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16. KEY

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		Design Authority									
		Design Agent									
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1	1	Cog. Mgr. J. R. Frederickson	J R Frederickson								
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18.	19.	20.	21. DOE APPROVAL (if required)
M. J. Packer (signature) 7/21/98 Signature of EDT Originator / Date	J. R. Frederickson (signature) 7/23/98 Authorized Representative for Receiving Organization / Date	J. R. Frederickson (signature) 7/22/98 Design Authority/ Cognizant Manager / Date	Ctrl. No. [] Approved [] Approved w/comments [] Disapproved w/comments

MCO GAS COMPOSITION FOR LOW REACTIVE SURFACE AREAS

M. J. Packer
DE&S Hanford Inc.
Richland, WA 99352
U.S. Department of Energy Contract DE-AC06-96RL13200

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Key Words: Reactive Surface Area, Backfill Overpressure, MCO

Abstract: This calculation adjusts modelled output (HNF-SD-SNF-TI-040, Rev. 2) by considering lower reactive fuel surface areas and by increasing the input helium backfill overpressure from 0.5 to 1.5 atm (2.5 atm abs) to verify that MCO gas-phase oxygen concentrations can remain below 4 mole % over a 40 year interim period under a 'worst case' condition of zero reactive surface area. Added backfill gas will dilute any gases generated during interim storage and is a strategy within the current design capability. The zero reactive surface area represents a hypothetical 'worst case' example where there is no fuel scrap and/or damaged spent fuel rods in an MCO. Also included is a hypothetical case where only K East fuel exists (no $Al(OH)_3$) in an MCO with an added backfill overpressure of 0.5 atm (1.5 atm abs).

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REVIEW CHECKLIST

Document Reviewed: "MCO Gas Composition for Low Reactive Surface Areas," HNF-3035, Rev. 0, M. J. Packer

Scope of Review: Assumptions, Methodology, Conclusions

Yes	No	NA		
[X]	[ ]	[ ]	*	Previous reviews complete and cover analysis, up to scope of this review, with no gaps.
[X]	[ ]	[ ]		Problem completely defined.
[X]	[ ]	[ ]		Accident scenarios developed in a clear and logical manner.
[X]	[ ]	[ ]		Necessary assumptions explicitly stated and supported.
[X]	[ ]	[ ]		Computer codes and data files documented.
[X]	[ ]	[ ]		Data used in calculations explicitly stated in document.
[X]	[ ]	[ ]		Data checked for consistency with original source information as applicable.
[X]	[ ]	[ ]		Mathematical derivation checked including dimensional consistency of results.
[X]	[ ]	[ ]		Models appropriate and used within range of validity or use outside range of established validity justified.
[ ]	[ ]	[X]		Hand calculations checked for errors. Spreadsheet results should be treated exactly the same as hand calculations.
[X]	[ ]	[ ]		Software input correct and consistent with document reviewed.
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[ ]	[ ]	[X]		Limits/criteria/guidelines applied to analysis results are appropriate and referenced. Limits/criteria/guidelines checked against references.
[X]	[ ]	[ ]		Safety margins consistent with good engineering practices.
[X]	[ ]	[ ]		Conclusions consistent with analytical results and applicable limits.
[X]	[ ]	[ ]		Results and conclusions address all points required in the problem statement.
[ ]	[ ]	[X]		Format consistent with appropriate NRC Regulatory Guide or other standards.
[ ]	[ ]	[X]	*	Review calculations, comments, and/or notes are attached.
[X]	[ ]	[ ]		**Document approved.**

M. G. Plys (signature)
Reviewer (Printed Name and Signature)

07/23/98
Date

*Any calculations, comments, or notes generated as part of this review should be signed, dated and attached to this checklist. Such material should be labeled and recorded in such a manner as to be intelligible to a technically qualified third party.

A-6002-359 (05/97)

REVIEW CHECKLIST

Document Reviewed: "MCO Gas Composition for Low Reactive Surface Areas," HNF-3035, Rev. 0, M.J. Packer

Scope of Review: Assumptions, Methodology, Conclusions

Yes	No	NA		
[X]	[ ]	[ ]	*	Previous reviews complete and cover analysis, up to scope of this review, with no gaps.
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[ ]	[ ]	[X]	*	Review calculations, comments, and/or notes are attached.
[X]	[ ]	[ ]		**Document approved.**

R. A. Sexton *Richard A. Sexton* 07/22/98

Reviewer (Printed Name and Signature) Date

*Any calculations, comments, or notes generated as part of this review should be signed, dated and attached to this checklist. Such material should be labeled and recorded in such a manner as to be intelligible to a technically qualified third party.

A-6002-359 (05/97)

1.0 INTRODUCTION AND PURPOSE

Interim storage of multi-canister overpacks (MCOs) containing spent nuclear fuel (SNF) generates issues of increasing gas compositions within the MCO, notably oxygen, because of it's flammability properties. The safe storage of the SNF in MCOs can be demonstrated by using conservative conditions with modelled values. Current thought is to provide 0.5 atm overpressure of helium to the MCOs prior to the 40 year interim storage. However, using 'worst case' conservative conditions, such as low reactive surface areas on the uranium fuel, the modelled results (Duncan and Plys 1998) show the oxygen concentrations to be above the 4% limit. This document proves, using conservative conditions with a zero reactive surface area and backfilling the MCO with 1.5 atm overpressure (2.5 atm abs) of helium prior to interim storage, the MCOs can maintain oxygen concentration levels below 4 mole %. Also, a hypothetical case exists with an MCO containing only K East fuel with a range of little to none reactive surface areas and an initial backfill overpressure of 0.5 atm (1.5 atm abs). Again this document demonstrates, using modelled parameters, that this condition remains well below 4 mole % oxygen over the 40 year storage period.

2.0 SCOPE

The subject scope includes input values from modelling calculations in HNF-SD-SNF-TI-040, Rev. 2 (Duncan and Plys 1998) with a revised (increased) helium backfill pressure to demonstrate that oxygen mole (or volume) concentrations, after 40 years of MCO storage, do not exceed 4% over a range of low reactive surface areas. Conservative input variables are utilized, including a zero reactive surface area, along with a bounding uranium oxide hydrate value (0.11 kg/m^2) which is correlated with the amount of oxygen generated per reactive surface area via radiolytic decomposition. The major modelling input revision is the increase of the initial helium backfill pressure in the MCO from 0.5 atm to 1.5 atm overpressure (or total 2.5 atm absolute). In principal, any oxygen generation rate can be mitigated through an appropriate backfill pressure (Duncan and Plys 1998). Also considered is the case of only K East fuel with no reactive surface area at 1.5 atm absolute backfill pressure.

3.0 KEY INPUTS AND ASSUMPTIONS

Revisions to modelling calculations are included in Appendix A (re-formatted MATHCAD™ file from Duncan and Plys) and noted in bold face type. Modelled input parameters include the following as noted in Appendix A:

Decay Power: A range of MCO decay power values, from 10 W to 770 W, is included in the calculations. An average MCO decay power is 396 W.

Radiolysis: $Al(OH)_3$ radiolysis is by gamma dose alone with $g(H_2)$ = 1.2 molecules/100 eV and $g(O_2)$ = 0.225 molecules/100 eV.

$UO_3 \cdot xH_2O$ radiolysis is by alpha, beta, and gamma sources with $g(H_2) = 0.165$, 0.05, and 1.2, respectively. $UO_3 \cdot xH_2O$ $g(O_2)$ values are 0.083, 0.025, and 0.11 for alpha, beta, and gamma, respectively.

Conservative values are included such as 8 kg aluminum hydroxide, 0.11 kg water/m^2 reactive surface area from uranium oxide hydrate, 200 g free water, and a range of low (and zero) reactive surface areas. The minimal to zero area is associated with minimal to no fuel scrap and undamaged fuel rods. Note that the 200 grams of free water remains as a constant over the range of reactive surface areas, including zero reactive area. This term is bounding since the amount of free water is associated with the cracks in the damaged fuel surface (reactive surface area). Helium backfill overpressure is increased from 0.5 atm to 1.5 atm (2.5 atm abs) prior to interim storage.

A separate conservative case is demonstrated assuming no $Al(OH)_3$ with minimal to zero reactive surface areas at a helium backfill pressure of 1.5 atm absolute.

4.0 CONCLUSION

The plot in Appendix A, on page A-11, shows that use of an initial helium backfill pressure of 2.5 atm absolute in the MCO results in acceptable oxygen mole concentrations per low (and zero) reactive surface areas under conservative conditions. The 'worst case' condition of zero reactive surface area using this initial helium backfill pressure results in an oxygen concentration less than 4% over 40 years. A comparison plot, on page A-12, shows the results from an initial helium backfill overpressure of 0.5 atm (1.5 atm abs) in an MCO using conservative input values. Page A-14 shows the results (oxygen below 3%) from the hypothetical condition with an MCO filled with only K East fuel and minimal to zero reactive surface areas at an initial helium backfill pressure of 1.5 atm absolute.

5.0 REFERENCE

D. R. Duncan and M. G. Plys, 1998, "MCO Internal Gas Composition and Pressure During Interim Storage," HNF-SD-SNF-TI-040, Rev. 2, DE&S Hanford, Richland, WA.

MCO O2% AND MAXIMUM PRESSURIZATION: RADIOLYSIS AND GETTERING OF O2
Goal is O2 concentration at end-of-life, or max concentration, so H2 gettering not considered.

RANGE OF Q AND A, DATABOOK G(O2) VALUES, 8 KG AL(OH)3,
BOUNDING 0.11 kg H2O / m^2 FROM UO3.2H2O, 200 G RESIDUAL H2O (NO UO3.2H2O DECOMP)

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FOR: Hanford Spent Nuclear Fuel Project - Duke Engineering & Services Hanford
- Richland, WA
Contact: Darrell Duncan 509-372-1013.
DATE: June, 1998.

Calculation Technical Basis and Assumptions:

1. Decay power varies per 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	

2. Average MCO decay power is 396 W, bounding power is 776 W, and fuel mass is 6339 kg. Alpha, beta, and gamma fractions from 1995 above are applied for all total MCO powers. So for example, alpha power in an average MCO is = (26.3/133.7) * 396 = 77.9 W.

3. MCO temperature is directly related to decay power as a function of time -- so O2 gettering is related to.

4. Al(OH)3 radiolysis is by gamma dose alone with g(H2) = 1.2 molecules / 100 ev [HNF-SNF-CN-006]. g(O2) is either 0.225 [same ref] or 0.6, conservative stoichiometric value. Al/U gamma absorption = 35%.

5. Uranium Oxide Hydrates are represented by UO3.2H2O.

6. UO3.2H2O NOT ALLOWED TO DECOMPOSE THERMALLY - RESIDUAL H2O EVAPORATE.

7. UO3.xH2O radiolysis is by alpha, beta, and gamma sources with g(H2) = 0.165, 0.05 and 1.2 respectively, using the 11% water fraction when x=2 [HNF-SD-SNF-CN-006]. U hydrate/U gamma absorption = 86%.

8. UO3.xH2O g(O2) values are: 0.083, 0.025, and 0.11 for alpha, beta, gamma respectively from [same ref], but a gamma value of 0.6 is a conservative stoichiometric value.

9. No hydrogen gettering - only occurs when Oxygen is depleted. This is OK because it allows the maximum presssure to be calculated, before substantial H2 gettering, and the max. O2 concentration.

10. Oxygen gettering by Ritchie's moist air correlation, since H2O present, with a minimum limit of Trimble's dry air correlation.

11. Bounding values are: **1.5 atm backfill overpressure**, 2.8 kg water from Al(OH)3 with no removal, 0.77 kg water from UO3.2H2O 7 m^2. Inputs may differ from bounds. Best-estimate is 0.055 kg H2O / m^2 from UO3.2H2O; bound is 0.11 kg/m^2. Bounding area is 8 m^2.

** *Note on units: time in years, mass in grams, area in m^2, with appropriate conversions used.*

1.0 INPUT AND DERIVED VALUES

Avogadro's number:	$Na := 6.022 \cdot 10^{23}$
Conversion factor J/100 ev:	$Jev := 1.6 \cdot 10^{-17}$
MCO volume, m^3,	$V_{mco} = 0.5$
and backfill temperature, K:	$T_{bf} = 298$
Fuel Mass (grams):	$M_f := 6.339 \cdot 10^{6}$
UO3 Hydrate mass per unit area gram/m^2:	$m = 110$ BOUNDING 0.11kg/m^2 !
Max g H2O from UO3.xH2O & max g Al(OH)3:	$UH_{max} = 770$ $AL_{max} = 8000$
Free H2O, g, bounding value:	$m_{fw} = 200$
Amount of water from UO4.2H2O if no AL(OH), g:	$m_{uo4} = 54$
Molecular weights of Al(OH)3 and UO3 hydrate:	$M_{ah} = 78$ $M_{uh} = 322$ $M_w = 18$
g(H2) & g(O2) value for Al(OH)3, molec/100 eV:	$g_{ahy} = 1.2$ $g_{oay} = 0.225$
g(H2) values for UO3 hydrates, molec/100 eV	$g_{hu\alpha} = 0.165$ $g_{hu\beta} = 0.05$ $g_{hu\gamma} = 1.2$
g(O2) values for UO3 hydrates, molec/100 eV	$g_{ou\alpha} = 0.083$ $g_{ou\beta} = 0.025$ $g_{ou\gamma} = 0.11$
g(H2) values for free H2O, molec/100 eV	$g_{hw\alpha} = 1.6$ $g_{hw\beta} = 0.53$ $g_{hw\gamma} = 0.5$

g(O2) values for free H2O, molec/100 eV

$$g_{ow\alpha} = 0.8$$
$$g_{ow\beta} = 0.265$$
$$g_{ow\gamma} = 0.25$$

Relative gamma absorption for Al, U, H2O:

$$rQ_{a\gamma} = 0.35$$
$$rQ_{u\gamma} = 0.86$$
$$rQ_{w\gamma} = 0.38$$

Power fraction for Al(OH)3. Multiplies initial power; decays with time per below.

$$fQ_{a\gamma} = rQ_{a\gamma} \cdot \frac{42.4}{133.7}$$
$$fQ_{a\gamma} = 0.111$$
$$fQ_{u\alpha} = \frac{26.3}{133.7}$$
$$fQ_{u\beta} = \frac{65}{133.7}$$
$$fQ_{u\gamma} = rQ_{u\gamma} \cdot \frac{42.4}{133.7}$$

Power fractions for U hydrates, Each independently decayed with time.

$$fQ_{u\alpha} = 0.1967$$
$$fQ_{u\beta} = 0.4862$$
$$fQ_{u\gamma} = 0.2727$$

Power fractions for for free H2O, each independently decayed with time.

$$fQ_{w\alpha} := fQ_{u\alpha}$$
$$fQ_{w\beta} := fQ_{u\beta}$$
$$fQ_{w\gamma} = rQ_{w\gamma} \cdot \frac{42.4}{133.7}$$
$$fQ_{w\gamma} = 0.1205$$

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

$$\lambda_\alpha := \frac{-1}{45} \cdot \ln\left(\frac{32}{26.3}\right)$$
$$\lambda_\alpha = -4.3593 \cdot 10^{-3}$$
$$\lambda_\beta := \frac{-1}{45} \cdot \ln\left(\frac{22}{65}\right)$$
$$\lambda_\beta = 0.0241$$

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

$$\lambda_q = 0.0149$$

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

$$\lambda_\gamma = 0.0242$$

2.1 FUNCTIONS FOR REMAINING MASS DUE TO RADIOLYSIS

2.1.1 Al(OH)3 radiolysis fractions and example for 396 W in 6339 kg (W/g unit used):

$$\lambda_{ao} := \frac{2}{3} \cdot M_f^{-1} \cdot M_{ah} \cdot (Jev \cdot Na)^{-1} \cdot (3600 \cdot 24 \cdot 365)$$

$$\lambda_{ao} = 2.6849 \cdot 10^{-5}$$

$$\Lambda_a(Q,t) := \frac{\lambda_{ao} \cdot g_{ha\gamma} \cdot fQ_{a\gamma} \cdot Q}{\lambda_\gamma} \cdot \left(e^{-\lambda_\gamma \cdot t} - 1\right)$$

$$F_a(Q,t) := e^{\Lambda_a(Q,t)}$$

Fraction (mass or moles) Al(OH)3 left as function of MCO power, time

$$F_a(396, 40) = 0.9643$$

Fraction left in average MCO after 40 years: 3.6% decomposition.

$$dF_{ha}(Q,t) := -\lambda_{ao} \cdot g_{ha\gamma} \cdot fQ_{a\gamma} \cdot Q \cdot e^{-\lambda_\gamma \cdot t}$$

Derivative of fraction: Used for H2 radiolysis rate

$$dF_{ha}(396, 20) = -8.7361 \cdot 10^{-4}$$

About -0.09% per year implies -3.6% over 40 years

$$dF_{oa}(Q,t) := -\lambda_{ao} \cdot g_{oa\gamma} \cdot fQ_{a\gamma} \cdot Q \cdot e^{-\lambda_\gamma \cdot t}$$

Derivative of fraction: Used for O2 radiolysis rate

2.1.2 UO3.2H2O radiolysis fractions and example for 396 W:

$$\lambda_{uo} := M_f^{-1} \cdot M_{uh} \cdot (Jev \cdot Na)^{-1} \cdot (3600 \cdot 24 \cdot 365)$$

$$\lambda_{uo} = 1.6626 \cdot 10^{-4}$$

$$\Lambda_u(Q,t) := \frac{\lambda_{uo} \cdot g_{hu\gamma} \cdot fQ_{u\gamma} \cdot Q}{\lambda_\gamma} \cdot \left(e^{-\lambda_\gamma \cdot t} - 1\right) + \frac{\lambda_{uo} \cdot g_{hu\beta} \cdot fQ_{u\beta} \cdot Q}{\lambda_\beta} \cdot \left(e^{-\lambda_\beta \cdot t} - 1\right) + \frac{\lambda_{uo} \cdot g_{hu\alpha} \cdot fQ_{u\alpha} \cdot Q}{\lambda_\alpha} \cdot \left(e^{-\lambda_\alpha \cdot t} - 1\right)$$

$$F_u(Q,t) := e^{\Lambda_u(Q,t)}$$

Fraction (mass or moles) U hydrate left as function of MCO power, time

$$F_u(396, 40) = 0.503$$

Fraction left in average MCO after 40 years: 50% decomposition.
Derivative of fraction for H2 radiolysis rate:

$$dF_{hu}(Q,t) := -\lambda_{uo} \cdot g_{hu\gamma} \cdot fQ_{u\gamma} \cdot Q \cdot e^{-\lambda_\gamma t} - \lambda_{uo} \cdot g_{hu\beta} \cdot fQ_{u\beta} \cdot Q \cdot e^{-\lambda_\beta t} - \lambda_{uo} \cdot g_{hu\alpha} \cdot fQ_{u\alpha} \cdot Q \cdot e^{-\lambda_\alpha t}$$

$$dF_{hu}(396, 20) = -0.0166$$

About -1.6% per year implies >50% over 40 years (rate varies strongly) O2 production from radiolysis of UO3.2H2O:

$$dF_{ou}(Q,t) := -\lambda_{uo} \cdot g_{ou\gamma} \cdot fQ_{u\gamma} \cdot Q \cdot e^{-\lambda_\gamma t} - \lambda_{uo} \cdot g_{ou\beta} \cdot fQ_{u\beta} \cdot Q \cdot e^{-\lambda_\beta t} - \lambda_{uo} \cdot g_{ou\alpha} \cdot fQ_{u\alpha} \cdot Q \cdot e^{-\lambda_\alpha t}$$

2.1.3 Free water decomposition

$$\lambda_{wo} := M_f^{-1} \cdot M_w \cdot (Jev \cdot Na)^{-1} \cdot (3600 \cdot 24 \cdot 365)$$

$$\lambda_{wo} = 9.2939 \cdot 10^{-6}$$

$$\Lambda_w(Q,t) := \frac{\lambda_{wo} \cdot g_{hw\gamma} \cdot fQ_{w\gamma} \cdot Q}{\lambda_\gamma} \cdot \left(e^{-\lambda_\gamma t} - 1\right) + \frac{\lambda_{wo} \cdot g_{hw\beta} \cdot fQ_{w\beta} \cdot Q}{\lambda_\beta} \cdot \left(e^{-\lambda_\beta t} - 1\right) + \frac{\lambda_{wo} \cdot g_{hw\alpha} \cdot fQ_{w\alpha} \cdot Q}{\lambda_\alpha} \cdot \left(e^{-\lambda_\alpha t} - 1\right)$$

$$F_w(Q,t) := e^{\Lambda_w(Q,t)}$$

Fraction (mass or moles) U hydrate left as function of MCO power, time

$$F_w(396, 40) = 0.9225$$

Fraction left in average MCO after 40 years: 8% decomposition.

Derivative of fraction for H2 radiolysis rate:

$$dF_{hw}(Q,t) := -\lambda_{wo} \cdot g_{hw\gamma} \cdot fQ_{w\gamma} \cdot Q \cdot e^{-\lambda_\gamma t} - \lambda_{wo} \cdot g_{hw\beta} \cdot fQ_{w\beta} \cdot Q \cdot e^{-\lambda_\beta t} - \lambda_{wo} \cdot g_{hw\alpha} \cdot fQ_{w\alpha} \cdot Q \cdot e^{-\lambda_\alpha t}$$

$$dF_{hw}(396, 20) = -1.9866 \cdot 10^{-3}$$

About -0.2% per year implies 8% over 40 years O2 production from radiolysis of free H2O

$$dF_{ow}(Q,t) := -\lambda_{wo} \cdot g_{ow\gamma} \cdot fQ_{w\gamma} \cdot Q \cdot e^{-\lambda_\gamma t} - \lambda_{wo} \cdot g_{ow\beta} \cdot fQ_{w\beta} \cdot Q \cdot e^{-\lambda_\beta t} - \lambda_{wo} \cdot g_{ow\alpha} \cdot fQ_{w\alpha} \cdot Q \cdot e^{-\lambda_\alpha t}$$

2.2 FUNCTIONS FOR U GETTERING RATE AND WATER VAPOR PRESSURE
Water vapor pressure:

$$fP_{sat}(T) := e^{\left(25.339 - \frac{5154.7}{T}\right)}$$

$fP_{sat}(323) = 1.1851 \cdot 10^{4}$ 50 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/cm^2/hr, converted to grams O2 per m^2 per year.; McGillivray units of kg/m^2/s similarly converted.

$K_{rit}(T) := 10^{13.8808 - 5769.6 \cdot T^{-1}} \cdot 10 \cdot 876$ Ritchie

$K_{trim}(T) := 10^{7.19 - 3732 \cdot T^{-1}} \cdot 10 \cdot 876$ Trimble

$T_{cor} := (5769.6 - 3732) \cdot (13.8808 - 7.19)^{-1}$

$T_{cor} = 304.5376$

Switch correlations here

$fK_{o}(T) := if\left(T \geq T_{cor}, K_{rit}(T), K_{trim}(T)\right)$

$fK_{o}(323) \cdot 0.1 \cdot (8766)^{-1} = 1.0429 \cdot 10^{-4}$ OK @ 50 C in mg/cm^2/hr Shows no discontinuity

$fK_{o}(323) \cdot 10^{-3} \cdot \left(3.15 \cdot 10^{7}\right)^{-1} = 2.9024 \cdot 10^{-10}$ *OK @ 50 C in kg/m^2/s*

$fK_{o}\left(T_{cor} + 0.01\right) \cdot 10^{-3} \cdot \left(3.15 \cdot 10^{7}\right)^{-1} = 2.4014 \cdot 10^{-11}$

$fK_{o}\left(T_{cor} - 0.01\right) \cdot 10^{-3} \cdot \left(3.15 \cdot 10^{7}\right)^{-1} = 2.3958 \cdot 10^{-11}$

2.3 RELATIONSHIP BETWEEN MCO POWER AND GAS TEMPERATURE

For 396 W MCO, Conservative low temperature drops are:
13 C delta-T vault gas to Tube wall; 15 C across gap; 3 C to scrap average;
so hmax for delta-Tmin: 396 / (13+15+3) = 396 / 31 = 12.8. Conservative value is 13 W/K.
Min. Getter temperature, given MCO power, vault entrance

$$FTmin(Q_0,t) = \frac{Q_0 \cdot \exp(-\lambda_q \cdot t)}{13} + 12$$

2.4 HYDRATE PARTIAL DECOMPOSITION DETERMINES INITIAL PRESSURE, INVENTORY
*** Residual free water assumed to prevent UO3.2H2O decomposition ***
NOTE: Area used by these functions is fuel reactive area, NOT any additional getter area.

$$N_{wa}(m_{ah}) := 1.5 \cdot m_{ah} \cdot M_{ah}^{-1}$$

Aluminum hydroxide water moles
Function for moles of UO3.2HO plus UO4.2H2O givem m = kg/m^2 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.

$$n_{wu}(m, A, m_a) := \left[\mathrm{if}\left[(m \cdot A) > UH_{max}, UH_{max}, m \cdot A\right] + m_{uo4} \cdot \left(1 - \frac{m_a}{AL_{max}}\right)\right] \cdot \frac{1}{M_w}$$

$$N_{wu}(Q, A, m_a) := n_{wu}(m, A, m_a)$$

Hydrate moles - NO adjustment for thermal decomposition

$$N_{st}(Q) := \left| \begin{array}{l} T_o \leftarrow fTmin(Q, 0) + 273 \\ fP_{sat}(T_o) \cdot V_{mco} \cdot (8.314 T_o)^{-1} \end{array} \right.$$

Initial steam from free water, Assumed sufficient!

$$N_{fw} := m_{fw} \cdot M_w^{-1}$$

Initial free water moles, No adjustment for evaporation

2.5 FUNCTIONS FOR IRON GETTER

Parabolic kinetic rate law, Units are m^2/yr. Answer at 50 C is 1.9*10^-19 cm^2/s, or 6e-16 m^2/yr. If Mathcad says zero, then change 'zero tolerance' in menu

$$fK_{Fe}(T) := 3.15 \cdot 10^{7} \cdot 10^{-4} \cdot 5.56631 0^{-11} \cdot e^{-6295.6 \cdot T^{-1}}$$

$$fK_{Fe}(323) = 6.0122 \cdot 10^{-16}$$

Getter area, m^2, given current moles and net molar production rate

$$fA_{get}(n_{o2}, dn_{o2}, T) := 10^{-6} \cdot \frac{55.85}{7.8} \cdot \frac{3}{2} \cdot \sqrt{2 \cdot n_{o2} \cdot dn_{o2} \cdot fK_{Fe}(T)^{-1}}$$

3.0 FUNCTIONS FOR GAS EVOLUTION WITH TIME, MCO POWER, GETTER AREA, Al(OH)3:

3.1 H2+H2O: With no hydrogen gettering, H2 + H2O is a function of time until O2 runs out:

$$fN_{h2}(Q, A, m_a, t) := N_{st}(Q) + N_{wu}(Q, A, m_a) \cdot (1 - F_u(Q, t)) + N_{wa}(m_a) \cdot (1 - F_a(Q, t)) + N_{fw} \cdot (1 - F_w(Q, t))$$

3.2 O2: Oxygen gettering depends upon time-dependent MCO temperature, and must be integrated. 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.

$$
dO2dt(t,Y) := \left|
\begin{array}{l}
Q \leftarrow Y_0 \\
A \leftarrow Y_1 \\
m_a \leftarrow Y_2 \\
R \leftarrow Y_3 \\
Y_4 \leftarrow \mathrm{if}\left[\left(Y_4 < 0\right), 0, Y_4\right] \\
N_{o2} \leftarrow Y_4 \\
N_u \leftarrow N_{wu}\left(Q, A, m_a\right) \cdot F_u(Q,t) \\
N_a \leftarrow N_{wa}\left(m_a\right) \cdot F_a(Q,t) \\
N_w \leftarrow N_{fw} \cdot F_w(Q,t) \\
sorca \leftarrow -dF_{oa}(Q,t) \cdot N_a \\
sorcu \leftarrow -dF_{ou}(Q,t) \cdot N_u \\
sorcw \leftarrow -dF_{ow}(Q,t) \cdot N_w \\
T_{get} \leftarrow fTmin(Q,t) + 273 \\
sink \leftarrow (R \cdot A) \cdot fK_o\left(T_{get}\right) \cdot 32^{-1} \\
net \leftarrow sorca + sorcu + sorcw - sink \\
dO2dt \leftarrow \left|
\begin{array}{l}
net \ \ \mathrm{if} \ \left(N_{o2} > 0\right) + (net > 0) \\
0 \ \ \mathrm{otherwise}
\end{array}\right.
\end{array}\right.
$$

First, assign scrutable names to elements of Y:
Q = Power, A = Fuel Area, ma = Al(OH)3 mass,
R = Rate law multiplier, No2 = O2 moles

Make O2 moles > 0 for numerical purposes. Current UO3 hydrate, Al(OH)3, and free water moles
Current source rates from radiolysis
Current gettering rate by U surfaces
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). Definition of rate of change: Here the trick is used, dY/dt=0 for constants

$$F(t,Y) := (0 \ \ 0 \ \ 0 \ \ 0 \ \ dO2dt(t,Y))^T$$

Integrating function to just get O2 moles at t years:

Test function for average MCO, bound Al(OH)3:

$$fN_{o2}(Q, A, m_a, R, t) := \begin{vmatrix} Y \leftarrow \begin{bmatrix} Q & A & m_a & R & 30 \cdot 10^{-5} \end{bmatrix}^T \\ last \leftarrow t \\ Z \leftarrow Rkadapt(Y, 0, t, last, F) \\ \left(Z^{<5>}\right)_{last} \end{vmatrix}$$

$fN_{o2}(400, 1, 8000, 1, 40) = 0.3075$

$fN_{o2}(400, 2, 8000, 1, 40) = 7.4381 \cdot 10^{-3}$

Conclusion: Average MCO will NOT have oxygen buildup!

4.0 RESULTS: 8 AL(OH)3, 0.11 kg/m^2, RATE MULT=1, **2.5 atm total from He backfill**

$m_a = 8000$ Al(OH)3 bounding mass, grams

$R = 1.0$ Rate law multiplier

Parametric variation for various power and getter areas:
Power 10 to 770 W, general increments of 50 in the range,
Area up to 5 m^2 with 0.25 increments below 1.5

$Q = 16$ $Q_q := 50 \cdot q$ $Q_0 = 10$. $Q_{16} = 770$

The reactive surface area range is at 0, 0.005, 0.01, 0.025, 0.05, and 0.1 m^2

$a := 0..5$ $A := (0\ \ 0.005\ \ 0.01\ \ 0.025\ \ 0.05\ \ 0.1)^T$

Hydrogen: $nh2_{q,a} := fN_{h2}(Q_q, A_a, m_a, 40)$

Oxygen: $no2_{q,a} := fN_{o2}(Q_q, A_a, m_a, R, 40)$

Helium backfill: $P_{bf} = 2.5$

$$n_{he} := P_{bf} \cdot 10^5 \cdot V_{mco} \cdot (8.314 T_{bf})^{-1}$$

$$n_{he} = 50.4526$$

Functions for concentration and pressure:

$$ntot_{q,a} := n_{he} + no2_{q,a} + nh2_{q,a}$$

$$O2\%_{a,q} := no2_{q,a} \cdot \left(ntot_{q,a}\right)^{-1}$$

O2 Mass in grams

$$MO2_{a,q} := \left(\text{if}\left(no2_{q,a} > 0, no2_{q,a}, 0\right)\right) \cdot 3$$

$$O2\%_{a,q} := \text{if}\left(O2\%_{a,q} > 0, 100 \cdot O2\%_{a,q}, 0\right)$$

$$P_{a,q} := ntot_{q,a} \cdot 8.314 \left(fTmin\left(Q_q, 40\right) + 273\right) \cdot V_{mco}^{-1} \cdot 10^{-5}$$

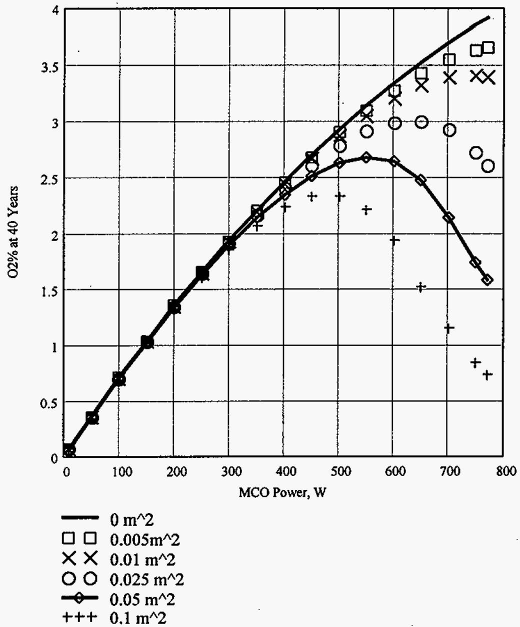
O2 Generation rate at time t, grams/year GIVEN calculation of no2 already (above) as an input:

$$fdn_{o2}\left(Q, A, m_a, R, A_{get}, no2, t\right) := \begin{vmatrix} Y \leftarrow \begin{bmatrix} Q & A & m_a & R & A_{get} & no2 \end{bmatrix}^T \\ dn \leftarrow dO2dt(t, Y) \end{vmatrix}$$

Required getter Area, m^2:

$$AFE_{a,q} := fA_{get}\left(\frac{MO2_{a,q}}{32}, fdn_{o2}\left(Q_q, A_a, m_a, R, 0, \frac{MO2_{a,q}}{32}, 40\right), fTmin\left(Q_q, 40\right) + 273\right)$$

Oxygen Percentage at 40 Years as a Function of MCO Power for Various Reactive Surface Areas, Case of: 8 kg Al(OH)3, 0.11 kg/m^2 water from UO3.2H2O, 200 g Free H2O, **BF Helium at 2.5 atm**



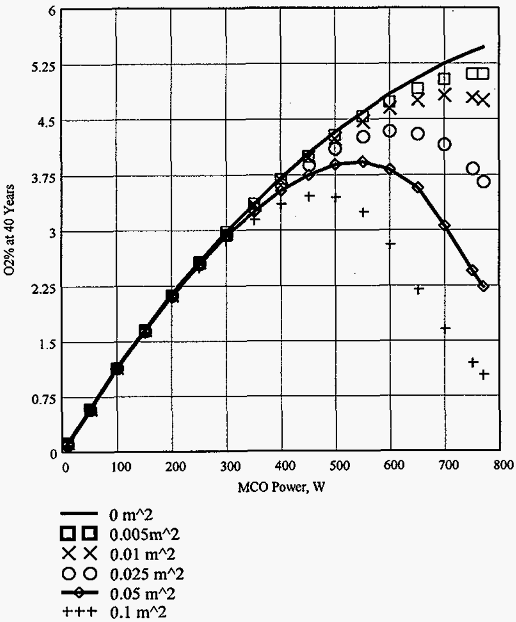
RESULTS : 8 kg AL(OH)3, 0.11 kg/m^2, RATE MULT = 1.0, **2.5 atm He BACKFILL**
Oxygen concentration as function of area, m^2 (row=constant A) and power, W (column=constant Q)

	Q	10	50	100	150	200	250	300	350	400	450	500	550	600	650	700	750	770
A																		
0		0.1	0.4	0.7	1	1.4	1.7	1.9	2.2	2.5	2.7	2.9	3.1	3.3	3.5	3.7	3.9	3.9
.005		0.1	0.4	0.7	1	1.4	1.6	1.9	2.2	2.4	2.7	2.9	3.1	3.3	3.4	3.5	3.6	3.7
.01		0.1	0.4	0.7	1	1.4	1.6	1.9	2.2	2.4	2.7	2.9	3.1	3.2	3.3	3.4	3.4	3.4
.025		0.1	0.4	0.7	1	1.3	1.6	1.9	2.2	2.4	2.6	2.8	2.9	3	3	2.9	2.7	2.6
.05		0.1	0.4	0.7	1	1.3	1.6	1.9	2.1	2.3	2.5	2.6	2.7	2.6	2.5	2.1	1.7	1.6
0.1		0	0.3	0.7	1	1.3	1.6	1.9	2.1	2.2	2.3	2.3	2.2	1.9	1.5	1.2	0.8	0.7

MCO Pressure (atm abs) Over 40 Years, A in units of m^2, Q in units of Watts

	Q	10	50	100	150	200	250	300	350	400	450	500	550	600	650	700	750	770
A																		
0		2.4	2.5	2.5	2.6	2.7	2.8	2.9	3	3.1	3.2	3.3	3.4	3.5	3.5	3.6	3.7	3.7
.005		2.4	2.5	2.5	2.6	2.7	2.8	2.9	3	3.1	3.2	3.3	3.4	3.5	3.5	3.6	3.7	3.7
.01		2.4	2.5	2.5	2.6	2.7	2.8	2.9	3	3.1	3.2	3.3	3.4	3.5	3.5	3.6	3.7	3.7
.025		2.4	2.5	2.5	2.6	2.7	2.8	2.9	3	3.1	3.2	3.3	3.4	3.5	3.5	3.6	3.7	3.7
.05		2.4	2.5	2.5	2.6	2.7	2.8	2.9	3	3.1	3.2	3.3	3.4	3.4	3.4	3.5	3.6	3.7
0.1		2.4	2.5	2.5	2.6	2.7	2.8	2.9	3	3.1	3.2	3.3	3.3	3.4	3.4	3.5	3.6	3.6

Oxygen Percentage at 40 Years as a Function of MCO Power for Various Reactive Surface Areas, Case of: 8 kg Al(OH)3, 0.11 kg/m^2 water from UO3.2H2O, 200 g Free H2O, **1.5 atm abs He Backfill**



4.0 RESULTS: 8 AL(OH)3, 0.11 kg/m^2, RATE MULT=1, **1.5 atm He BACKFILL**

$m_a := 0$ **Al(OH)3 no mass, grams**

$R = 1.0$ Rate law multiplier

Parametric variation for various power and getter areas:
Power 10 to 770 W, general increments of 50 in the range,
Area up to 5 m^2 with 0.25 increments below 1.5

$q = 0..16 \; Q_q := 50 \cdot q$ $Q_0 = 10$ $Q_{16} = 770$

$a := 0..5$ $A := (0\ \ 0.005\ \ 0.01\ \ 0.025\ \ 0.05\ \ 0.1)^T$

Hydrogen: $nh2_{q,a} := fN_{h2}(Q_q, A_a, m_a, 40)$

Oxygen: $no2_{q,a} := fN_{o2}(Q_q, A_a, m_a, R, 40)$

Helium backfill: $P_{bf} = 1.5$

$n_{he} := P_{bf} \cdot 10^5 \cdot V_{mco} \cdot (8.314 T_{bf})^{-1}$ $n_{he} = 30.2716$

Functions for concentration and pressure:

$ntot_{q,a} := n_{he} + no2_{q,a} + nh2_{q,a}$

$O2\%_{a,q} := no2_{q,a} \cdot (ntot_{q,a})^{-1}$

O2 Mass in grams

$MO2_{a,q} = (\text{if}(no2_{q,a} > 0, no2_{q,a}, 0)) \cdot 32$

$O2\%_{a,q} := \text{if}(O2\%_{a,q} > 0, 100 \cdot O2\%_{a,q}, 0)$

$P_{a,q} := ntot_{q,a} \cdot 8.314 \left(fTmin(Q_q, 40) + 273\right) \cdot V_{mco}^{-1} \cdot 10^{-5}$

O2 Generation rate at time t, grams/year GIVEN calculation of no2 already (above) as an input:

$$fdn_{o2}(Q, A, m_a, R, A_{get}, no2, t) := \left| \begin{array}{l} Y \leftarrow [Q\ \ A\ \ m_a\ \ R\ \ A_{get}\ \ no2]^T \\ dn \leftarrow dO2dt(t, Y) \end{array} \right.$$

Required getter Area, m^2:

$$AFE_{a,q} := fA_{get}\left(\frac{MO2_{a,q}}{32}, fdn_{o2}\left(Q_q, A_a, m_a, R, 0, \frac{MO2_{a,q}}{32}, 40\right), fTmin(Q_q, 40) + 273\right)$$

Oxygen Percentage at 40 Years as a Function of MCO Power for Various Reactive Surface Areas, Case of: **(KE fuel only) no Al(OH)3**, 0.11 kg/m^2 water from UO3.2H2O, 200 g Free H2O