg}}{(2200-2100)K}\cdot(T-2100K) + Hzr_3(2100K)$$

$$Hzr_5(T) := Hzr_4(2200K) + \frac{356 \frac{joule}{kg}}{K}\cdot(T-2200K)$$

$$H_{Zr}(T) := \begin{cases} Hzr_1(T) & \text{if } [(T \ge 300K) \wedge (T < 1100K)] \\ Hzr_2(T) & \text{if } [(T \ge 1100K) \wedge (T < 1250K)] \\ Hzr_3(T) & \text{if } [(T \ge 1250K) \wedge (T < 2100K)] \\ Hzr_4(T) & \text{if } [(T \ge 2100K) \wedge (T < 2200K)] \\ Hzr_5(T) & \text{if } ((T \ge 2200K)) \\ 0\frac{joule}{kg} & \text{otherwise} \end{cases}$$





Zircaloy enthalpy as a function of temperature.

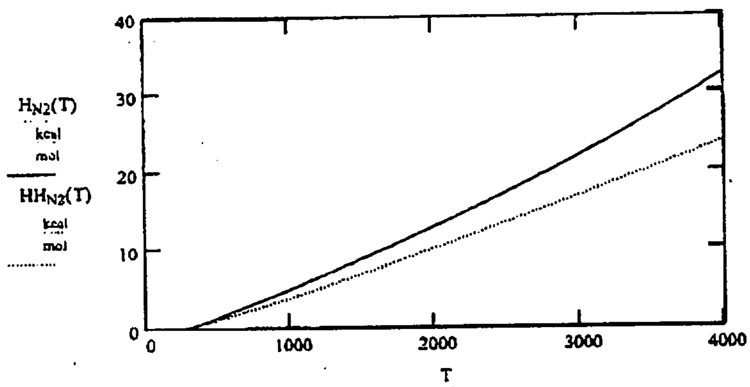
Nitrogen Enthalpy

$$H_{N2}(T) := \left[6.76\cdot\frac{T}{K} + \frac{1}{2}\cdot\left(0.606\cdot10^{-3}\right)\cdot\left(\frac{T}{K}\right)^2 + \frac{1}{3}\cdot\left(0.13\cdot10^{-6}\right)\cdot\left(\frac{T}{K}\right)^3 - 2.044\cdot10^3\right]\frac{cal}{mol}$$

CRC Handbook

$$HH_{N2}(T) := \left[1.117\cdot10^3\cdot\left(\frac{T}{K}\right) - 2.880\cdot10^5\cdot\ln\left(\frac{T}{K}\right) - 5.348\cdot10^7\cdot\left(\frac{K}{T}\right) + 1.506\cdot10^6\right]\cdot\frac{joule}{kg}\cdot MW_{N2}$$

MELCOR Properties



Whole Core Properties **

$580 \cdot mass_{clad} = 2.895 \times 10^4 kg$ Mass of cladding in 580-element core

$\frac{580 \cdot mass_{clad}}{\rho_{Zr}} = 4.454 m^3$ Volume of cladding Zr in 580-element core

$580 \cdot mass_{canister} = 2.496 \times 10^4 kg$ Mass of canister in 580-element core

$\frac{580 \cdot mass_{canister}}{\rho_{Zr}} = 3.84 m^3$ Volume of canister Zr in 580-element core

$(mass_{canister} + mass_{clad}) \cdot 580 = 5.391 \times 10^4 kg$ Mass of Total Zr in 580-element core

$\frac{[(mass_{canister} + mass_{clad}) \cdot 580]}{\rho_{Zr}} = 8.294 m^3$ Volume of Total Zr in 580-element core

Calculate the Energy From Oxidizing a Single Fuel Assembly ***********************************

$f_{oxy} = 0.36$ Fraction of available Zr which becomes oxidized.

$\Delta H_{oxy} := 1.2065 \cdot 10^7 \cdot \frac{joule}{kg}$ Heat of reaction for Zr in Oxygen $\Delta H_{oxy} = 2.882 \times 10^3 \frac{cal}{gm}$

$E_{clad} := f_{oxy} \cdot mass_{clad} \cdot \Delta H_{oxy}$ $E_{canister} := f_{oxy} \cdot mass_{canister} \cdot \Delta H_{oxy}$ $MJ \equiv 10^6 joule$

$E_{oxy} := E_{clad} + E_{canister}$ $GJ \equiv 10^9 \cdot joule$

$KW \equiv 1000 \cdot watt$

$E_{clad} = 216.78 MJ$

$E_{canister} = 186.935 MJ$

$E_{oxy} = 0.404 GJ$

Analysis of Burning a fraction of the Zr available **

$Zr + O_2 \Rightarrow ZrO_2$

$mass_{Zr} := (1 - f_{oxy}) \cdot (mass_{canister} + mass_{clad})$ Mass of Zr remaining after oxidation of f_{oxy} fraction

$moles_{Zr} := f_{oxy} \cdot \left(\frac{mass_{clad} + mass_{canister}}{MW_{Zr}} \right)$ Total moles of Zr in a fuel assembly participating in oxidation.

Air Composition
21% Oxygen
79% Nitrogen

$moles_{Zr} = 366.904\ mol$

$moles_{O2} := moles_{Zr}$ Moles of oxygen consumed in buring f_{oxy} fraction of the available Zr metal.

$moles_{N2} := \frac{79}{21} \cdot moles_{O2}$ Moles of nitrogen associated with the air- burning of f_{oxy} fraction of the available Zr metal.

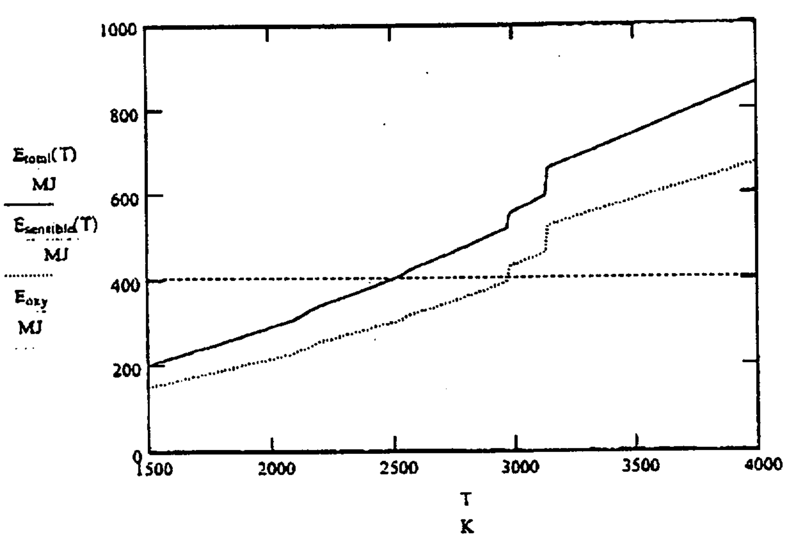
$mass_{ZrO2} := f_{oxy} \cdot (mass_{clad} + mass_{canister}) \cdot \frac{MW_{ZrO2}}{MW_{Zr}}$ Mass of ZrO_2 formed after oxidizing the fraction of Zr metal

$$E_{total}(T) := (mass_{ZrO2} \cdot H_{ZrO2}(T) + mass_{Zr} \cdot H_{Zr}(T) + mass_{fuel} \cdot H_{UO2}(T) + moles_{N2} \cdot H_{N2}(T))$$

$$E_{sensible}(T) := mass_{ZrO2} \cdot H_{ZrO2}(T) + mass_{fuel} \cdot H_{UO2}(T) + mass_{Zr} \cdot H_{Zr}(T)$$

$T := 1500K, 1510K .. 4000K$

$f_{oxy} \equiv 0.36$



The graph to the left shows the partitioning of energy from the oxidation of a fraction of the Zr in a fuel assembly. The energy produced by oxidation, Eoxy is partitioned between the fuel assembly debris and an amount of nitrogen associated with the oxygen in the air. The red curve shows tha total energy of debris and nitrogen, and the blue curve shows the sensible heat retained in the debris alone. The difference in the red and blue curve is an estimate of the plume energy, since this is the energy content of the nitrogen.

In the above energy partition, I have assumed that the fuel assembly will slump after exceeding 2500K in bulk temperature. After slumping, the geometry is assumed to alter so that continued exposure to air is precluded. The energy required to cause this slumping is attained after reaching about 33% oxidation of the available Zr metal, including the channel boxes (BWR fuel). The plume energy would be the energy transported by the nitrogen portion of the air which was involved in the oxidation reactions.

$\text{Plume\_Energy} := \text{moles}_{N2} \cdot H_{N2}(2500K)$ These values are on a per assembly basis.

$\text{Plume\_Energy} = 100.707\ MJ$

If we assume that the $\text{Burn\_Duration} := 30\text{min}$ then the power to the plume can be estimated as....

$\text{Plume\_Power} := \dfrac{\text{Plume\_Energy}}{\text{Burn\_Duration}}$ $\text{Plume\_Power} = 55.948\ KW$ per assembly

If an entire core of assemblies is involved, the numbers are multiplied by the number of asemblies. However another way to express the results might be in a fraction of the chemical energy that goes to the plume.

$$\text{Plume\_fraction} := \frac{E_{oxy} - E_{sensible}(2500K)}{E_{oxy}}$$

So, in summary, we expect that a fraction of each fuel assembly would be involved in air oxidation, that fraction limited by the degradation of the assembly after surpassing 2500K. That fraction is equal to

$f_{oxy} = 0.36$

And, of this fraction of the Zr producing chemical energy, the amount going into the plume is estimated to be:

$\text{Plume\_fraction} = 0.252$

A final note is that I have assumed that the heat is strictly partitioned between fuel, clad, canister, the oxide reaction products and the nitrogen. Heat losses could allow a bit more oxidation energy to be liberated before resulting in fuel slumping, so an additional factor might be included to account for this.

A highly conservative assumption would be to assume that the sensible heat associated with 2500K is retained in the fuel debris, but that the entire amount of zircaloy in the assembly is oxidized. In this case....

$$\text{Emax}_{oxy} := (\text{mass}_{clad} + \text{mass}_{canister}) \cdot \Delta H_{oxy}$$

$\text{Emax}_{oxy} = 1.121\ GJ$

$$E_{debris}(T) := \left[(\text{mass}_{clad} + \text{mass}_{canister}) \cdot \frac{MW_{ZrO2}}{MW_{Zr}} \cdot H_{ZrO2}(T) \right] + \text{mass}_{fuel} \cdot H_{UO2}(T)$$

$E_{debris}(2500K) = 0.353\ GJ$

In this conservative case, the oxidized fraction is assumed to be 100% and the fraction of the oxidation energy going into the plume is

$$\frac{Emax_{oxy} - E_{debris}(2500K)}{Emax_{oxy}} = 0.685$$

Plume fraction of oxidation energy under highly conservative assumptions.

Executive Summary **

We would expect that the fuel assemblies will collapse by overheating at about 2500K which we would expect to happen after attaining something on the order of 33% oxidation of the available zircaloy. On the basis of an entire core of 580 BWR assemblies, this amounts to

Total Energy = $f_{oxy} \cdot 580 \cdot Emax_{oxy} = 234\ GJ$

Sensible Heat in Debris = $580 \cdot E_{sensible}(2500K) = 175\ GJ$ mixture of Zr, oxidized ZrO_2 and UO_2

Plume Energy = $580 \cdot \left(f_{oxy} \cdot Emax_{oxy} - E_{sensible}(2500K)\right) = 59\ GJ$

where, $f_{oxy} = 0.36$

An estimate of an upper bound would be to assume 100% oxidation of the available zircaloy with retention of sensible heat in the debris material. In this case, the energy associated with oxidizing an entire core of asemblies would partiton as follows:

Total Energy = $580 \cdot Emax_{oxy} = 650\ GJ$

Sensible Heat in Debris = $580 \cdot E_{debris}(2500K) = 205\ GJ$ fully oxidized ZrO_2 and UO_2

Plume Energy = $580 \cdot \left(Emax_{oxy} - E_{debris}(2500K)\right) = 445\ GJ$

It should be pointed out that the upper bound requires considerably more air to remove heat than participates in the oxidation. It is doubtful that such effective drafting could be realized.