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August 7, 2000

Mr. Jason H. Schaperow
Office of Nuclear Regulatory Research
Division of Systems Analysis and Regulatory Effectiveness
Safety Margins and Systems Analysis Branch
U.S. Nuclear Regulatory Commission
Mail Stop: T-10K8
Washington, DC 20555-0001

Subject: Analysis of Plume Energy from Air Oxidation in Spent Fuel Storage Pool

Dear Jason,

Enclosed is an analysis of air oxidation of exposed BWR fuel elements in a spent fuel storage tank where the cooling/shielding water is presumed to have been lost following a non-specific seismic event of very low likelihood. The problem posed was to evaluate the energy content of a plume of hot gases rising off of fuel assemblies that are undergoing vigorous oxidation in air. The starting point of the analysis was a conservative estimate of the plume energy that you made based on the assumption that 100% of the oxidation energy was carried away by the plume. The intent of the present analysis was to remove some of the conservatism in your bounding estimate by evaluating the sensible heat that must surely remain within the significant mass of the fuel assemblies. The analysis I performed is essentially a heat balance performed on the fuel bundles with the objective of partitioning the available oxidation energy between the sensible heat of the fuel debris and the plume rising from the damaged fuel assemblies. The analysis is provided in an attachment titled "Analysis of Plume Energy Associated with Spent Fuel Pool Storage Accident." The results of the analysis are summarized as follows.

Since it is known that the fuel assemblies will become so highly degraded by the time their temperature has reached 2500K that the assemblies will collapse into a rubblized geometry, I have taken this to be the maximum temperature that is likely to be attained by the fuel while oxidation is occurring. After this, the degraded geometry will prevent further access of air into the debris. I estimate that only about 30 to 40% oxidation of the available zircaloy will bring the fuel assemblies to the neighborhood of 2500K. Oxidation of 580 BWR fuel assemblies to this state would produce about 234 GJ of chemical energy of which 175 GJ would be retained in the *partially oxidized* fuel debris as sensible heat, leaving 59GJ available to heat the plume gases. Rates can be estimated by assuming that these energies are released over a period of about ½

I-29

hour. A more conservative analysis results from assuming that 100% zircaloy oxidation nevertheless takes place (however unphysical this may be), and that a total of 650 GJ of chemical heat is liberated in the 580 fuel assemblies. Retaining 205 GJ of sensible heat in the 2500K, *fully oxidized* fuel assemblies leaves **445GJ** available for heating the plume. A more detailed integrated analysis could be performed using MELCOR, however, I believe that these estimates bound the plume energy. Please see the attached Mathcad file for the details of the analysis.

It was a pleasure to perform this interesting analysis. If you have any questions or comments, or need any further assistance, please feel free to call me at 505-284-3989.

Sincerely,



Randall O. Gauntt
Modeling and Analysis Department - 6415
Mail Stop 0739

Enclosure

Copy to:

USNRC	Ali Behbahani
USNRC	C. G. Tinkler, Jr.
MS0747	Allen Camp (6410)
MS0742	J. R. Guth (6414)
MS0739	File Copy 5.2.5

Analysis of Plume Energy Associated with Spent Fuel Pool Storage Accident

R.O. Gauntt 7/13/2000

Fuel and Canister Dimensions *****

$$r_{o_clad} := 6.135 \text{ mm}$$

$$r_{fuel} := \frac{0.410}{2} \cdot \text{in}$$

$$r_{i_clad} := 5.322 \text{ mm}$$

$$\text{can_perimeter} := 4.5215 \cdot \text{in}$$

$$\text{assembly_length} := 4.1 \text{ m}$$

$$\Delta t_{\text{canister}} := 0.12 \cdot \text{in}$$

Fuel Properties *****

$$\rho_{Zr} := 6500 \frac{\text{kg}}{\text{m}^3}$$

$$C_{p_{UO_2}} := 370 \frac{\text{joule}}{\text{kg} \cdot \text{K}}$$

$$\rho_{UO_2} := 0.95 \cdot 10.96 \cdot \frac{\text{gm}}{\text{cm}^3}$$

$$\rho_{ZrO_2} := 5.6 \cdot \frac{\text{gm}}{\text{cm}^3}$$

$$MW_{Zr} := 91.2 \frac{\text{gm}}{\text{mol}}$$

$$MW_{N_2} := 28 \cdot \frac{\text{gm}}{\text{mol}}$$

$$MW_{ZrO_2} := 123.2 \cdot \frac{\text{gm}}{\text{mol}}$$

$$MW_{O_2} := 32 \cdot \frac{\text{gm}}{\text{mol}}$$

Fuel Assembly Properties *****

$$\text{mass}_{\text{clad}} := 64\pi \cdot (r_{o_clad}^2 - r_{i_clad}^2) \cdot \text{assembly_length} \cdot \rho_{Zr}$$

$$\text{mass}_{\text{canister}} := \text{assembly_length} \cdot \text{can_perimeter} \cdot \Delta t_{\text{canister}} \cdot \rho_{Zr}$$

$$\text{mass}_{\text{fuel}} := 62 \cdot \pi \cdot r_{\text{fuel}}^2 \cdot \text{assembly_length} \cdot \rho_{UO_2}$$

$$\text{mass}_{\text{canister}} = 43.039 \text{ kg}$$

$$\text{mass}_{\text{clad}} = 49.91 \text{ kg}$$

$$\text{mass}_{\text{fuel}} = 225.442 \text{ kg}$$

Enthalpy (Internal Energy) of Zircaloy, UO₂ and ZrO₂ ***
 Properties from MATPRO**

UO₂ Internal Energy *****

$$\begin{aligned}
 K_1 &:= 296.7 \cdot K^{-1} & \theta &:= 535.285 \cdot K & \Delta H_{f_UO2} &:= 2.74 \cdot 10^5 \cdot \frac{\text{joule}}{\text{kg}} \\
 K_2 &:= 2.43 \cdot 10^{-2} \cdot K^{-2} & E_D &:= 1.577 \cdot 10^5 \cdot \frac{\text{joule}}{\text{mol}} & C_{p_UO2} &:= 503 \cdot \frac{\text{joule}}{\text{kg} \cdot K} \\
 K_3 &:= 8.745 \cdot 10^7 & R &:= 8.3143 \cdot \frac{\text{joule}}{\text{mol} \cdot K} & &
 \end{aligned}$$

$$H_{\text{solid_UO2}}(T) := \left[\frac{K_1 \cdot \theta}{\left(e^{\frac{\theta}{T}} - 1 \right)} + \frac{K_2 \cdot T^2}{2} + K_3 \cdot e^{\left(\frac{-E_D}{R \cdot T} \right)} \right] \cdot \frac{\text{joule}}{\text{kg}}$$

$$H_{UO2}(T) := \Phi(3138K - T) \cdot H_{\text{solid_UO2}}(T) + \Phi(T - 3138K) \cdot \left[H_{\text{solid_UO2}}(3138K) + \Delta H_{f_UO2} + (T - 3138K) \cdot C_{p_UO2} \right]$$

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

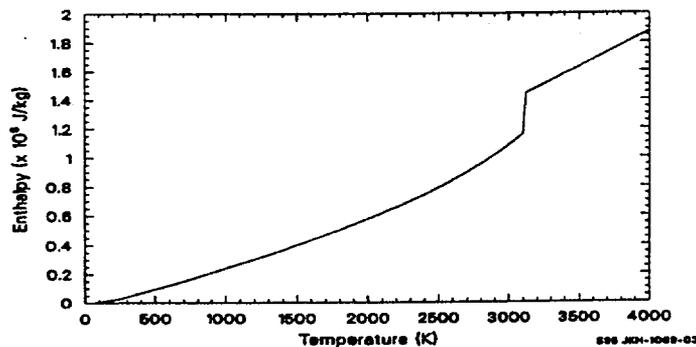
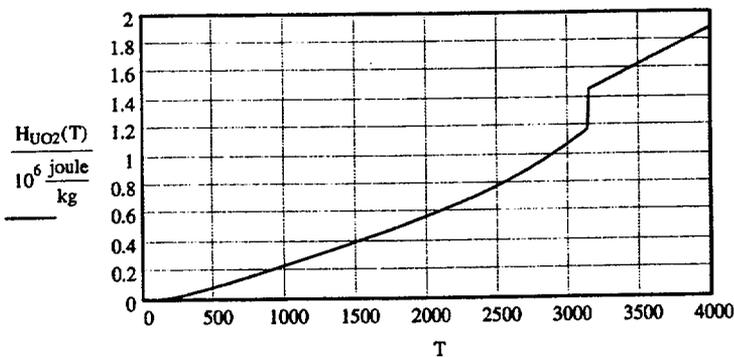


Figure 2-3. Enthalpy of UO₂ as a function of temperature to 4,000 K.



Zircaloy Oxide Internal Energy

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

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

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

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

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

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

$$H_{ZrO_2}(T) := \begin{cases} H_1(T) & \text{if } [(T > 273.0K) \wedge (T < 1478.0K)] \\ H_2(T) & \text{if } [(T > 1478.01K) \wedge (T < 2000.0K)] \\ H_3(T) & \text{if } [(T \geq 2000.0K) \wedge (T < 2558.0K)] \\ H_4(T) & \text{if } [(T \geq 2558.0K) \wedge (T < 2973.0K)] \\ H_5(T) & \text{if } [(T \geq 2973.01K) \wedge (T < 4100.0K)] \\ 0.0 \frac{\text{joule}}{\text{kg}} & \text{otherwise} \end{cases}$$

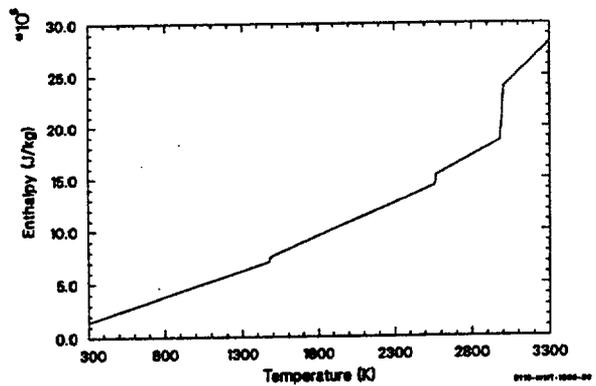
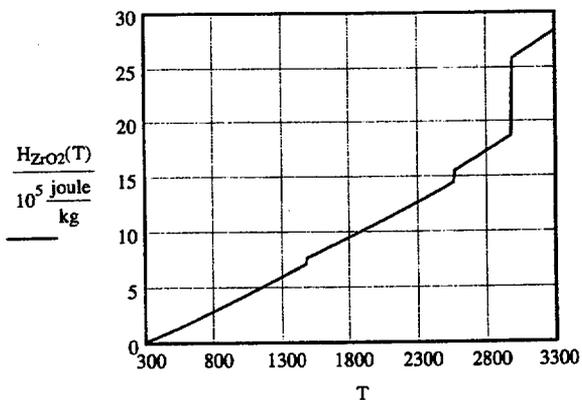


Figure 5-3. Zircaloy oxide enthalpy as a function of temperature.

Enthalpy of Zr

$$H_{Zr_1}(T) := \frac{(2.6 - 0) \cdot 10^5 \text{ joule}}{\text{kg}} \cdot (T - 300\text{K})$$

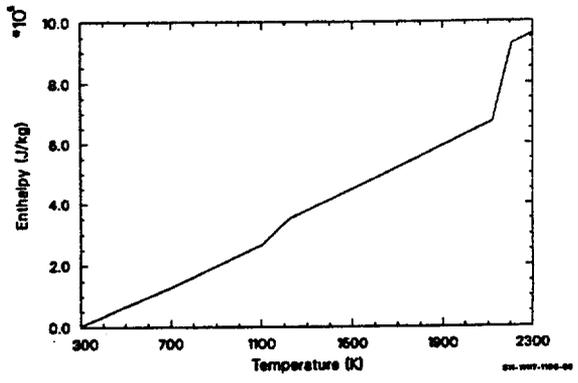
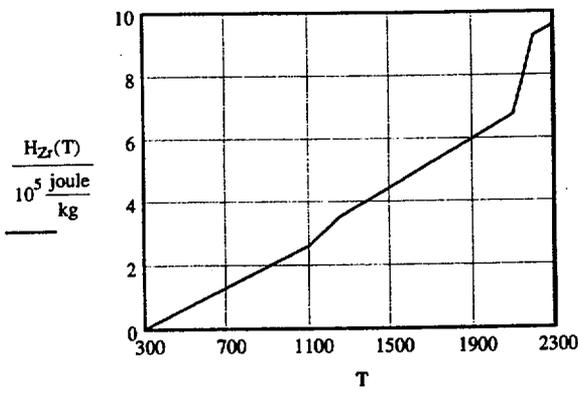
$$H_{Zr_2}(T) := \frac{(3.5 - 2.6) \cdot 10^5 \text{ joule}}{\text{kg}} \cdot (T - 1100\text{K}) + H_{Zr_1}(1100\text{K})$$

$$H_{Zr_3}(T) := \frac{(6.75 - 3.5) \cdot 10^5 \text{ joule}}{\text{kg}} \cdot (T - 1250\text{K}) + H_{Zr_2}(1250\text{K})$$

$$H_{Zr_4}(T) := \frac{(9.25 - 6.75) \cdot 10^5 \text{ joule}}{\text{kg}} \cdot (T - 2100\text{K}) + H_{Zr_3}(2100\text{K})$$

$$H_{Zr_5}(T) := H_{Zr_4}(2200\text{K}) + \frac{356 \text{ joule}}{\text{kg}} \cdot (T - 2200\text{K})$$

$$H_{Zr}(T) := \begin{cases} H_{Zr_1}(T) & \text{if } [(T \geq 300\text{K}) \wedge (T < 1100\text{K})] \\ H_{Zr_2}(T) & \text{if } [(T \geq 1100\text{K}) \wedge (T < 1250\text{K})] \\ H_{Zr_3}(T) & \text{if } [(T \geq 1250\text{K}) \wedge (T < 2100\text{K})] \\ H_{Zr_4}(T) & \text{if } [(T \geq 2100\text{K}) \wedge (T < 2200\text{K})] \\ H_{Zr_5}(T) & \text{if } (T \geq 2200\text{K}) \\ 0 \frac{\text{joule}}{\text{kg}} & \text{otherwise} \end{cases}$$

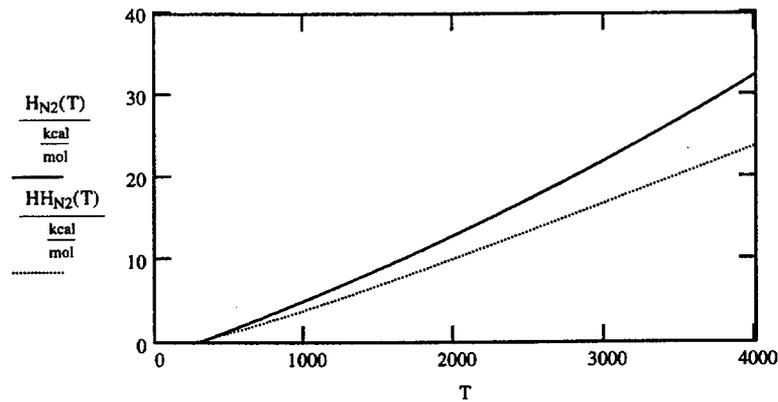


Zircaloy enthalpy as a function of temperature.

Nitrogen Enthalpy*****

$$H_{N_2}(T) := \left[6.76 \cdot \frac{T}{K} + \frac{1}{2} \cdot (0.606 \cdot 10^{-3}) \cdot \left(\frac{T}{K} \right)^2 + \frac{1}{3} \cdot (0.13 \cdot 10^{-6}) \cdot \left(\frac{T}{K} \right)^3 - 2.044 \cdot 10^3 \right] \frac{\text{cal}}{\text{mol}} \quad \text{CRC Handbook}$$

$$HH_{N_2}(T) := \left[1.117 \cdot 10^3 \cdot \left(\frac{T}{K} \right) - 2.880 \cdot 10^5 \cdot \ln \left(\frac{T}{K} \right) - 5.348 \cdot 10^7 \cdot \left(\frac{K}{T} \right) + 1.506 \cdot 10^6 \right] \cdot \frac{\text{joule}}{\text{kg}} \cdot MW_{N_2} \quad \text{MELCOR Properties}$$



Whole Core Properties *****

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

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

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

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

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

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

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

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

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

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

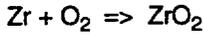
$E_{\text{oxy}} := E_{\text{clad}} + E_{\text{canister}}$ GJ $\equiv 10^9$ joule
KW $\equiv 1000$ watt

$E_{\text{clad}} = 216.78 \text{ MJ}$

$E_{\text{canister}} = 186.935 \text{ MJ}$

$E_{\text{oxy}} = 0.404 \text{ GJ}$

Analysis of Burning a fraction of the Zr available *****



$mass_{Zr} := (1 - f_{oxy}) \cdot (mass_{canister} + mass_{clad})$

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

$moles_{Zr} = 366.904 \text{ mol}$

$moles_{O_2} := moles_{Zr}$

Moles of oxygen consumed in burning f_{oxy} fraction of the available Zr metal.

$moles_{N_2} := \frac{79}{21} \cdot moles_{O_2}$

Moles of nitrogen associated with the air- burning of f_{oxy} fraction of the available Zr metal.

$mass_{ZrO_2} := f_{oxy} \cdot (mass_{clad} + mass_{canister}) \cdot \frac{MW_{ZrO_2}}{MW_{Zr}}$

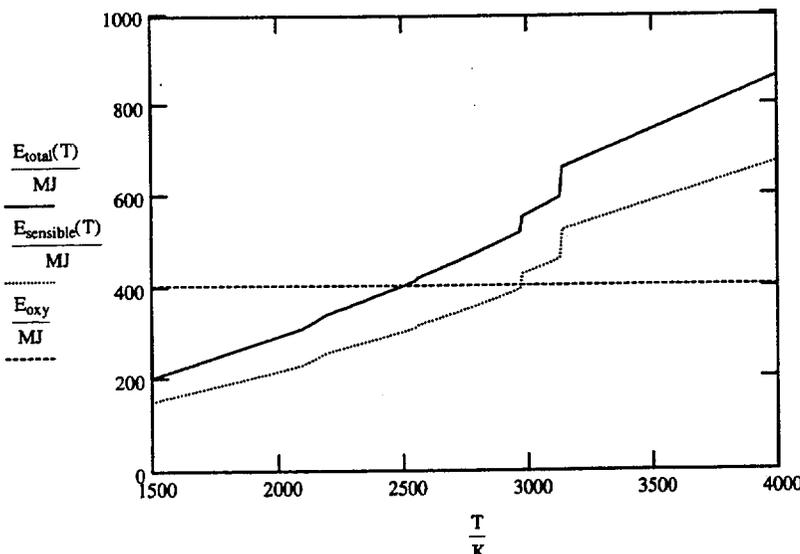
Mass of ZrO_2 formed after oxidizing the fraction of Zr metal

$E_{total}(T) := (mass_{ZrO_2} \cdot H_{ZrO_2}(T) + mass_{Zr} \cdot H_{Zr}(T) + mass_{fuel} \cdot H_{UO_2}(T) + moles_{N_2} \cdot H_{N_2}(T))$

$E_{sensible}(T) := mass_{ZrO_2} \cdot H_{ZrO_2}(T) + mass_{fuel} \cdot H_{UO_2}(T) + mass_{Zr} \cdot H_{Zr}(T)$

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

$f_{oxy} \equiv 0.36$



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, E_{oxy} is partitioned between the fuel assembly debris and an amount of nitrogen associated with the oxygen in the air. The red curve shows the 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.

$$\text{Plume_Energy} := \text{moles}_{\text{N}_2} \cdot H_{\text{N}_2}(2500\text{K})$$

These values are on a per assembly basis.

$$\text{Plume_Energy} = 100.707 \text{ MJ}$$

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

$$\text{Plume_Power} := \frac{\text{Plume_Energy}}{\text{Burn_Duration}} \quad \text{Plume_Power} = 55.948 \text{ KW} \quad \text{per assembly}$$

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

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

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

$$f_{\text{oxy}} = 0.36$$

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....

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

$$E_{\text{max_oxy}} = 1.121 \text{ GJ}$$

$$E_{\text{debris}}(T) := \left[(\text{mass}_{\text{clad}} + \text{mass}_{\text{canister}}) \cdot \frac{MW_{\text{ZrO}_2}}{MW_{\text{Zr}}} \cdot H_{\text{ZrO}_2}(T) \right] + \text{mass}_{\text{fuel}} \cdot H_{\text{UO}_2}(T)$$

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

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

$$\frac{E_{\text{max}_{\text{oxy}}} - E_{\text{debris}(2500\text{K})}}{E_{\text{max}_{\text{oxy}}}} = 0.685$$

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 36% oxidation of the available zircaloy. On the basis of an entire core of 580 BWR assemblies, this amounts to

$$\begin{aligned} \text{Total Energy} &= f_{\text{oxy}} \cdot 580 \cdot E_{\text{max}_{\text{oxy}}} = 234 \text{ GJ} \\ \text{Sensible Heat in Debris} &= 580 \cdot E_{\text{sensible}(2500\text{K})} = 175 \text{ GJ} \quad \text{mixture of Zr, oxidized ZrO}_2 \text{ and UO}_2 \\ \text{Plume Energy} &= 580 \cdot (f_{\text{oxy}} \cdot E_{\text{max}_{\text{oxy}}} - E_{\text{sensible}(2500\text{K})}) = 59 \text{ GJ} \\ \text{where,} \quad f_{\text{oxy}} &= 0.36 \end{aligned}$$

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 assemblies would partition as follows:

$$\begin{aligned} \text{Total Energy} &= 580 \cdot E_{\text{max}_{\text{oxy}}} = 650 \text{ GJ} \\ \text{Sensible Heat in Debris} &= 580 \cdot E_{\text{debris}(2500\text{K})} = 205 \text{ GJ} \quad \text{fully oxidized ZrO}_2 \text{ and UO}_2 \\ \text{Plume Energy} &= 580 \cdot (E_{\text{max}_{\text{oxy}}} - E_{\text{debris}(2500\text{K})}) = 445 \text{ GJ} \end{aligned}$$

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.

8/2/00

Today, at 3:15 p.m., I called R. Gauntt regarding his ltr on "Plume Heat Content of SFP Accidents." He said he would try to prepare the cover letter today.

~~Followup 8/22/00~~

From: Jason Schaperow
To: GWIA:rogaunt@[sandia.gov]
Date: Tue, Aug 8, 2000 9:26 AM
Subject: Re: Plume Energy

There seems to be a problem printing out the cover letter and analysis. (The cover letter does not print out and the analysis only prints out the first three pages.) I will wait for the copy coming in the mail.

Thanks.
Jason

>>> "Gauntt, Randall O" <rogaunt@sandia.gov> 08/07 7:39 PM >>>
Jason,
Here is the cover letter and the analysis.
They are coming in the mail also.

cover letter:

ftp://ftp.sandia.gov/outgoing/gauntt/Plume_Energy_Cover_Letter.pdf

analysis: ftp://ftp.sandia.gov/outgoing/gauntt/Plume_Energy_Analysis.pdf

Randy

CC: Ali Behbahani, Charles Tinkler

From: "Gauntt, Randall O" <rogaunt@sandia.gov>
To: "Jason Schaperow" <JHS1@nrc.gov>, "Gauntt, Randa...
Date: Tue, Aug 8, 2000 10:35 AM
Subject: RE: Plume Energy

Sorry,
I did not put the correct title on the paper anyway.
I fixed it.

Randy

By the way, if your Acrobat viewer can display all of the pages on your screen, then failure to print them on your local printer is a local problem, not one with the transmitted file. The pdf format is really a nice way to communicate - it's a shame to let a local problem with the computers constrain us. If your acrobat viewer sees all of the pages, you should have your computer guys check it out. Forward the file to them and ask them to trouble shoot their printers or their Acrobat installation. Just a suggestion. I would give them something to do.

-----Original Message-----

From: Jason Schaperow [mailto:JHS1@nrc.gov]
Sent: August 08, 2000 7:26 AM
To: rogaunt@sandia.gov
Cc: Ali Behbahani; Charles Tinkler
Subject: Re: Plume Energy

There seems to be a problem printing out the cover letter and analysis. (The cover letter does not print out and the analysis only prints out the first three pages.) I will wait for the copy coming in the mail.

Thanks.
Jason

>>> "Gauntt, Randall O" <rogaunt@sandia.gov> 08/07 7:39 PM >>>
Jason,
Here is the cover letter and the analysis.
They are coming in the mail also.

cover letter:
ftp://ftp.sandia.gov/outgoing/gauntt/Plume_Energy_Cover_Letter.pdf

analysis: ftp://ftp.sandia.gov/outgoing/gauntt/Plume_Energy_Analysis.pdf

Randy

CC: "Ali Behbahani" <AXB.twf5_po.TWFN_DO@nrc.gov>, "Ch..."