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JMW 11/12/07

Maintained by Oleg Povetko

SCIENTIFIC NOTEBOOK

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INITIAL ENTRIES

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Project Title: Radionuclide Release Rates and Solubility Limits. Support Prelicensing Transition to License Application Review – ENG4 ISI

Participants: Oleg Povetko (OP), Alexei Kouznetsov (AK),(Independent Consultant, Calgary, Canada), Vladislav Golikov (VG),(Consultant, Federal Radiological Center, Institute of Radiation Hygiene, St. Petersburg, Russia)

Objective: document activities related to the analyses of generation of radiolytic species in waste packages at potential Yucca Mountain repository for postclosure period

Goal of Project
The goal of this project is to provide independent scoping evaluations for potential of radiolytic species generation inside failed waste packages. The species are generated in the radiation environment inside the waste package cavity in voids filled with air and water vapor.

08/08/2007 (OP)

I made literature search and identified the following DOE report pertinent to radiolysis species generation.
"Radiolytic Species Generation from Internal Waste Package Criticality, rev 00, 2001" . Initiated review of this document.

08/20/2007 (OP)

I initiated modeling of 21-PWR TAD WP for radiolysis studies.

08/24/2007 (AK) (OP)

Consultant conducted literature search on neutron and gamma radiolysis. He examined more thoroughly DOE AMR "Radiolytic Specie Generation from Internal Waste Package Criticality, CAL-EBS-NU-000017 REV 00", 2001.

Beginning of AK entry.

#08/22/2007
Examined literature on the neutron and gamma radiolysis:
"Radiolytic Specie Generation from Internal Waste Package Criticality, CAL-EBS-NU-000017 REV 00",

- Химические изменения, которые претерпевают некоторые материалы при облучении, известное как **радиолиз** или **радиолитическое разложение**, наблюдается, когда такие материалы, как пластмасса или резина, подвергаются **облучению**, что **приводит к образованию ряда новых химических соединений**.
- **Радиолиз** также вызывает усиленное выделение некоторых химических веществ, содержащихся в материалах отходов.
- Радиолиз воды и органических соединений вызывает образование водорода, а также других воспламеняющихся или токсичных химических веществ. Такое радиолитическое разложение является одним из основных источников опасности возникновения пожаров и/или взрывов в некоторых емкостях с высокоактивными отходами на предприятиях Хэнфорда и Саванна-Ривер-Сайт.
- От образования и накопления опасных химических веществ в результате радиолиза пострадали хранилище с плутонием в Роки-Флэтс и хранилища с ТРУ-отходами на ряде других объектов.
- Одной из причин было разложение изделий из пластмассы под действием радиолиза на воспламеняющиеся и токсичные газы.
- Фактически, радиолиз может сделать отходы со временем более опасными или сделать опасными отходы, первоначально неопасные.

Translation Follows ALW 6/12/09

- Radiation effects on the corrosion of metals and alloys include, among other things, radiolysis of the local gaseous and aqueous environment to produce both oxidizing and reducing radicals.

- Radiolysis processes in moist air environments lead to the fixation of nitrogen as NO, NO_2, and especially HNO_3 (Reed and Van Konynenburg 1988, pp. 393-404).
- Nitric acid is assumed to be the principal corrosive radiolytic chemical specie and is produced in an irradiated air-water vapor ystem when the hydroxyl radicals generated from the water vapor convert nitrogen dioxides, hat are formed by the radiolytic reaction between nitrogen and oxygen, to nitric acids.
- Radiolysis producing a local depression of the pH resulting in localized corrosion of cladding terial is included in the localized corrosion model as a special feature, YMP FEP NO. .1.02.15.00 (CRWMS M&O 2000d, Section 6.2.5).
- Zircaloy has excellent corrosion resistance to nitric acid and hydrogen peroxide, the concentration of these species can be enhanced by radiolysis during n internal WP criticality, potentially accelerating the corrosion effects in the cladding material.

The purpose of this calculation is to provide a detailed calculation the potential for generation of radiolytic species during a **postulated static criticality event in a WP**.

No new entries on this page

Radiolytic production of particular chemical species depends upon

- the radiation environment,
- the chemical components present, and
- the physical environment where the radiolytic reactions are occurring.

The yield of any given chemical species is characterized by a single parameter, "**G**", identified as the **G-factor** (Reed and Van Konynenburg 1991, pp. 1396-1403).

Definition:
The **"G" value** represents the number of molecules of a chemical species produced per **100 eV** of
absorbed radiation energy in the volume containing the irradiated environment.

Measurements of the **"G" factor** for production of **nitrogen dioxide** (one-to-one production ratio for nitric acid) from mixed neutron-gamma radiation range from approximately **0.5 to 2.5** molecules/100 eV of absorbed energy (Reed and Van Konynenburg 1991, p. 1399).

Assumption:

1. 21-pressurized water reactor (PWR) WP, containing commercial spent nuclear fuel (CSNF) assemblies, was assumed to have failed and subsequently partially filled with water
2. The steel basket structure was assumed to have fully degraded with the degradation products settling to the bottom of the WP
3. Hematite (Fe_2O_3) is assumed to be the only ironbearing degradation product formed from the original basket material (Assumption 3.1)
4. In a separate suite of evaluations, the contribution to the degradation product volume from diaspore generated by oxidized aluminum from the thermal shunt plates is also considered.
5. The packing fraction of the hematite, or the hematite-diaspore mixture, was assumed to be 0.58 (Assumption 3.2), with the remaining space filled with water.
6. For evaluations involving mixtures, complete reaction of the Fe and Al in the donating structures provides a mole fraction of 0.8439 (mass fraction = **0.9350**) for the hematite in the degradation product mixture material.
7. Degradation products were assumed to be present outside the fuel pins in assemblies below the degradation product-water mixture level, but not within the guide tube and instrument tube spaces of those assemblies.
8. The water level above the degradation product-water mixture was assumed to extend sufficiently high to maintain criticality, leaving an air-water vapor space at the top of the WP.
9. The radiant energy deposition in the air-water vapor space was calculated with the MCNP code (Briesmeister, 1997) using the KCODE option and tracking the transport of both neutron and gamma particles.
10. The gamma interactions include photon and electron processes leading to dissociation of the gas molecules and generation of nitric acids in the air-water vapor space.

Method

A series of these tallies have been specified in the MCNP input decks to obtain estimates for the following physical quantities:

1. Total, neutron, and gamma energy depositions, in MeV, in the moist air regions of the waste package
2. Average energy released per fission for the waste package
3. Average number of neutrons released per fission for the waste package
4. k_{eff} for each of the SNF regions: the fuel pins surrounded by degradation products (lower region), the fuel pins surrounded by water (middle region), and the fuel pins surrounded by moist air (top region) (see Figure 5.4 for region definition).

Information is collected for both gamma and neutron events using "f6" and "f4" tally types

No new entries on this page

3. ASSUMPTIONS

3.1 It is assumed that the steel in the basket assembly and fuel assembly end fittings is fully
degraded. Hematite (Fe_2O_3) and Diaspore (ALO(OH)) are assumed to be the only degradation products remaining from the steel internals. The rational for this assumption is that these minerals have a very low solubility whereas other degradation products with higher solubilities are more likely to be transported out of the WP. This minimizes the amount of neutron absorber materials in the WP which is conservative. This assumption is used in Sections 2 and 5.

3.2 It is assumed that the porosity of packed particles resulting from degradation of the steel
and aluminum internal structure of a 21 PWR WP is 42%. The rationale for this assumption is that measurements of the porosity of compacted granular materials (sand) was limited to approximately 42% before onset of container distortion (CRWMS M&O 1998b, p. 15). This assumption is used in Sections 2, 5, and 6.

3.3 It is assumed that the "G" factor for radiolytic production of nitric acid has the same value for neutron radiation as for gamma radiation. The rationale for this assumption is that radiolytic specie production is proportional to the absorbed energy rather than the effective dose. This assumption is used in Sections 2, 5, and 6.

3.4 It is assumed that the spacing between fuel assemblies in an asymmetric arrangement (resting on the WP) is 0.25 cm. The rationale for this assumption is that degradation products from the basket structure remaining between assemblies will prevent direct contact between assemblies This assumption is used in Sections 5 and 6.

3.5 It is assumed that the stainless steel inner shell of the WP is not degraded. The rationale
for this assumption is that it is conservative. Degradation products from the WP shell would increase the total volume of the hematite in the WP, thus decreasing the moist air space available for radiolytic reactions. This assumption is used in Sections 5 and 6.

3.6 It is assumed that the Babcock and Wilcox (B&W) Mark B 15x15 fuel design used for
this calculation is representative of the fuel types anticipated for potential disposition in the MGR. The basis for this assumption is this assembly type has been used for WP source term (CRWMS M&O 1999a, Section 3) and radiolysis calculations (BSC 2001b, Section 5.2). This assumption is used in Section 5.

3.7 It is assumed that the instrument tube in a B&W Mark B fuel assembly is the same length
as the fuel pins. The rationale for this assumption is that it is conservative allowing slightly more moderator within the assemblies immersed in the degradation products. This assumption is used in Section 5.

End of AK entry.

No new entries on this page

09/03/2007

In order to develop MCNP model I initiated the following working files containing all current collected information necessary for model building.

a-h.i
fuel_comp.xls
21-PWR-EDAII-A-0914_cor.xls
deg_comp.xls

No new entries on this page

10/01/2007 (AK)(OP)

#09/12/07
Obtained, examined and analyzed data on relative humidity, WP and drift wall temperatures available from TPA output, CNWRA reports and ACNW presentations.
Extracted necessary data from physics handbooks.
Performed calculations to determine water vapor parameters. Data is needed as MCNP model input.

Waste package drift wall temperatures and vapour pressures and densities

Table 09/12/07-1. Drift Wall Temperatures

Time[yr]	0.5	Mean
...		
8.56430E+01	1.46320E+02	1.46560E+02
8.99580E+01	1.46120E+02	1.46360E+02
9.43740E+01	1.45730E+02	1.45970E+02
9.88940E+01	1.45200E+02	1.45430E+02
1.03520E+02	1.40570E+02	1.40790E+02
1.08250E+02	1.38910E+02	1.39130E+02
...		
4.48250E+02	1.17840E+02	1.17980E+02
4.61060E+02	1.17450E+02	1.17590E+02
4.74160E+02	1.17060E+02	1.17200E+02
4.87570E+02	1.16610E+02	1.16750E+02
5.01300E+02	1.16110E+02	1.16250E+02
5.15350E+02	1.15590E+02	1.15730E+02
...		
1.85430E+03	7.99960E+01	8.01100E+01
1.90000E+03	7.91490E+01	7.92620E+01
1.94680E+03	7.83050E+01	7.84180E+01
1.99470E+03	7.74770E+01	7.75900E+01
2.04370E+03	7.66960E+01	7.68090E+01
2.09390E+03	7.59460E+01	7.60590E+01
...		
9.76900E+03	4.56260E+01	4.56950E+01
1.00000E+04	4.53450E+01	4.54140E+01
1.04500E+04	4.47640E+01	4.48310E+01
...		
1.00000E+05	2.51610E+01	2.51670E+01

Interpolation to 100 Years:

0.5	Mean
1.44093E+02	1.44321E+02

Interpolation to 500 Years:

0.5	Mean
1.16157E+02	1.16297E+02

Interpolation to 2000 Years:

0.5	Mean
7.73925E+01	7.75055E+01

(See SN September 2007 Radiolysis.xls, Sheet "drift wall temperature")

No new entries on this page

Table 09/12/07-2. Table 16. Drift Wall Temperatures and Correspondence Vapour Pressures and Densities

Time	Drift Wall temperature	X	Vapour Pressure*	Vapour Density**
Years	centigrades	x = 1.0 - (t+273.0)/647.3	Pa==n/m^2	g/cm^3
100	144.0930437	0.35564183	4.03886E+05	0.020795827
500	116.1573416	0.398799102	1.74788E+05	0.009645758
2,000	77.39252449	0.458686043	4.23425E+04	0.002595206
10,000	45.345	0.508195582	9.69178E+03	0.000653816
100,000	25.161	0.539377414	3.17352E+03	0.000228581

*Vapor Pressure= 221.2E+5 *exp((vpa * x +vpb * x**(1.5) + vpc * x**3 +vpd * x**6)/ (1 - x))
Vpa = - 7.76451;
Vpb = 1.45838;
Vpc = - 2.7758;
Vpd = - 1.23303;

** Vapor Density= $P * \mu / R / T$;
Where:
μ = 17.8559 (for H_2O)
R = 831,441 ± 0,00026 [Дж/(моль·К]

(See SN September 2007 Radiolysis.doc, Sheet "Radiolise Results")

No new entries on this page

#09/15/07
Developed ORIGEN-ARP depletion model based on South Texas reactor campaigr based on data avalaible from "PWR Source Term Generation and Evaluation , Rev 0B, 2004" AMR

I. Assembly Type and its Operating Parameters

Source:	*PWR Source Term Generation and Evaluation*
Document Identifier	*000-00C-MGR0-00100-000-00B*
Pages:	*Page 24 of 33*

The moderator temperature	578	K
Density of the moderator	0.7136	g/cm^3
Input average boron concentration	552.6316	ppm

Operational history of the assembly in the reactorone cycle and new libraries at least every 100 days

Thermal Reactor Power	2568	MWt
Assemblies in a core	177	
Power/Assembly	14.50847	MWt
MTU per Assembly	0.46363	MTU
Enrichement	5%	
Assembly	15 × 15 for Babcock & Wilcox and	
BurnUp	78.25865 GWd/MTU	
BurnUp Days	2500.818	days

Fuel Type is selected from the list of fuel types and is input for all compositions listed on the first composition screen.

The fuel assembly types include:

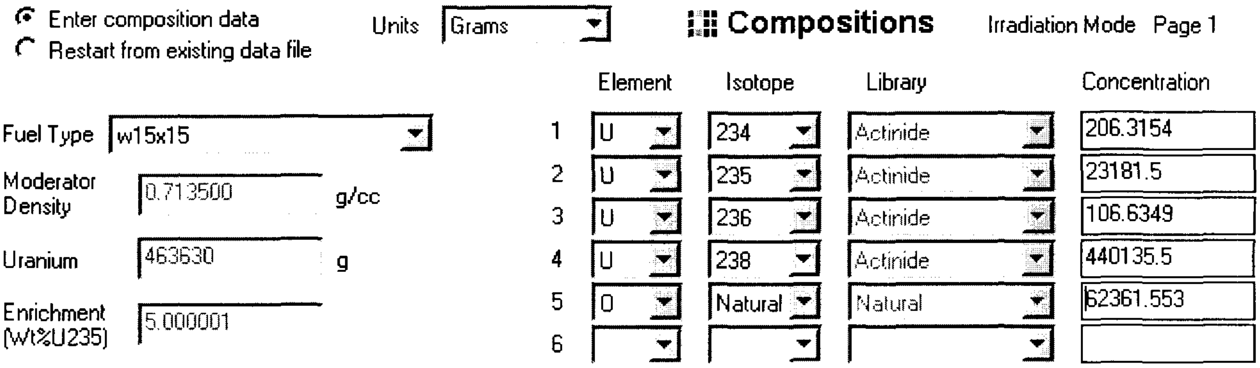
8 × 8 (for BWR fuel),PWR fuel).
14 × 14 (for ABB Combustion Engineering–type PWR fuel with large water holes)
w15x15 15 × 15 for Babcock & Wilcox and
17 × 17 - Westinghouse–type

No new entries on this page

#09/16/07
Performed ORIGEN-ARP calculations to determine gamma and neutron sources inside WP for 5-100,000 years for maximum CSNF assembly. Documented results. Data is needed as MCNP model input

II. OrigenARP Input and Output Parameters

II.1 Compositions:



Enter composition data
Restart from existing data file

Units: Grams

Compositions — Irradiation Mode — Page 1

Fuel Type: w15x15
Moderator Density: 0.713500 g/cc
Uranium: 463630 g
Enrichment (Wt%U235): 5.000001

	Element	Isotope	Library	Concentration
1	U	234	Actinide	206.3154
2	U	235	Actinide	23181.5
3	U	236	Actinide	106.6349
4	U	238	Actinide	440135.5
5	O	Natural	Natural	62361.553
6				

No new entries on this page

II.2 Input Summary:

Number of Isotopes = 5
Input Option = Entering data using form
Input Units = grams

Library: w15x15
Enrichment Factor (Wt%U235) = 5.000001
Moderator Density (g/cc) = 0.713500

Nuclide	ID	Library	Concentration
U 234	922340	Actinide	206.315400
U 235	922350	Actinide	23181.500000
U 236	922360	Actinide	106.634900
U 238	922380	Actinide	440135.500000
O	80000	Natural	62361.553000

Neutron Group = 44GrpENDF5
Number of groups = 44

2.0000000e+007	8.1873000e+006	6.4340000e+006	4.8000000e+006	3.0000000e+006
2.4790000e+006	2.3540000e+006	1.8500000e+006	1.4000000e+006	9.0000000e+005
4.0000000e+005	1.0000000e+005	2.5000000e+004	1.7000000e+004	3.0000000e+003
5.5000000e+002	1.0000000e+002	3.0000000e+001	1.0000000e+001	8.1000000e+000
6.0000000e+000	4.7500000e+000	3.0000000e+000	1.7700000e+000	1.0000000e+000
6.2500000e-001	4.0000000e-001	3.7500000e-001	3.5000000e-001	3.2500000e-001
2.7500000e-001	2.5000000e-001	2.2500000e-001	2.0000000e-001	1.5000000e-001
1.0000000e-001	7.0000000e-002	5.0000000e-002	4.0000000e-002	3.0000000e-002
2.5300000e-002	1.0000000e-002	7.5000000e-003	3.0000000e-003	1.0000000e-005

Gamma Group = 44GrpENDF5
Number of groups = 44

2.0000000e+007	1.4000000e+007	1.2000000e+007	1.0000000e+007	8.0000000e+006
7.5000000e+006	7.0000000e+006	6.5000000e+006	6.0000000e+006	5.5000000e+006
5.0000000e+006	4.5000000e+006	4.0000000e+006	3.5000000e+006	3.0000000e+006
2.5000000e+006	2.3499990e+006	2.1499990e+006	2.0000000e+006	1.7999990e+006
1.6599990e+006	1.5699990e+006	1.5000000e+006	1.4399990e+006	1.3299990e+006
1.1999990e+006	1.0000000e+006	7.9999990e+005	6.9999990e+005	5.9999990e+005
5.1199990e+005	5.0999990e+005	4.4999990e+005	3.9999990e+005	2.9999990e+005
1.9999990e+005	1.4999990e+005	9.9999940e+004	7.4999940e+004	6.9999940e+004
6.0000000e+004	4.5000000e+004	3.0000000e+004	2.0000000e+004	9.9999960e+003

Number of cases = 8

No new entries on this page

```
Case Number #1  -- Irradiation
====================================================

Title: Case: 0-1000 days
Basis: 0.46363 MTU


Time units  =      Days

OUTPUT OPTIONS

Tables = Nuclides

Output:

      Light Elements
      Actinides
      Fission Products

Output units = grams
Table cutoff = 0.000010

Power                Cumulative     Write Results
MW/Basis                Time         to Dataset
=======              =========      =============
1.4508470e+001       1.0000000e+002     No
1.4508470e+001       2.0000000e+002     No
1.4508470e+001       3.0000000e+002     No
1.4508470e+001       4.0000000e+002     No
1.4508470e+001       5.0000000e+002     No
1.4508470e+001       6.0000000e+002     No
1.4508470e+001       7.0000000e+002     No
1.4508470e+001       8.0000000e+002     No
1.4508470e+001       9.0000000e+002     No
1.4508470e+001       1.0000000e+003     Yes
```

No new entries on this page

Case Number #2 -- Irradiation
==

Title: case 1000 - 2000 days
Basis: 0.46363 MTU

Time units = Days

OUTPUT OPTIONS

Tables = Nuclides

Output:

Light Elements
Actinides
Fission Products

Output units = grams
Table cutoff = 0.000010

Power MW/Basis	Cumulative Time	Write Results to Dataset
1.4508470e+001	1.0000000e+002	No
1.4508470e+001	2.0000000e+002	No
1.4508470e+001	3.0000000e+002	No
1.4508470e+001	4.0000000e+002	No
1.4508470e+001	5.0000000e+002	No
1.4508470e+001	6.0000000e+002	No
1.4508470e+001	7.0000000e+002	No
1.4508470e+001	8.0000000e+002	No
1.4508470e+001	9.0000000e+002	No
1.4508470e+001	1.0000000e+003	Yes

No new entries on this page

```
Case Number #3  -- Irradiation
====================================================

Title: 3 case 2000 - 2556.464
Basis: 0.46363 MTU


Time units  =       Days

OUTPUT OPTIONS

Tables = Nuclides

Output:

      Light Elements
      Actinides
      Fission Products

Output units = grams
Table cutoff = 0.000010

Power               Cumulative     Write Results
MW/Basis               Time         to Dataset
=======             =========      =============
1.4508470e+001      5.5646400e+001     No
1.4508470e+001      1.1129280e+002     No
1.4508470e+001      1.6693920e+002     No
1.4508470e+001      2.2258560e+002     No
1.4508470e+001      2.7823200e+002     No
1.4508470e+001      3.3387840e+002     No
1.4508470e+001      3.8952480e+002     No
1.4508470e+001      4.4517120e+002     No
1.4508470e+001      5.0081760e+002     No
```

No new entries on this page

Case Number #4 -- Decay
==

Title: 100 Years
Basis: 0.46363 MTU

Beginning time	=	0.000000
Time units	=	Years
Neutron source	=	UO2
Bremsstrahlung	=	UO2
Library Type	=	Total

Output Options:
No output is requested for this case.

Cumulative Time	Source Spectra	Save Results
1.0000000e-001	No	No
3.0000000e-001	No	No
1.0000000e+000	No	No
3.0000000e+000	No	No
1.0000000e+001	No	No
3.0000000e+001	No	No
1.0000000e+002	Yes	Yes

Case Number #5 -- Decay
==

Title: 500 Years
Basis: 0.46363 MTU

Beginning time	=	100.000000
Time units	=	Years
Neutron source	=	UO2
Bremsstrahlung	=	UO2
Library Type	=	Total

Output Options:
No output is requested for this case.

Cumulative Time	Source Spectra	Save Results
3.0000000e+002	No	No
5.0000000e+002	Yes	Yes

No new entries on this page

```
Case Number #6  -- Decay
====================================================

Title: 2000 Years
Basis: 0.46363 MTU

Beginning time      =   500.000000
Time units          =   Years
Neutron source      =   UO2
Bremsstrahlung      =   UO2
Library Type        =   Total

Output Options:
No output is requested for this case.

Cumulative Time     Source Spectra     Save Results
===============     ==============     ============
1.0000000e+003           No                No
2.0000000e+003           Yes               Yes

Case Number #7  -- Decay
====================================================

Title: 10000 Years
Basis: 0.46363 MTU

Beginning time      =   2000.000000
Time units          =   Years
Neutron source      =   UO2
Bremsstrahlung      =   UO2
Library Type        =   Total

Output Options:
No output is requested for this case.

Cumulative Time     Source Spectra     Save Results
===============     ==============     ============
3.0000000e+003           No                No
1.0000000e+004           Yes               Yes

Case Number #8  -- Decay
====================================================

Title: 100000 Years
Basis: 0.46363 MTU

Beginning time      =   10000.000000
Time units          =   Years
Neutron source      =   UO2
Bremsstrahlung      =   UO2
Library Type        =   Total

Output Options:
No output is requested for this case.

Cumulative Time     Source Spectra     Save Results
===============     ==============     ============
3.0000000e+004           No                No
1.0000000e+005           Yes               Yes
```

No new entries on this page

II.3 OrigenARP Input/Output Data:

Origen ARP\PWR_P14.inp – Input file;
Origen ARP\PWR_P14.out – Output File;

Table 09/16/07-1. OrigenARP output data for 100 years down (case 4)

	Scale ID	Nuclide/ A.W.	Years MCNP ID	100 Y (g/basis)	at/cm^3
light elements					
	O	15.8575	8016.62c	6.23600E+04	1.24296E-02
actinides					
	u235	233.025	92235.66c	1.54300E+03	2.09290E-05
	u236	234.018	92236.66c	3.37800E+03	4.56243E-05
	u238	236.006	92238.66c	4.13700E+05	5.54049E-03
	np237	235.0118	93237.66c	6.52800E+02	8.77962E-06
	pu238	236.0045	94238.66c	1.75400E+02	2.34906E-06
	pu239	236.9986	94239.66c	2.84000E+03	3.78755E-05
	pu240	237.992	94240.66c	1.80800E+03	2.40116E-05
	pu241	238.978	94241.66c	7.52300E+00	9.94990E-08
	pu242	239.979	94242.66c	7.75500E+02	1.02140E-05
	am243	240.9734	95243.66c	2.81900E+02	3.69753E-06
fission products					
34	se 82			3.42300E+01	
35	br 81	80.2212	35081.55c	2.09100E+01	8.23854E-07
36	kr 83	82.2018	36083.66c	3.19800E+01	1.22965E-06
36	kr 84	83.1906	36084.66c	1.26700E+02	4.81380E-06
36	kr 85			3.36900E-02	
36	kr 86	85.1726	36086.66c	1.81134E+02	6.72179E-06
37	rb 85	84.1824	37085.66c	1.21400E+02	4.55809E-06
37	rb 87	86.1624	37087.66c	2.43300E+02	8.92503E-06
38	sr 88			3.35200E+02	
38	sr 90			4.26300E+01	
39	y 89	88.142	39089.66c	4.46000E+02	1.59933E-05
40	zr 90	89.132	40090.66c	5.09200E+02	1.80568E-05
40	zr 91	90.122	40091.66c	5.92100E+02	2.07658E-05
40	zr 92	91.112	40092.66c	6.55400E+02	2.27361E-05
40	zr 93	92.1083	40093.66c	7.10600E+02	2.43844E-05
40	zr 94	93.096	40094.66c	8.10900E+02	2.75310E-05
40	zr 96	95.081	40096.66c	8.47100E+02	2.81596E-05
42	mo 95			7.40900E+02	
42	mo 96			9.38900E+01	
42	mo 97			8.58900E+02	
42	mo 98			8.95400E+02	
42	mo100	95.116	42000.66c	3.61009E+03	1.19964E-04
43	tc 99	98.15	43099.66c	7.53700E+02	2.42713E-05
44	ru100			2.23700E+02	
44	ru101	100.039	44101.50c	3.04880E+03	9.63263E-05
44	ru102			9.45200E+02	
44	ru104			6.75900E+02	
44	ru106			2.99900E-28	

45	rh103	102.021	45103.66c	3.84200E+02	1.19029E-05
46	pd104	103.0114	46104.66c	4.37000E+02	1.34085E-05
46	pd105	104.0039	46105.66c	4.83500E+02	1.46937E-05
46	pd106	104.9937	46106.66c	5.02300E+02	1.51212E-05
46	pd107			2.88300E+02	
46	pd108	106.9769	46108.66c	4.78800E+02	1.41465E-05
46	pd110	108.961	46110.66c	6.55800E+01	1.90233E-06
47	ag109	107.969	47109.66c	8.96600E+01	2.62473E-06
48	cd110	108.959	48110.66c	8.36200E+01	2.42567E-06
48	cd111	109.952	48111.66c	3.27400E+01	9.41154E-07
50	sn126	117.6704	50000.42c	2.17200E+01	5.83415E-07
52	te128			9.82700E+01	
52	te130			4.13100E+02	
53	i127	125.8143	53127.66c	4.94100E+01	1.24128E-06
53	i129	127.798	53129.60c	1.69900E+02	4.20199E-06
54	xe131	129.781	54131.66c	3.14400E+02	7.65697E-06
54	xe132	130.771	54132.66c	1.37300E+03	3.31852E-05
54	xe134	132.755	54134.66c	1.66300E+03	3.95938E-05
54	xe136	134.74	54136.66c	2.44800E+03	5.74249E-05
55	cs133	131.764	55133.66c	1.07100E+03	2.56908E-05
55	cs135	133.747	55135.60c	5.16700E+02	1.22107E-05
55	cs137	135.731	55137.60c	1.26700E+02	2.95041E-06
56	ba134			3.09400E+02	
56	ba136			5.93700E+01	
56	ba137			1.25400E+03	
56	ba138	136.715	56138.66c	3.02877E+03	7.00222E-05
57	la139			1.29600E+03	
58	ce140			1.36300E+03	
58	ce142			1.19300E+03	
59	pr141	139.697	59141.50c	1.17600E+03	2.66076E-05
60	nd142			4.84000E+01	
60	nd143	141.682	60143.50c	6.59100E+02	1.47035E-05
60	nd144			1.61900E+03	
60	nd145	143.668	60145.50c	2.24300E+03	4.93463E-05
60	nd146			8.48900E+02	
60	nd148	146.646	60148.50c	1.44610E+03	3.11683E-05
60	nd150			2.01500E+02	
61	pm147	145.653	61147.50c	3.01400E-10	6.54047E-18
62	sm147	145.653	62147.66c	1.65200E+02	3.58489E-06
62	sm148			2.18500E+02	
62	sm150	148.629	62150.50c	5.19000E+02	1.10370E-05
62	sm152	150.615	62152.50c	1.54410E+02	3.24035E-06
62	sm154			4.43100E+01	
63	eu153	151.608	63153.66c	1.31100E+02	2.73317E-06
63	eu154	152.6	63154.66c	9.98400E-03	2.06793E-10
64	gd156	154.583	64156.66c	2.01000E+02	4.10979E-06
64	gd158	156.567	64158.66c	3.89000E+01	7.85298E-07

No new entries on this page

Table 09/16/07-2. OrigenARP output data for 500 years down (case 5)

Scale ID	Nuclide/ A.W.	Years MCNP ID	500 Y (g/basis)	at/cm^3
O	15.8575	8016.62c	6.23600E+04	1.24296E-02
u234	232.03	92234.66c	4.41E+02	6.00322E-06
u235	233.025	92235.66c	1.58E+03	2.13631E-05
u236	234.018	92236.66c	3.45E+03	4.66102E-05
u238	236.006	92238.66c	4.14E+05	5.54049E-03
np237	235.0118	93237.66c	1.06E+03	1.41889E-05
pu239	236.9986	94239.66c	2.82E+03	3.75821E-05
pu240	237.992	94240.66c	1.74E+03	2.30687E-05
pu242	239.979	94242.66c	7.75E+02	1.02100E-05
am241	238.986	95241.66c	4.56E+02	6.02555E-06
am243	240.9734	95243.66c	2.72E+02	3.56112E-06
br 81	80.2212	35081.55c	2.09E+01	8.23854E-07
se 82			3.42E+01	
kr 83	82.2018	36083.66c	3.20E+01	1.22965E-06
kr 84	83.1906	36084.66c	1.27E+02	4.81380E-06
rb 85	84.1824	37085.66c	1.21E+02	4.55809E-06
kr 86	85.1726	36086.66c	1.81E+02	6.72054E-06
rb 87	86.1624	37087.66c	2.43E+02	8.92503E-06
sr 88	88	37087.66c	3.35E+02	1.20395E-05
y 89	88.142	39089.66c	4.46E+02	1.59933E-05
zr 90	89.132	40090.66c	5.52E+02	1.95674E-05
zr 91	90.122	40091.66c	5.92E+02	2.07658E-05
zr 92	91.112	40092.66c	6.55E+02	2.27361E-05
zr 93	92.1083	40093.66c	7.11E+02	2.43810E-05
zr 94	93.096	40094.66c	8.11E+02	2.75310E-05
mo 95			7.41E+02	
zr 96	95.081	40096.66c	8.47E+02	2.81596E-05
mo 96			9.39E+01	
mo 97			8.59E+02	
mo 98			8.95E+02	
tc 99	98.15	43099.66c	7.53E+02	2.42391E-05
mo100	95.116	42000.66c	3.61E+03	1.19964E-04
ru100			2.24E+02	
ru101	100.039	44101.50c	1.04E+03	3.29692E-05
ru102			9.45E+02	
ru103	102.022	44103.50c	2.01E+03	6.21256E-05
ru104			6.76E+02	
pd104	103.0114	46104.66c	4.37E+02	1.34085E-05
pd105	104.0039	46105.66c	4.84E+02	1.46937E-05
pd106	104.9937	46106.66c	5.02E+02	1.51212E-05
pd107			2.88E+02	
pd108	106.9769	46108.66c	4.79E+02	1.41465E-05
ag109	107.969	47109.66c	8.97E+01	2.62473E-06
pd110	108.961	46110.66c	6.56E+01	1.90233E-06

cd110	108.959	48110.66c	8.36E+01	2.42567E-06
cd111	109.952	48111.66c	3.27E+01	9.41154E-07
sn126	117.6704	50000.42c	2.17E+01	5.81804E-07
i127	125.8143	53127.66c	4.94E+01	1.24128E-06
te128			9.83E+01	
i129	127.798	53129.60c	1.70E+02	4.20199E-06
te130			4.13E+02	
xe131	129.781	54131.66c	3.14E+02	7.65697E-06
xe132	130.771	54132.66c	1.37E+03	3.31852E-05
cs133	131.764	55133.66c	1.07E+03	2.56908E-05
xe134	132.755	54134.66c	1.66E+03	3.95938E-05
ba134			3.09E+02	
cs135	133.747	55135.60c	5.17E+02	1.22083E-05
xe136	134.74	54136.66c	2.45E+03	5.74249E-05
ba136			5.94E+01	
ba137			1.38E+03	
ba138	136.715	56138.66c	3.16E+03	7.29583E-05
la139			1.30E+03	
ce140			1.36E+03	
pr141	139.697	59141.50c	1.18E+03	2.66076E-05
ce142			1.19E+03	
nd142			4.84E+01	
nd143	141.682	60143.50c	6.59E+02	1.47035E-05
nd144			1.62E+03	
nd145	143.668	60145.50c	3.09E+03	
nd146			8.49E+02	
sm147	145.653	62147.66c	1.65E+02	3.58489E-06
nd148	146.646	60148.50c	3.96E+02	8.52867E-06
sm148			2.19E+02	
nd150			2.02E+02	
sm150	148.629	62150.50c	5.19E+02	1.10370E-05
sm152	150.615	62152.50c	1.10E+02	2.31049E-06
eu153	151.608	63153.66c	1.75E+02	3.65694E-06
sm154			4.43E+01	
gd154	152.599	64154.66c	3.78E+01	7.83556E-07
gd156	154.583	64156.66c	2.01E+02	4.10979E-06
gd158	156.567	64158.66c	3.89E+01	7.85298E-07

No new entries on this page

Table 09/16/07-3. OrigenARP output data for 2000 years down (case 6)

Scale ID	Nuclide/ A.W.	Years MCNP ID	2000 Y (g/basis)	at/cm^3
O	15.8575	8016.62c	6.23600E+04	1.24296E-02
u234	232.03	92234.66c	4.46E+02	6.08087E-06
u235	233.025	92235.66c	1.69E+03	2.29636E-05
u236	234.018	92236.66c	3.70E+03	4.99868E-05
u238	236.006	92238.66c	4.14E+05	5.54049E-03
np237	235.0118	93237.66c	1.46E+03	1.96761E-05
pu239	236.9986	94239.66c	2.73E+03	3.64485E-05
pu240	237.992	94240.66c	1.48E+03	1.96954E-05
pu242	239.979	94242.66c	7.74E+02	1.01876E-05
am243	240.9734	95243.66c	2.36E+02	3.09286E-06
se 82			3.42E+01	
br 81	80.2212	35081.55c	2.09E+01	8.23854E-07
kr 83	82.2018	36083.66c	3.20E+01	1.22965E-06
kr 84	83.1906	36084.66c	1.27E+02	4.81380E-06
kr 86	85.1726	36086.66c	1.81E+02	6.72054E-06
rb 85	84.1824	37085.66c	1.21E+02	4.55809E-06
rb 87	86.1624	37087.66c	2.43E+02	8.92503E-06
sr 88	88	37087.66c	3.35E+02	1.20395E-05
y 89	88.142	39089.66c	4.46E+02	1.59933E-05
zr 90	89.132	40090.66c	5.52E+02	1.95674E-05
zr 91	90.122	40091.66c	5.92E+02	2.07658E-05
zr 92	91.112	40092.66c	6.55E+02	2.27361E-05
zr 93	92.1083	40093.66c	7.10E+02	2.43638E-05
zr 94	93.096	40094.66c	8.11E+02	2.75310E-05
zr 96	95.081	40096.66c	8.47E+02	2.81596E-05
mo 95			7.41E+02	
mo 96			9.39E+01	
mo 97			8.59E+02	
mo 98			8.95E+02	
mo100	95.116	42000.66c	3.61E+03	1.19964E-04
tc 99	98.15	43099.66c	7.49E+02	2.41200E-05
ru100			2.24E+02	
ru101	100.039	44101.50c	1.04E+03	3.29692E-05
ru102			9.45E+02	
ru103	102.022	44103.50c	2.01E+03	6.21256E-05
ru104			6.76E+02	
pd104	103.0114	46104.66c	4.37E+02	1.34085E-05
pd105	104.0039	46105.66c	4.84E+02	1.46937E-05
pd106	104.9937	46106.66c	5.02E+02	1.51212E-05
pd107			2.88E+02	
pd108	106.9769	46108.66c	4.79E+02	1.41436E-05
pd110	108.961	46110.66c	6.56E+01	1.90233E-06
ag109	107.969	47109.66c	8.97E+01	2.62473E-06

cd110	108.959	48110.66c	8.36E+01	2.42567E-06
cd111	109.952	48111.66c	3.27E+01	9.41154E-07
sn126	117.6704	50000.42c	2.14E+01	5.75894E-07
te128			9.83E+01	
te130			4.13E+02	
i127	125.8143	53127.66c	4.94E+01	1.24128E-06
i129	127.798	53129.60c	1.70E+02	4.20199E-06
xe131	129.781	54131.66c	3.14E+02	7.65697E-06
xe132	130.771	54132.66c	1.37E+03	3.31852E-05
xe134	132.755	54134.66c	1.66E+03	3.95938E-05
xe136	134.74	54136.66c	2.45E+03	5.74249E-05
cs133	131.764	55133.66c	1.07E+03	2.56908E-05
cs135	133.747	55135.60c	5.16E+02	1.22036E-05
ba134			3.09E+02	
ba136			5.94E+01	
ba137			1.38E+03	
ba138	136.715	56138.66c	3.16E+03	7.29583E-05
la139			1.30E+03	
ce140			1.36E+03	
ce142			1.19E+03	
pr141	139.697	59141.50c	1.18E+03	2.66076E-05
nd142			4.84E+01	
nd143	141.682	60143.50c	6.59E+02	1.47035E-05
nd144			1.62E+03	
nd145	143.668	60145.50c	2.24E+03	4.93463E-05
nd146			8.49E+02	
nd148	146.646	60148.50c	1.45E+03	3.11683E-05
nd150			2.02E+02	
sm147	145.653	62147.66c	1.65E+02	3.58489E-06
sm148			2.19E+02	
sm150	148.629	62150.50c	5.19E+02	1.10370E-05
sm152	150.615	62152.50c	1.54E+02	3.24035E-06
sm154			4.43E+01	
eu153	151.608	63153.66c	1.31E+02	2.73317E-06
gd154	152.599	64154.66c	3.78E+01	7.83556E-07
gd156	154.583	64156.66c	2.01E+02	4.10979E-06
gd158	156.567	64158.66c	3.89E+01	7.85298E-07

No new entries on this page

Table 09/16/07-4. OrigenARP output data for 10000 years down (case 7)

Scale ID	Nuclide/ A.W.	Years MCNP ID	(g/basis)	10,000 Y at/cm^3
O	15.8575	8016.62c	6.24E+04	1.24296E-02
u234	232.03	92234.66c	4.37E+02	5.95146E-06
u235	233.025	92235.66c	2.26E+03	3.06407E-05
u236	234.018	92236.66c	4.53E+03	6.12105E-05
u238	236.006	92238.66c	4.14E+05	5.54049E-03
np237	235.0118	93237.66c	1.50E+03	2.02276E-05
pu239	236.9986	94239.66c	2.28E+03	3.03937E-05
pu240	237.992	94240.66c	6.37E+02	8.45719E-06
pu242	239.979	94242.66c	7.64E+02	1.00572E-05
am243	240.9734	95243.66c	1.11E+02	1.45724E-06
se 82			3.42E+01	
br 81	80.2212	35081.55c	2.09E+01	8.23854E-07
kr 83	82.2018	36083.66c	3.20E+01	1.22965E-06
kr 84	83.1906	36084.66c	1.27E+02	4.81380E-06
kr 86	85.1726	36086.66c	1.81E+02	6.72054E-06
rb 85	84.1824	37085.66c	1.21E+02	4.55809E-06
rb 87	86.1624	37087.66c	2.43E+02	8.92503E-06
sr 88	88	37087.66c	3.35E+02	1.20395E-05
y 89	88.142	39089.66c	4.46E+02	1.59933E-05
zr 90	89.132	40090.66c	5.52E+02	1.95674E-05
zr 91	90.122	40091.66c	5.92E+02	2.07658E-05
zr 92	91.112	40092.66c	6.55E+02	2.27361E-05
zr 93	92.1083	40093.66c	7.08E+02	2.42780E-05
zr 94	93.096	40094.66c	8.11E+02	2.75310E-05
zr 96	95.081	40096.66c	8.47E+02	2.81596E-05
mo 95			7.41E+02	
mo 96			9.39E+01	
mo 97			8.59E+02	
mo 98			8.95E+02	
mo100	95.116	42000.66c	3.61E+03	1.19964E-04
tc 99	98.15	43099.66c	7.30E+02	2.34952E-05
ru100			2.24E+02	
ru101	100.039	44101.50c	1.04E+03	3.29692E-05
ru102			9.45E+02	
ru103	102.022	44103.50c	2.01E+03	6.21256E-05
ru104			6.76E+02	
pd104	103.0114	46104.66c	4.37E+02	1.34085E-05
pd105	104.0039	46105.66c	4.84E+02	1.46937E-05
pd106	104.9937	46106.66c	5.02E+02	1.51212E-05
pd107			2.88E+02	
pd108	106.9769	46108.66c	4.79E+02	1.41377E-05
pd110	108.961	46110.66c	6.56E+01	1.90233E-06

ag109	107.969	47109.66c	8.97E+01	2.62473E-06
cd110	108.959	48110.66c	8.36E+01	2.42567E-06
cd111	109.952	48111.66c	3.27E+01	9.41154E-07
sn126	117.6704	50000.42c	2.03E+01	5.44736E-07
te128			9.83E+01	
te130			4.13E+02	
i127	125.8143	53127.66c	4.94E+01	1.24128E-06
i129	127.798	53129.60c	1.70E+02	4.19951E-06
xe131	129.781	54131.66c	3.14E+02	7.65697E-06
xe132	130.771	54132.66c	1.37E+03	3.31852E-05
xe134	132.755	54134.66c	1.66E+03	3.95938E-05
xe136	134.74	54136.66c	2.45E+03	5.74249E-05
cs133	131.764	55133.66c	1.07E+03	2.56908E-05
cs135	133.747	55135.60c	5.15E+02	1.21729E-05
ba134			3.09E+02	
ba136			5.94E+01	
ba137			1.38E+03	
ba138	136.715	56138.66c	3.16E+03	7.29583E-05
la139			1.30E+03	
ce140			1.36E+03	
ce142			1.19E+03	
pr141	139.697	59141.50c	1.18E+03	2.66076E-05
nd142			4.84E+01	
nd143	141.682	60143.50c	6.59E+02	1.47035E-05
nd144			1.62E+03	
nd145	143.668	60145.50c	2.24E+03	4.93463E-05
nd146			8.49E+02	
nd148	146.646	60148.50c	1.45E+03	3.11683E-05
nd150			2.02E+02	
sm147	145.653	62147.66c	1.65E+02	3.58489E-06
sm148			2.19E+02	
sm150	148.629	62150.50c	5.19E+02	1.10370E-05
sm152	150.615	62152.50c	1.54E+02	3.24035E-06
sm154			4.43E+01	
eu153	151.608	63153.66c	1.31E+02	2.73317E-06
gd154	152.599	64154.66c	3.78E+01	7.83556E-07
gd156	154.583	64156.66c	2.01E+02	4.10979E-06
gd158	156.567	64158.66c	3.89E+01	7.85298E-07

No new entries on this page

Table 09/16/07-5. OrigenARP output data for 100000 years down (case 8)

Scale ID	Nuclide/ A.W.	Years MCNP ID	(g/basis)	100,000 Y at/cm^3
O	15.8575	8016.62c	6.24E+04	1.24296E-02
u234	232.03	92234.66c	3.44E+02	4.68461E-06
u235	233.025	92235.66c	4.43E+03	6.00471E-05
u236	234.018	92236.66c	5.15E+03	6.94899E-05
u238	236.006	92238.66c	4.14E+05	5.54183E-03
np237	235.0118	93237.66c	1.47E+03	1.97299E-05
pu239	236.9986	94239.66c	1.83E+02	2.44323E-06
pu242	239.979	94242.66c	6.47E+02	8.51756E-06
se 82			3.42E+01	
br 81	80.2212	35081.55c	2.09E+01	8.23854E-07
kr 83	82.2018	36083.66c	3.20E+01	1.22965E-06
kr 84	83.1906	36084.66c	1.27E+02	4.81380E-06
kr 86	85.1726	36086.66c	1.81E+02	6.72054E-06
rb 85	84.1824	37085.66c	1.21E+02	4.55809E-06
rb 87	86.1624	37087.66c	2.43E+02	8.92503E-06
sr 88	88	37087.66c	3.35E+02	1.20395E-05
y 89	88.142	39089.66c	4.46E+02	1.59933E-05
zr 90	89.132	40090.66c	5.52E+02	1.95674E-05
zr 91	90.122	40091.66c	5.92E+02	2.07658E-05
zr 92	91.112	40092.66c	6.55E+02	2.27361E-05
zr 93	92.1083	40093.66c	6.79E+02	2.33069E-05
zr 94	93.096	40094.66c	8.11E+02	2.75310E-05
zr 96	95.081	40096.66c	8.47E+02	2.81596E-05
mo 95			7.41E+02	
mo 96			9.39E+01	
mo 97			8.59E+02	
mo 98			8.95E+02	
mo100	95.116	42000.66c	3.61E+03	1.19964E-04
tc 99	98.15	43099.66c	5.43E+02	1.74830E-05
ru 99			2.11E+02	
ru100			2.24E+02	
ru101	100.039	44101.50c	2.88E+03	9.08573E-05
ru102			9.45E+02	
ru104			6.76E+02	
rh103	102.022	44103.50c	3.84E+02	1.19028E-05
pd104	103.0114	46104.66c	4.37E+02	1.34085E-05
pd105	104.0039	46105.66c	4.84E+02	1.46937E-05
pd106	104.9937	46106.66c	5.02E+02	1.51212E-05
pd107			2.85E+02	
pd108	106.9769	46108.66c	4.76E+02	1.40549E-05
pd110	108.961	46110.66c	6.56E+01	1.90233E-06

ag109	107.969	47109.66c	8.97E+01	2.62473E-06
cd110	108.959	48110.66c	8.36E+01	2.42567E-06
cd111	109.952	48111.66c	3.27E+01	9.41154E-07
te128			9.83E+01	
te130			4.13E+02	
i127	125.8143	53127.66c	4.94E+01	1.24128E-06
i129	127.798	53129.60c	1.69E+02	4.18220E-06
xe131	129.781	54131.66c	3.14E+02	7.65697E-06
xe132	130.771	54132.66c	1.37E+03	3.31852E-05
xe134	132.755	54134.66c	1.66E+03	3.95938E-05
xe136	134.74	54136.66c	2.45E+03	5.74249E-05
cs133	131.764	55133.66c	1.07E+03	2.56908E-05
cs135	133.747	55135.60c	5.01E+02	1.18467E-05
ba134			3.09E+02	
ba136			5.94E+01	
ba137			1.38E+03	
ba138	136.715	56138.66c	3.16E+03	7.29583E-05
la139			1.30E+03	
ce140			1.36E+03	
ce142			1.19E+03	
pr141	139.697	59141.50c	1.18E+03	2.66076E-05
nd142			4.84E+01	
nd143	141.682	60143.50c	6.59E+02	1.47035E-05
nd144			1.62E+03	
nd145	143.668	60145.50c	2.24E+03	4.93463E-05
nd146			8.49E+02	
nd148	146.646	60148.50c	1.45E+03	3.11683E-05
nd150			2.02E+02	
sm147	145.653	62147.66c	1.65E+02	3.58489E-06
sm148			2.19E+02	
sm150	148.629	62150.50c	5.19E+02	1.10370E-05
sm152	150.615	62152.50c	1.54E+02	3.24035E-06
sm154			4.43E+01	
eu153	151.608	63153.66c	1.31E+02	2.73317E-06
gd154	152.599	64154.66c	3.78E+01	7.83556E-07
gd156	154.583	64156.66c	2.01E+02	4.10979E-06
gd158	156.567	64158.66c	3.89E+01	7.85298E-07

Table 09/16/07-6.
Smeared by Assembly Nuclides Densities for the Fuel Clad, Guide Tube and Instrument Tube

Scale ID	A.W.	MCNP ID	Nuclides Densities [at/cm^3]
cr	51.549	24000.50c	7.72271E-06
fe	55.365	26000.55c	1.43800E-05
Zr	90.436	40000.66c	4.32181E-03
sn	117.6704	50000.42c	4.73643E-05

See SN September 2007 Radiolysis.xls, Sheet "Neutron Nuclides Densities"

Table 09/16/07-7. OrigenARP output data for 500 years down (case 5) accommodated for the photon transport libraries

Scale ID	Nuclide A.W.	MCNP ID	500 Years (g/basis)	at/cm^3
O	15.8575	8000.04p	6.23600E+04	1.24296E-02
u234	232.03		4.41E+02	6.00322E-06
u235	233.025		1.58E+03	2.13631E-05
u236	234.018		3.45E+03	4.66102E-05
u238	236.006		4.14E+05	5.54049E-03
		92000.04p		5.61446E-03
np237	235.0118	93000.04p	1.06E+03	1.41889E-05
pu239	236.9986		2.82E+03	3.75821E-05
pu240	237.992		1.74E+03	2.30687E-05
pu242	239.979		7.75E+02	1.02100E-05
		94000.04p		7.08607E-05
am241	238.986		4.56E+02	6.02555E-06
am243	240.9734		2.72E+02	3.56112E-06
		95000.04p		9.58666E-06
se 82	78.2817	34000.04p	3.42E+01	1.38208E-06
br 81	80.2212	35000.04p	2.09E+01	8.23854E-07
kr 83	82.2018		3.20E+01	1.22965E-06
kr 84	83.1906		1.27E+02	4.81380E-06
kr 86	85.1726		1.81E+02	6.72054E-06
		36000.04p		1.27640E-05
rb 85	84.1824		1.21E+02	4.55809E-06
rb 87	86.1624		2.43E+02	8.92503E-06
		37000.04p		1.34831E-05
sr 88	86.8674	38000.04p	3.35E+02	1.21964E-05
y 89	88.142	39000.04p	4.46E+02	1.59933E-05
zr 90	89.132		5.52E+02	1.95674E-05
zr 91	90.122		5.92E+02	2.07658E-05
zr 92	91.112		6.55E+02	2.27361E-05
zr 93	92.1083		7.11E+02	2.43810E-05
zr 94	93.096		8.11E+02	2.75310E-05
zr 96	95.081		8.47E+02	2.81596E-05
		40000.04p		1.43141E-04
mo 95	90		7.41E+02	2.60197E-05
mo 96	91		9.39E+01	3.26109E-06
mo 97	92		8.59E+02	2.95080E-05
mo 98	93		8.95E+02	3.04312E-05

mo100	95.116		1.02E+03	3.39279E-05
		42000.04p		1.23148E-04
tc 99	98.15	43000.04p	7.53E+02	2.42391E-05
ru100	99		2.24E+02	7.14194E-06
ru101	100.039		8.20E+02	2.59014E-05
ru102	101		9.45E+02	2.95793E-05
ru103	102.022		3.84E+02	1.19028E-05
ru104	103		6.76E+02	2.07410E-05
		44000.04p		9.52665E-05
pd104	103.0114		4.37E+02	1.34085E-05
pd105	104.0039		4.84E+02	1.46937E-05
pd106	104.9937		5.02E+02	1.51212E-05
pd107	106		2.88E+02	8.59655E-06
pd108	106.9769		1.91E+02	5.62847E-06
pd110	108.961		6.56E+01	1.90233E-06
		46000.04p		5.93508E-05
ag109	107.969	47000.04p	8.97E+01	2.62473E-06
cd110	108.959		8.36E+01	2.42567E-06
cd111	109.952		3.27E+01	9.41154E-07
		48000.04p		3.36683E-06
sn126	117.6704	50000.04p	2.17E+01	5.81804E-07
te128	126.504		9.83E+01	2.45529E-06
te130	126.504		4.13E+02	1.03213E-05
		52000.04p		1.27766E-05
i127	125.8143		4.94E+01	1.24128E-06
i129	127.798		1.70E+02	4.20199E-06
		53000.04p		5.44327E-06
xe131	129.781		3.14E+02	7.65697E-06
xe132	130.771		1.37E+03	3.31852E-05
xe134	132.755		1.66E+03	3.95938E-05
xe136	134.74		2.45E+03	5.74249E-05
		54000.04p		1.37861E-04
cs133	131.764		1.07E+03	2.56908E-05
cs135	133.747		5.17E+02	1.22083E-05
		55000.04p		3.78991E-05
ba134	133		3.09E+02	7.35282E-06
ba136	135		5.94E+01	1.39001E-06
ba137	136		1.38E+03	3.20952E-05
ba138	136.715		1.41E+03	3.25053E-05
		56000.04p		7.33434E-05
la139	137.712	57000.04p	1.30E+03	2.97453E-05
ce140	138.916		1.36E+03	3.10119E-05
ce142	138.916		1.19E+03	2.71440E-05

		58000.04p		5.81559E-05
pr141	139.697	59000.04p	1.18E+03	2.66076E-05
nd142	140.682		4.84E+01	1.08741E-06
nd143	141.682		6.11E+02	1.36238E-05
nd144	142.668		1.62E+03	3.58679E-05
nd145	143.668		6.24E+02	1.37281E-05
nd146	144.646		8.49E+02	1.85496E-05
nd148	146.646		3.96E+02	8.52867E-06
nd150	148.646		2.02E+02	4.28457E-06
		60000.04p		9.56701E-05
sm147	145.653		1.65E+02	3.58489E-06
sm148	146.64		2.19E+02	4.70960E-06
sm150	148.629		3.01E+02	6.39037E-06
sm152	150.615		1.10E+02	2.31049E-06
sm154	152.615		4.43E+01	9.17677E-07
		62000.04p		1.79130E-05
eu153	151.608	63000.04p	1.31E+02	2.73317E-06
gd154	152.599		3.78E+01	7.83556E-07
gd156	154.583		2.01E+02	4.10979E-06
gd158	156.567		3.89E+01	7.85298E-07
		64000.04p		5.67865E-06

Table 09/16/07-8.
Smeared by Assembly Nuclides Densities for the Fuel Clad, Guide Tube and Instrument Tube

Scale ID	A.W.	MCNP ID	Nuclides Densities [at/cm^3]
cr	51.549	24000.04p	7.72271E-06
fe	55.365	28000.04p	1.43800E-05
Zr	90.436	40000.04p	4.32181E-03
sn	117.6704	50000.04p	4.73643E-05

See SN September 2007 Radiolysis.xls, Sheet "Photon Nuclides Densities"

All Photon Calculation Cases Uses the Same Material Composition

No new entries on this page

Table 09/16/07-9. Total neutron spectra for basis = 0.46363 MTU [neutrons/sec/basis]

grp	Start MeV	End MeV	100 Years n/sec/basis	500 Years n/sec/basis	2000 Years n/sec/basis	10,000 Years n/sec/bas s	100,000 Years n/sec/basis
1	1.00E-11	3.00E-09	5.137E-05	4.468E-05	3.602E-05	1.181E-05	7.537E-07
2	3.00E-09	7.50E-09	4.330E-05	3.187E-05	2.574E-05	8.548E-06	6.446E-07
3	7.50E-09	1.00E-08	2.264E-05	1.506E-05	1.217E-05	4.079E-06	3.400E-07
4	1.00E-08	2.53E-08	1.447E-04	8.317E-05	6.737E-05	2.301E-05	2.317E-06
5	2.53E-08	3.00E-08	4.828E-05	2.502E-05	2.031E-05	7.052E-06	8.192E-07
6	3.00E-08	4.00E-08	1.092E-04	5.404E-05	4.390E-05	1.537E-05	1.896E-06
7	4.00E-08	5.00E-08	1.178E-04	5.570E-05	4.529E-05	1.598E-05	2.089E-06
8	5.00E-08	7.00E-08	2.598E-04	1.174E-04	9.555E-05	3.400E-05	4.700E-06
9	7.00E-08	1.00E-07	4.445E-04	1.919E-04	1.563E-04	5.610E-05	8.197E-06
10	1.00E-07	1.50E-07	8.683E-04	3.602E-04	2.937E-04	1.063E-04	1.631E-05
11	1.50E-07	2.00E-07	1.019E-03	4.191E-04	3.440E-04	1.309E-04	1.992E-05
12	2.00E-07	2.25E-07	5.565E-04	2.261E-04	1.856E-04	7.080E-05	1.092E-05
13	2.25E-07	2.50E-07	5.853E-04	2.361E-04	1.938E-04	7.388E-05	1.149E-05
14	2.50E-07	2.75E-07	6.127E-04	2.458E-04	2.017E-04	7.684E-05	1.203E-05
15	2.75E-07	3.25E-07	1.303E-03	5.191E-04	4.260E-04	1.621E-04	2.558E-05
16	3.25E-07	3.50E-07	6.883E-04	2.727E-04	2.238E-04	8.508E-05	1.352E-05
17	3.50E-07	3.75E-07	7.117E-04	2.811E-04	2.307E-04	8.765E-05	1.398E-05
18	3.75E-07	4.00E-07	7.344E-04	2.893E-04	2.373E-04	9.013E-05	1.442E-05
19	4.00E-07	6.25E-07	7.533E-03	2.938E-03	2.410E-03	9.131E-04	1.479E-04
20	6.25E-07	1.00E-06	1.567E-02	6.038E-03	4.950E-03	1.868E-03	3.073E-04
21	1.00E-06	1.77E-06	4.169E-02	1.591E-02	1.304E-02	4.902E-03	8.170E-04
22	1.77E-06	3.00E-06	8.709E-02	3.305E-02	2.706E-02	1.014E-02	1.704E-03
23	3.00E-06	4.75E-06	1.577E-01	5.963E-02	4.882E-02	1.824E-02	3.080E-03
24	4.75E-06	6.00E-06	1.327E-01	5.009E-02	4.100E-02	1.530E-02	2.590E-03
25	6.00E-06	8.10E-06	2.550E-01	9.614E-02	7.869E-02	2.932E-02	4.975E-03
26	8.10E-06	1.00E-05	2.614E-01	9.845E-02	8.057E-02	2.999E-02	5.097E-03
27	1.00E-05	3.00E-05	4.047E+00	1.519E+00	1.243E+00	4.617E-01	7.876E-02
28	3.00E-05	1.00E-04	2.616E+01	9.807E+00	7.834E+00	2.896E+00	4.950E-01
29	1.00E-04	5.50E-04	3.712E+02	1.386E+02	1.115E+02	4.120E+01	7.035E+00
30	5.50E-04	3.00E-03	4.713E+03	1.758E+03	1.418E+03	5.241E+02	8.948E+01
31	3.00E-03	1.70E-02	6.382E+04	2.381E+04	1.915E+04	7.081E+03	1.208E+03
32	1.70E-02	2.50E-02	5.384E+04	2.008E+04	1.613E+04	5.967E+03	1.018E+03
33	2.50E-02	1.00E-01	8.365E+05	3.122E+05	2.513E+05	9.297E+04	1.585E+04
34	1.00E-01	4.00E-01	6.016E+06	2.246E+06	1.813E+06	6.706E+05	1.142E+05
35	4.00E-01	9.00E-01	1.308E+07	4.872E+06	3.934E+06	1.453E+06	2.466E+05
36	9.00E-01	1.40E+00	1.311E+07	4.858E+06	3.906E+06	1.441E+06	2.419E+05
37	1.40E+00	1.85E+00	1.068E+07	3.929E+06	3.107E+06	1.146E+06	1.892E+05
38	1.85E+00	2.35E+00	1.042E+07	3.795E+06	2.913E+06	1.076E+06	1.734E+05
39	2.35E+00	2.48E+00	2.313E+06	8.360E+05	6.280E+05	2.321E+05	3.676E+04
40	2.48E+00	3.00E+00	8.331E+06	2.987E+06	2.217E+06	8.172E+05	1.280E+05
41	3.00E+00	4.80E+00	1.426E+07	5.043E+06	3.872E+06	1.407E+06	2.168E+05
42	4.80E+00	6.43E+00	3.714E+06	1.295E+06	1.053E+06	3.771E+05	5.453E+04
43	6.43E+00	8.19E+00	1.158E+06	3.922E+05	3.190E+05	1.129E+05	1.512E+04
44	8.19E+00	2.00E+01	3.903E+05	1.265E+05	1.027E+05	3.579E+04	4.292E+03
		Total	**8.44316E+07**	**3.07377E+07**	**2.41528E+07**	**8.87528E+06**	**1.43898E+06**

See SN September 2007 Radiolysis.xls, Sheet "Neutron Spectra"

No new entries on this page

Table 09/16/07-10. Total Photon Spectra for basis = 0.46363 MTU [photons/sec/basis]

grp	Start MeV	End MeV	100 Years p/sec/basis	500 Years p/sec/basis	2000 Years p/sec/basis	10000 Years p/sec/basis	100000 Years p/sec/basis
1	1.00000E-02	2.00000E-02	1.34600E+14	2.51900E+13	5.32600E+12	1.74200E+12	1.64100E+11
2	2.00000E-02	3.00000E-02	4.51400E+13	3.95200E+12	4.63500E+11	7.21100E+10	2.62500E+10
3	3.00000E-02	4.50000E-02	5.39900E+13	2.96800E+11	1.58600E+11	7.34700E+10	1.50900E+10
4	4.50000E-02	6.00000E-02	6.55500E+13	2.35800E+13	2.17600E+12	2.80300E+10	1.02200E+10
5	6.00000E-02	7.00000E-02	1.00100E+13	3.67900E+10	3.09000E+10	1.67000E+10	4.91800E+09
6	7.00000E-02	7.50000E-02	5.71700E+12	1.41200E+12	1.22600E+12	5.78600E+11	5.40800E+09
7	7.50000E-02	1.00000E-01	1.67800E+13	2.40200E+11	2.03900E+11	1.14100E+11	4.53500E+10
8	1.00000E-01	1.50000E-01	1.78800E+13	1.29300E+12	1.11100E+12	5.28700E+11	1.12300E+10
9	1.50000E-01	2.00000E-01	1.07300E+13	1.45800E+10	1.24200E+10	7.98400E+09	7.22100E+09
10	2.00000E-01	3.00000E-01	8.88900E+12	6.17800E+11	5.37000E+11	2.58100E+11	2.41700E+10
11	3.00000E-01	4.00000E-01	5.88400E+12	8.37000E+10	7.84500E+10	4.97100E+10	3.93500E+10
12	4.00000E-01	4.50000E-01	1.72800E+12	2.30400E+10	2.29000E+10	2.17700E+10	1.57200E+10
13	4.50000E-01	5.10000E-01	1.65500E+12	5.31100E+08	3.98200E+08	3.81100E+08	1.43200E+09
14	5.10000E-01	5.12000E-01	1.17100E+09	2.45200E+06	5.73400E+05	4.73400E+06	3.62500E+07
15	5.12000E-01	6.00000E-01	7.28800E+11	6.28300E+08	5.72100E+08	6.06500E+08	8.79000E+08
16	6.00000E-01	7.00000E-01	3.54200E+14	8.25000E+10	4.77300E+10	4.80000E+10	4.84700E+10
17	7.00000E-01	8.00000E-01	7.11500E+11	2.38900E+09	2.21800E+09	2.55800E+09	5.35400E+09
18	8.00000E-01	1.00000E+00	7.66100E+11	1.32700E+09	1.23200E+09	1.53700E+09	3.89000E+09
19	1.00000E+00	1.20000E+00	3.37200E+11	6.44600E+08	6.82700E+08	1.82500E+09	1.02800E+10
20	1.20000E+00	1.33000E+00	1.54800E+11	1.04700E+08	1.36800E+08	6.30000E+08	4.34300E+09
21	1.33000E+00	1.44000E+00	4.30700E+10	7.40400E+06	5.16900E+07	6.05200E+08	4.70200E+09
22	1.44000E+00	1.50000E+00	1.39700E+10	8.86600E+07	8.75200E+07	8.83200E+07	9.07500E+07
23	1.50000E+00	1.57000E+00	1.27200E+10	2.94800E+06	1.83200E+07	2.14200E+08	1.83700E+09
24	1.57000E+00	1.66000E+00	1.78200E+10	2.16500E+06	1.15900E+07	1.34900E+08	1.04700E+09
25	1.66000E+00	1.80000E+00	1.03800E+10	1.80100E+07	1.23400E+08	1.39000E+09	1.07900E+10
26	1.80000E+00	2.00000E+00	4.72200E+09	3.17700E+06	1.92900E+07	2.12700E+08	1.64400E+09
27	2.00000E+00	2.15000E+00	8.10600E+08	5.55000E+05	8.74500E+06	1.06000E+08	8.25300E+08
28	2.15000E+00	2.35000E+00	1.84100E+07	7.03700E+06	3.48000E+07	3.71400E+08	2.88000E+09
29	2.35000E+00	2.50000E+00	3.08600E+06	5.24300E+05	9.08200E+06	1.10100E+08	8.57900E+08
30	2.50000E+00	3.00000E+00	2.85700E+08	8.31900E+06	3.26500E+06	1.01900E+07	7.20800E+07
31	3.00000E+00	3.50000E+00	5.14800E+06	1.78200E+06	1.64500E+06	2.93200E+06	1.86200E+07
32	3.50000E+00	4.00000E+00	2.98300E+06	1.02600E+06	8.39900E+05	3.22700E+05	6.57000E+04
33	4.00000E+00	4.50000E+00	1.72800E+06	5.94500E+05	4.86900E+05	1.87100E+05	3.80900E+04
34	4.50000E+00	5.00000E+00	1.00100E+06	3.44500E+05	2.82200E+05	1.08400E+05	2.20800E+04
35	5.00000E+00	5.50000E+00	5.80400E+05	1.99700E+05	1.63600E+05	6.28600E+04	1.28000E+04
36	5.50000E+00	6.00000E+00	3.36400E+05	1.15700E+05	9.48600E+04	3.64400E+04	7.42300E+03
37	6.00000E+00	6.50000E+00	1.95000E+05	6.70700E+04	5.50000E+04	2.11300E+04	4.30400E+03
38	6.50000E+00	7.00000E+00	1.13000E+05	3.88800E+04	3.18900E+04	1.22500E+04	2.49500E+03
39	7.00000E+00	7.50000E+00	6.55100E+04	2.25400E+04	1.84900E+04	7.10100E+03	1.44700E+03
40	7.50000E+00	8.00000E+00	3.79800E+04	1.30600E+04	1.07200E+04	4.11700E+03	8.38900E+02
41	8.00000E+00	1.00000E+01	4.48400E+04	1.54300E+04	1.26600E+04	4.86300E+03	9.90900E+02
42	1.00000E+01	1.20000E+01	2.31700E+03	7.97200E+02	6.54400E+02	2.51400E+02	5.12300E+01
43	1.20000E+01	1.40000E+01	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
44	1.40000E+01	2.00000E+01	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
		Total:	7.35556E+14	5.68282E+13	1.14000E+13	3.55006E+12	4.68476E+11

See SN September 2007 Radiolysis.xls, Sheet "Gamma Spectra"

#09/22/07, #09/23/07
Refined MCNP model created for investigation radiolytic generation of nitric acid and other species inside
cavity of failed 21-PWR TAD WP within air-water vapor volume
Performed preliminary runs of the MCNP model.Documented results.

III. MCNP Calculations Cases

III.1. MCNP Input Data

Fuel Smeared in Dry Assembly with External Sources (Different Cases for Neutron and Gamma Transport)

Table 09/23/07-1. Common Cases Parameters:

Fuel Basket Plate:	11 mm Neutronit A978 analogous to 304B6 with 75%% B-10 and B-11	
Casc:	TAD canister	
Assembly:	Smeared Dry	
Filled With	Air + H2O	
BurnUp	78.25864508	GWd/MTU

Table 09/23/07-2. MCNP Input Case Codes

	Physics: (N/G)	Years of Decay	H2O in Air	Absorber Plates
	P	Y	H	AP
				11 mm Neutronit A978 analogous to 304B6 with 75%% B-10 and B-11
PN_Y100_H0_APB11	N	100	0	B11
PN_Y500_H0_APB11	N	500	0	B11
PN_Y2000_H0_APB11	N	2000	0	B11
PN_Y10000_H0_APB11	N	10000	0	B11
PN_Y100000_H0_APB11	N	100000	0	B11
PG_Y100_H0_APB11	G	100	0	B11
PG_Y500_H0_APB11	G	500	0	B11
PG_Y2000_H0_APB11	G	2000	0	B11
PG_Y10000_H0_APB11	G	10000	0	B11
PG_Y100000_H0_APB11	G	100000	0	B11

Table 09/23/07-3. MCNP Input/Output

MCNP Case Codes	MCNP Input	MCNP Output
PN_Y100_H0_APB11	MCNP\Neutron\PN_Y100_H0_APB11.inp	MCNP\Neutron\PN_Y100_H0_APB11.out
PN_Y500_H0_APB11	MCNP\Neutron\PN_Y500_H0_APB11.inp	MCNP\Neutron\PN_Y500_H0_APB11.out
PN_Y2000_H0_APB11	MCNP\Neutron\PN_Y2000_H0_APB11.inp	MCNP\Neutron\PN_Y2000_H0_APB11.out
PN_Y10000_H0_APB11	MCNP\Neutron\PN_Y10000_H0_APB11.inp	MCNP\Neutron\PN_Y10000_H0_APB11.out
PN_Y100000_H0_APB11	MCNP\Neutron\PN_Y100000_H0_APB11.inp	MCNP\Neutron\PN_Y100000_H0_APB11.out
PG_Y100_H0_APB11	MCNP\Gamma\PG_Y100_H0_APB11.inp	MCNP\Gamma\PG_Y100_H0_APB11.out
PG_Y500_H0_APB11	MCNP\Gamma\PG_Y500_H0_APB11.inp	MCNP\Gamma\PG_Y500_H0_APB11.out
PG_Y2000_H0_APB11	MCNP\Gamma\PG_Y2000_H0_APB11.inp	MCNP\Gamma\PG_Y2000_H0_APB11.out
PG_Y10000_H0_APB11	MCNP\Gamma\PG_Y10000_H0_APB11.inp	MCNP\Gamma\PG_Y10000_H0_APB11.out
PG_Y100000_H0_APB11	MCNP\Gamma\PG_Y100000_H0_APB11.inp	MCNP\Gamma\PG_Y100000_H0_APB11.out

III.2. MCNP Input Data Geometry

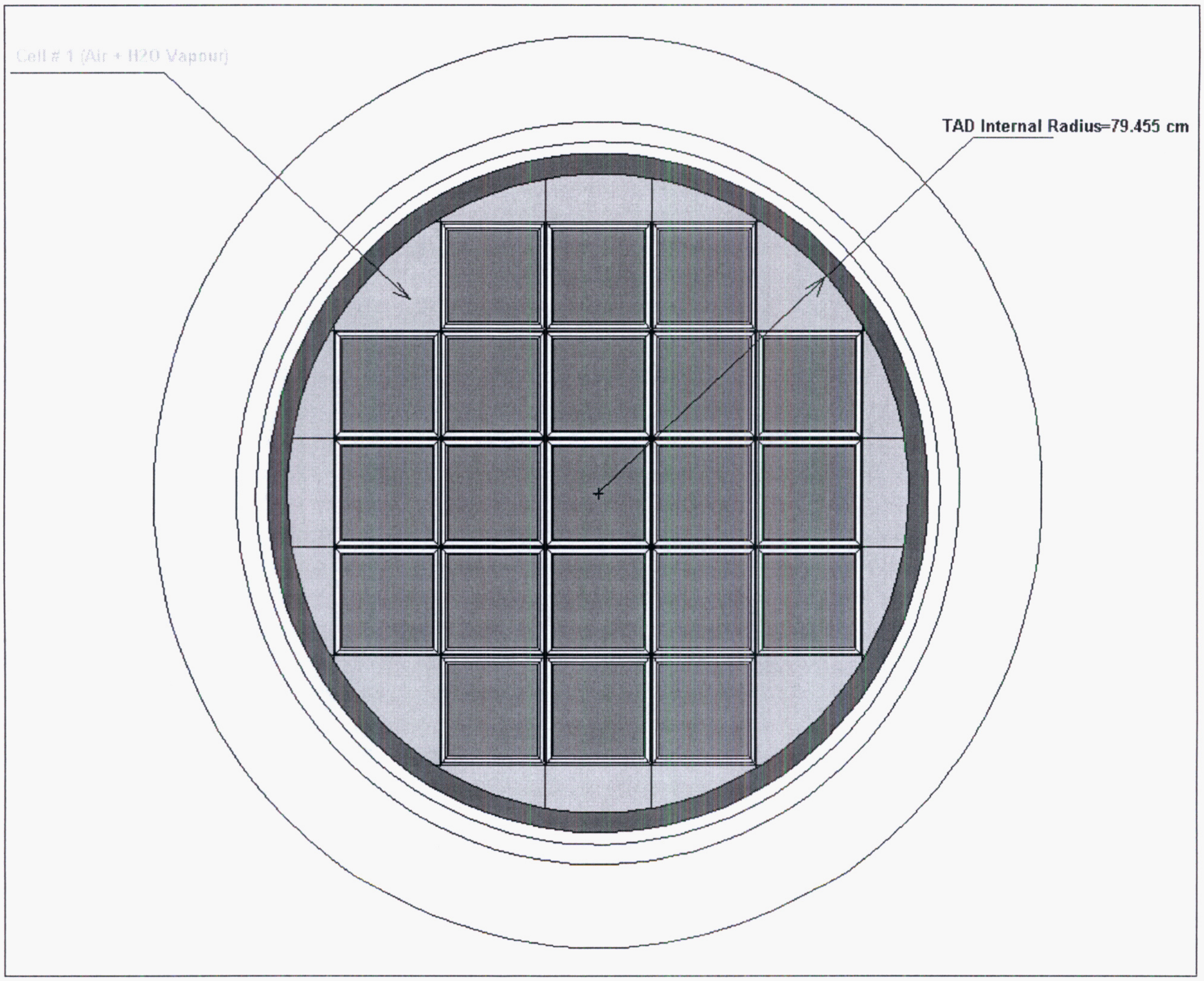


Figure 09/23/07-1. PWR-21 Radial Geometry

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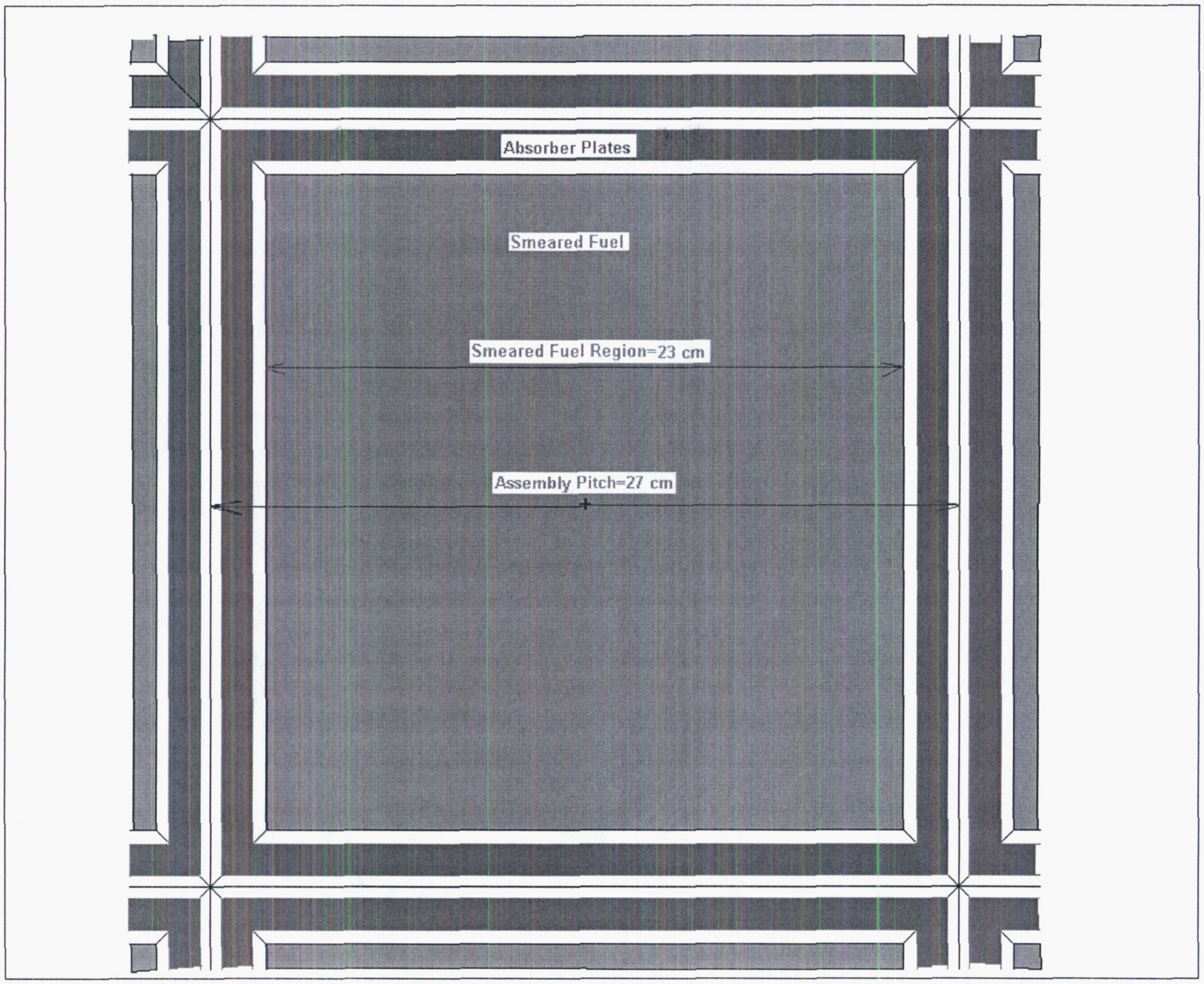

Figure 09/23/07-2. Assembly Radial Geometry

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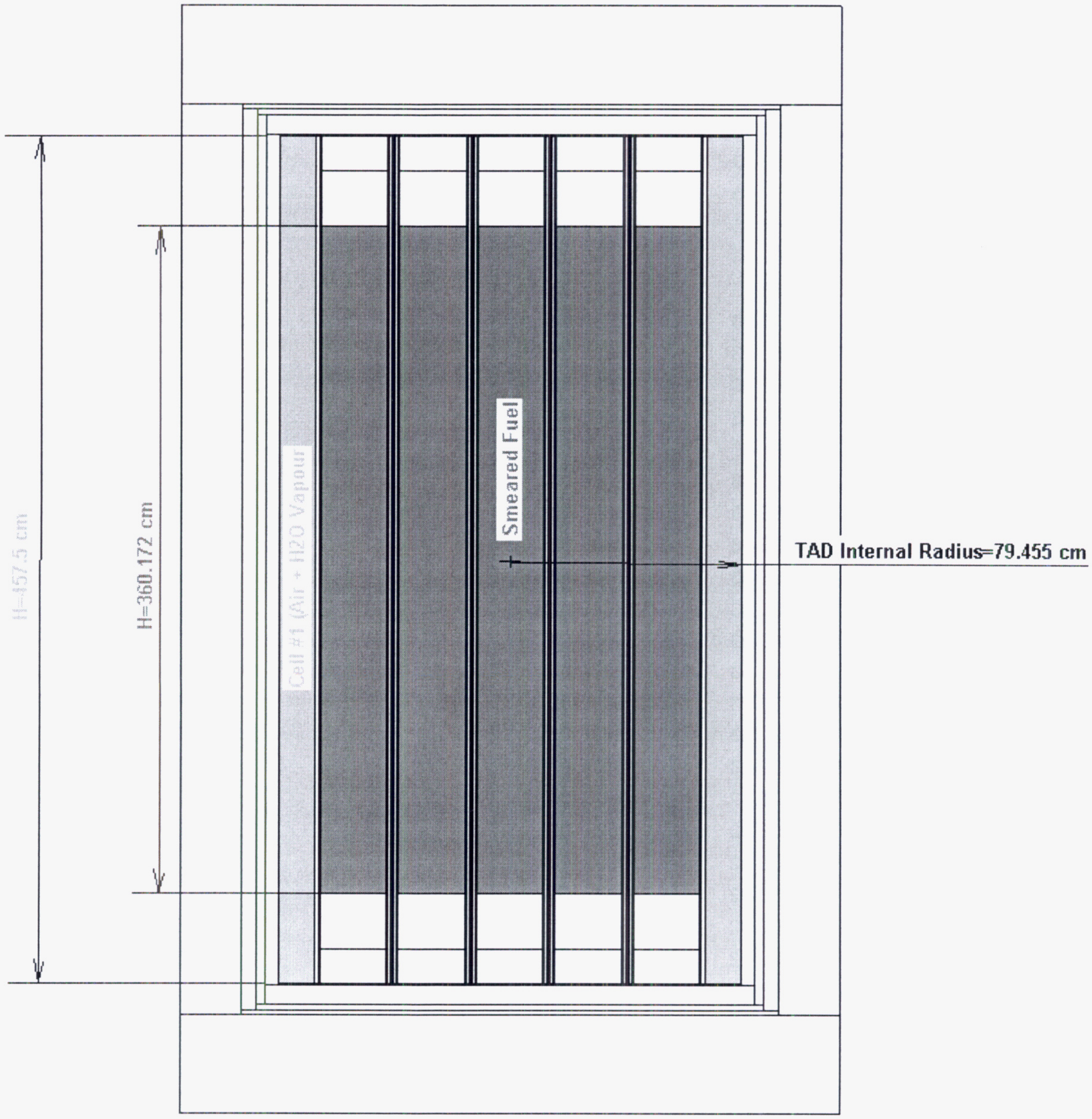

Figure 09/23/07-3. PWR-21 Axial Geometry

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III.3. MCNP Cell Parameters

Table 09/23/07-4. MCNP Outputted Cell Parameters

Cell	atom density	gram density	Input volume	calculated volume	Mass
1	**2.15408E-03**	**2.21868E-02**	**2.06981E+06**		**4.59225E+04**
1011	2.15408E-03	2.21868E-02		3.33518E+05	7.39969E+03
1012	2.15408E-03	2.21868E-02		3.33518E+05	7.39969E+03
1013	2.15408E-03	2.21868E-02		3.33518E+05	7.39969E+03
1021	2.15408E-03	2.21868E-02		3.33518E+05	7.39969E+03
1022	2.15408E-03	2.21868E-02		3.33518E+05	7.39969E+03
1023	2.15408E-03	2.21868E-02		3.33518E+05	7.39969E+03
1024	2.15408E-03	2.21868E-02		3.33518E+05	7.39969E+03
1025	2.15408E-03	2.21868E-02		3.33518E+05	7.39969E+03
1031	2.15408E-03	2.21868E-02		3.33518E+05	7.39969E+03
1032	2.15408E-03	2.21868E-02		3.33518E+05	7.39969E+03
1033	2.15408E-03	2.21868E-02		3.33518E+05	7.39969E+03
1034	2.15408E-03	2.21868E-02		3.33518E+05	7.39969E+03
1035	2.15408E-03	2.21868E-02		3.33518E+05	7.39969E+03
1041	2.15408E-03	2.21868E-02		3.33518E+05	7.39969E+03
1042	2.15408E-03	2.21868E-02		3.33518E+05	7.39969E+03
1043	2.15408E-03	2.21868E-02		3.33518E+05	7.39969E+03
1044	2.15408E-03	2.21868E-02		3.33518E+05	7.39969E+03
1045	2.15408E-03	2.21868E-02		3.33518E+05	7.39969E+03
1051	2.15408E-03	2.21868E-02		3.33518E+05	7.39969E+03
1052	2.15408E-03	2.21868E-02		3.33518E+05	7.39969E+03
1053	2.15408E-03	2.21868E-02		3.33518E+05	7.39969E+03
3	2.35422E-02	3.44986E+00		1.90531E+05	6.57305E+05
4	8.58620E-02	7.81992E+00		5.37562E+03	4.20369E+04
5	8.58620E-02	7.81992E+00		5.37562E+03	4.20369E+04
6	8.58620E-02	7.81992E+00		5.37562E+03	4.20369E+04
7	8.58620E-02	7.81992E+00		5.37562E+03	4.20369E+04
801	8.87710E-02	7.74452E+00		1.26316E+04	9.78255E+04
901	8.87710E-02	7.74452E+00		1.26316E+04	9.78255E+04
101	8.87710E-02	7.74452E+00		1.26316E+04	9.78255E+04
111	8.87710E-02	7.74452E+00		1.26316E+04	9.78255E+04
8	2.15408E-03	2.21868E-02		4.88015E+03	1.08275E+02
9	2.15408E-03	2.21868E-02		4.88015E+03	1.08275E+02
10	2.15408E-03	2.21868E-02		4.88015E+03	1.08275E+02
11	2.15E-03	2.22E-02		4.88E+03	1.08E+02
12	9.87E-02	1.78E+00		1.60E+04	2.84E+04
13	2.15E-03	2.22E-02		9.74E+03	2.16E+02
14	9.87E-02	1.78E+00		1.60E+04	2.84E+04
15	2.15E-03	2.22E-02		9.74E+03	2.16E+02
120	2.15E-03	2.22E-02		9.92E+03	2.20E+02
121	2.15E-03	2.22E-02		9.92E+03	2.20E+02
122	8.70E-02	7.96E+00		1.18E+06	9.40E+06
123	8.70E-02	7.96E+00		2.46E+05	1.96E+06
124	8.70E-02	7.96E+00		2.46E+05	1.96E+06
125	2.15E-03	2.22E-02		7.21E+04	1.60E+03
126	2.15E-03	2.22E-02		7.21E+04	1.60E+03
127	2.15E-03	2.22E-02		7.79E+05	1.73E+04
128	8.51E-02	8.69E+00		1.37E+06	1.19E+07

129	8.51E-02	8.69E+00	5.37E+04	4.67E+05
130	8.51E-02	8.69E+00	5.37E+04	4.67E+05
131	2.15E-03	2.22E-02	6.71E+06	1.49E+05
132	2.15E-03	2.22E-02	2.17E+06	4.81E+04
133	2.15E-03	2.22E-02	2.17E+06	4.81E+04
134	0.00E+00	0.00E+00	0.00E+00	0.00E+00

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Total Assemblies Volume= 7.00388E+06 cm^3 = Summ(Cell#1011 : Cell#1053)

Out of Assemblies Volume =

calculated volume of Cell #1 - Total Assemblies Volume =

9.07368E+06 - 7.00388E+06 = 206981 cm^3

See SN September 2007 Radiolysis.xls, sheet "MCNP Cells Volumes"

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V. Cells Absorbed Energies and Nitrogen Dioxide Production

Table 09/23/07-5. Cell #1 Neutron Radiation Power Calculation Results

Down Years	Neutron Spectrum Particles/ sec/basis	Assemblies	MCNP Case	MCNP F6 Tally:Neutron MeV/ g/Particle	Error	Neutron Radiation Power per Gram of Weight MeV/g/sec
100	8.44316E+07	21	PN_Y100_H0_APB11	1.20909E-06	0.0063	2.14379E+0
500	3.07377E+07	21	PN_Y500_H0_APB11	1.15635E-06	0.0062	7.46414E+0
2000	2.41528E+07	21	PN_Y2000_H0_APB11	9.33076E-07	0.0062	4.73265E+0
10000	8.87528E+06	21	PN_Y10000_H0_APB11	5.54051E-07	0.0063	1.03264E+0
100000	1.43898E+06	21	PN_Y100000_H0_APB11	3.20950E-07	0.0051	9.69862E+0

Table 09/23/07-6. Cell #1 Photon Radiation Power Calculation Results

Down Years	Gamma Spectrum Particles/ sec/basis	Assemblies	MCNP Case	MCNP F6 Tally:Gamma MeV/ g/Particle	Relative Error	Photon Radiation Power per Gram of Weigh MeV/g/sec
100	7.35556E+14	21	PG_Y100_H0_APB11	1.21864E-09	0.0092	1.88239E+0
500	5.68282E+13	21	PG_Y500_H0_APB11	6.67947E-12	0.0849	7.97122E+0
2000	1.14E+13	21	PG_Y2000_H0_APB11	2.06937E-1	0.0477	4.95408E+0
10000	3.55006E+12	21	PG_Y10000_H0_APB11	7.34349E-1	0.0322	5.47467E+0
100000	4.68476E+11	21	PG_Y100000_H0_APB11	1.41971E-09	0.0106	1.39671E+0

(See SN September 2007 Radiolysis.xls, Sheet "Radiolysis Results")

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Table 09/23/07-8. Nitrogen Dioxide Production in Cell #1 from Neutron Radiation

Down Years	Neutron Radiation Power per Gram of Weight* MeV/g/sec	Vapour Density** g/cm^3	G-Factor for production of nitrogen dioxide Moleculs/MeV	Nitrogen Dioxide Production in Cell #1 from Neutron Radiation Moleculs/cm^3/sec	Moleculs/sec	g/Year
100	2.14379E+03	2.07958E-02	10000	4.45819E+05	9.22302E+11	2.20440E-03
500	7.46414E+02	9.64576E-03	10000	7.19973E+04	1.48947E+11	3.55998E-04
2000	4.73265E+02	2.59521E-03	10000	1.22822E+04	2.54092E+10	6.07305E-05
10000	1.03264E+02	6.53816E-04	10000	6.75160E+02	1.39676E+09	3.33839E-06
100000	9.69862E+00	2.28581E-04	10000	2.21692E+01	4.58632E+07	1.09618E-07

* See Table 17 "Cell #1 Neutron Radiation Power Calculation Results"
** See Table 16 "Drift Wall Temperatures and Calculated Vapour Pressures and Densities"

Table Table 09/23/07-9. Nitrogen Dioxide Production in Cell #1 from Gamma Radiation

Down Years	Gamma Radiation Power per Gram of Weight* MeV/g/sec	Vapour Density** g/cm^3	G-Factor for production of nitrogen dioxide Moleculs/MeV	Nitrogen Dioxide Production in Cell #1 from Gamma Radiation Moleculs/cm^3/sec	Moleculs/sec	g/Year
100	1.88239E+07	2.07958E-02	10000	3.91460E+09	8.09844E+15	1.93561E+01
500	7.97122E+03	9.64576E-03	10000	7.68885E+05	1.59065E+12	3.80183E-03
2000	4.95408E+03	2.59521E-03	10000	1.28569E+05	2.65980E+11	6.35720E-04
10000	5.47467E+03	6.53816E-04	10000	3.57943E+04	7.40505E+10	1.76988E-04
100000	1.39671E+04	2.28581E-04	10000	3.19261E+04	6.60482E+10	1.57862E-04

* See Table 18 "Cell #1 Photon Radiation Power Calculation Results"
** See Table 16 "Drift Wall Temperatures and Calculated Vapour Pressures and Densities"

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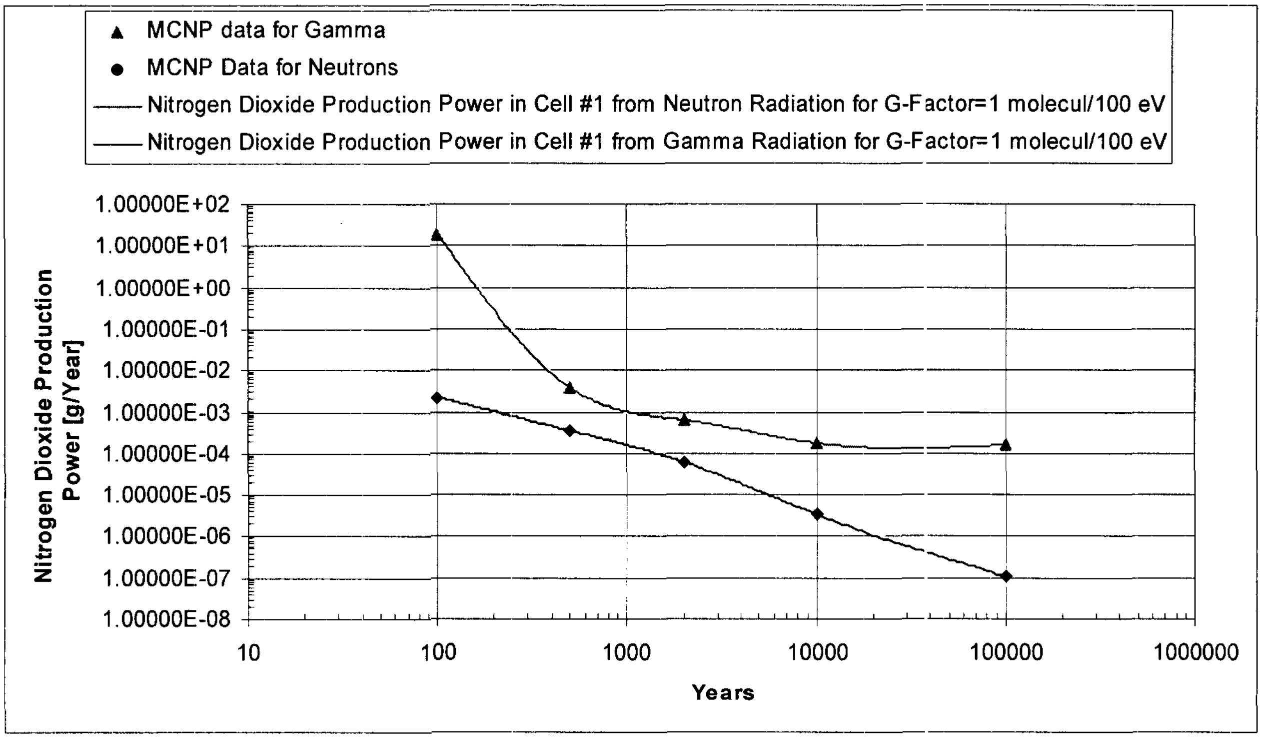

Figure 09/23/07-1. Nitrogen Dioxide Production Power

Spline Interpolation of the calculated results to perform integrating over time and presents at the Figure 09/23/07-1 has been performed by C# FunWork software (see solution at the FunWork_2005\FunWork\FunWork.sln and resultes at the FunWork_2005\FunWork\bin\Debug\Ln_G_Sec_SplineApproximation and FunWork_2005\FunWork\bin\Debug\Ln_G_Sec_Neutron_SplineApproximation)

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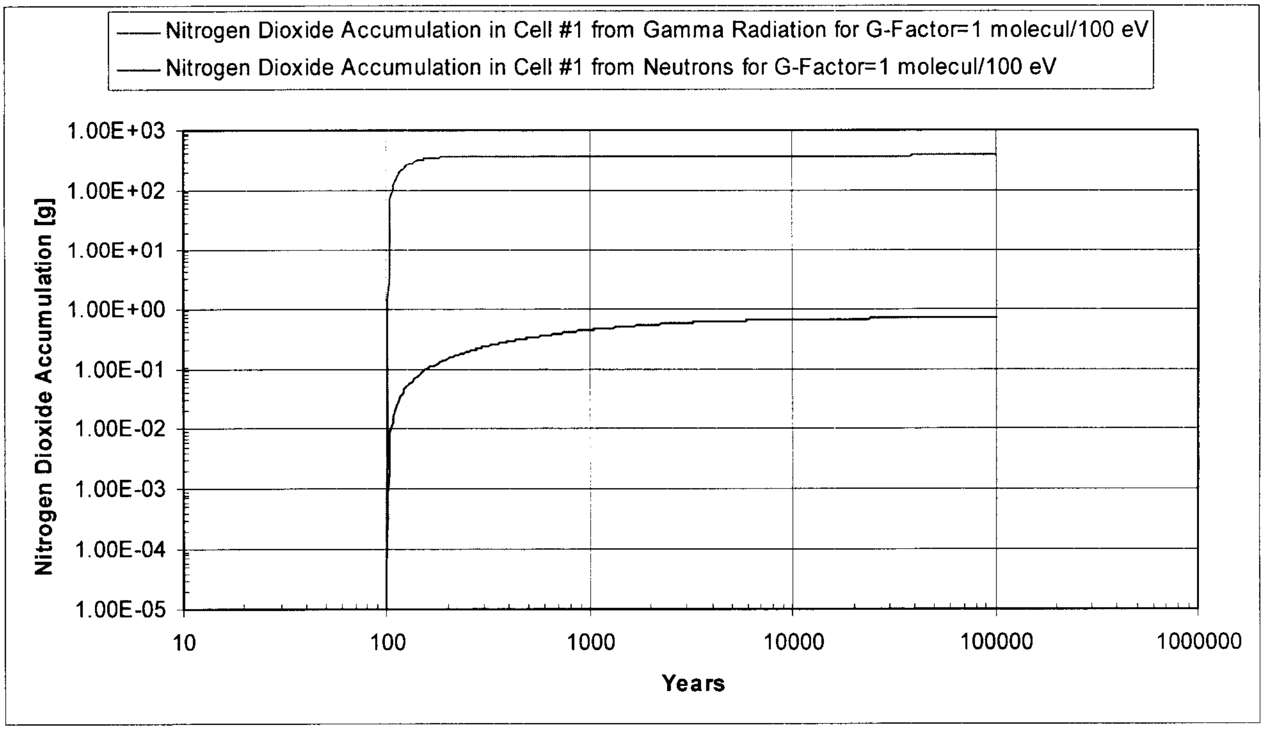

Figure 09/23/07-2. Nitrogen Dioxide Accumulation

See SN September 2007 Radiolysis.xls;
Sheet:" Radiolysis Results";
Cells: AB42:AB246 – Gamma;
Cells: AJ42:AJ246 – Neutrons;

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VI. Quality Assurance

Quality Assurance (QA) program has been applied to this analysis by:

- "Radcog", ver 02.17, testing calculations and
- Comparisons present results with data from "Radiolytic Specie Generation from Internal Waste Package Criticality", Document Identifier: CAL-EBS-NU-000017 REV 00, Page 32, Table 6.2;

VI.1. "Radcog" Testing calculations

21 Fuel assembly irradiate air-vapor volume inside TAD Internal (see Figure 09/23/07-3, Figure 09/23/07-4)

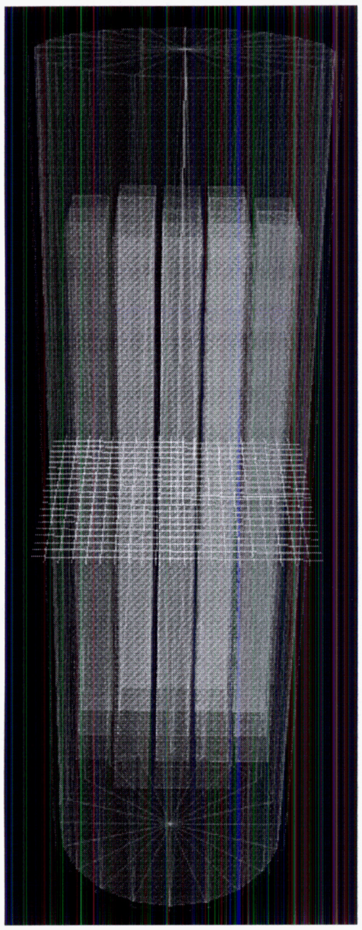

Figure 09/23/07-3. PWR-21 simplified geometry as inputted at "Radcog"

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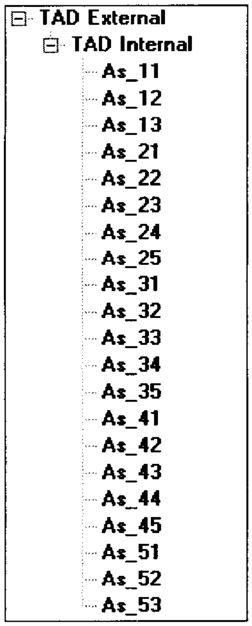

Figure 09/23/07-4. PWR-21 3D Elements and their hierarchy:

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Table Table 09/23/07-10. RadCog and MCNP Absorbed Dose Calculations Results

RadCog			MCNP		
Computer time = 10.78 minutes			Computer time = 15.53 minutes		
3-D Element:	Mev/g/particle:	Stat. Error(%):	Cell#	Mev/g/particle:	Stat. Error(%):
TAD Internal	3.67E-09	0.43	2	4.15E-09	0.17
As_11	2.46E-08	0.53	3	2.3E-08	0.23
As_12	2.48E-08	0.52	4	2.36E-08	0.23
As_13	2.45E-08	0.53	5	2.31E-08	0.23
As_21	2.48E-08	0.52	6	2.31E-08	0.23
As_22	2.56E-08	0.51	7	2.44E-08	0.23
As_23	2.57E-08	0.51	8	2.45E-08	0.23
As_24	2.57E-08	0.51	9	2.43E-08	0.23
As_25	2.48E-08	0.52	10	2.31E-08	0.23
As_31	2.52E-08	0.52	11	2.35E-08	0.23
As_32	2.59E-08	0.51	12	2.45E-08	0.23
As_33	2.59E-08	0.51	13	2.44E-08	0.23
As_34	2.58E-08	0.51	14	2.45E-08	0.23
As_35	2.45E-08	0.53	15	2.36E-08	0.23
As_41	2.43E-08	0.53	16	2.31E-08	0.23
As_42	2.56E-08	0.51	17	2.44E-08	0.23
As_43	2.57E-08	0.51	18	2.44E-08	0.23
As_44	2.55E-08	0.51	19	2.44E-08	0.23
As_45	2.43E-08	0.53	20	2.3E-08	0.23
As_51	2.45E-08	0.53	21	2.31E-08	0.23
As_52	2.47E-08	0.52	22	2.36E-08	0.23
As_53	2.44E-08	0.53	23	2.31E-08	0.23

Calculation has been produced for the Air+H2O Vapor Density = 2.19958E-02 g/cm^3 (100 years down)

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Table Table 09/23/07-11. Absorbed Doses at the Cell #1 (see Figure 09/23/07-1,2,3: PWR-21 Geometry)

Down	Gamma Radiation Power for Cell #1		NO2	NNO3	
			gram produced over 90,000	gram produced over 90,000	moles produced over 90,000
Years	MeV/g/sec	rad/hr	years	years	years*
100	18823947	1085.7	1742049	2386050	3819
500	7971.2	0.4597	342	468	7
2000	4954.1	0.2857	57.2	78.3	1.2
10000	5474.7	0.31576	15.9	21.8	0.34
100000	13967.1	0.80559	14.2	19.5	0.31

**"The 74-mole quantity of HNO3 from the hypothetical static criticality calculation compares toapproximately 20moles of HNO3 produced over 90,000 years at < 4 rad/hr from radionuclide decay (BSC 2001b, Section 6)."*

See "Radiolytic Specie Generation from Internal Waste Package Criticality", Document Identifier: CAL-EBS-NU-000017 REV 00, Page 31

No new entries on this page

12/03/2007 (OP)(AK)
The following draft report was shared with NRC for comments.

Radiolytic Specie Generation From Waste Package Residual Radionuclide Decay

Scoping Calculation to Estimate Radiolytic Production of Nitric Acid in Waste Package Emplaced in Repository After Permanent Closure

BACKGROUND

Radiolytic processes in moist air environments lead to the fixation of nitrogen as NO, NO_2, and especially HNO_3. Nitric acid is assumed to be one of the corrosive radiolytic chemical species and is produced in an irradiated air-water vapor system when the hydroxyl radicals generated from the water vapor convert nitrogen oxides, that are formed by the radiolytic reaction between nitrogen and oxygen, to nitric acid.

PURPOSE

Estimate radiolytic nitric acid production in 21-PWR TAD WP disposed of in Yucca Mountain geologic repository.

METHODOLOGY

1. ORIGEN-ARP depletion model is constructed based on South Texas reactor campaign. Neutron and gamma radiation spectra are determined as function of time in repository for $t>100$ years.
2. TPA simulation is executed. The amount of water vapor in drift air is extracted from the output postprocessing.
3. The MCNP irradiation model of 21-PWR TAD WP is created.
4. Neutron and gamma energy absorption in water/vapor mixture are calculated using MCNP simulation.

ASSUMPTIONS

1. WP is breached, so water vapor penetrates the WP through the breach.
2. Time of breach > 100 years

3. The amount of water is determined by the relative humidity inside the drift. The water vapor concentration in air inside WP is equal to the concentration of water vapor in drift air outside WP.
4. Neutron and gamma decay radiations are functions of decay time
5. G (NO_2)=1.0 molecules/100 eV of energy absorbed by the water vapor. Number of produced NO_2 molecules equals number of HNO_3 molecules.
6. Produced nitric acid remains stable for sufficiently long time.
7. Energy absorption takes place only in TAD canister cavity space between assemblies and canister walls.

RESULTS

I. Assembly Type and Its Operating Parameters for Burnup Calculations

ORIGEN-ARP depletion model is based on South Texas reactor campaign based on data available from "*PWR Source Term Generation and Evaluation , Rev 0B, 2004*" AMR

Source:	*PWR Source Term Generation and Evaluation*
Document Identifier	*000-00C-MGR0-00100-000-00B*
Pages:	*Page 24 of 33*

The moderator temperature	578	K
Density of the moderator	0.7136	g/cm^3
Input average boron concentration	552.6316	ppm

Operational history of the assembly in the reactor one cycle and new libraries at least every 100 days

Thermal Reactor Power	2568	MWt
Assemblies in a core	177	
Power/Assembly	14.50847	MWt
MTU per Assembly	0.46363	MTU
Enrichement	5%	
Assembly	15 × 15 for Babcock & Wilcox and	

BurnUp	78.25865 GWd/MTU
BurnUp Days	2500.818 days

Fuel Type has been selected from the list of fuel types as ***"w15x15"*** - 15 × 15 for Babcock & Wilcox.

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II. OrigenARP Input and Output Parameters

OrigenARP calculations are performed for the assembly operation parameters.

OrigenARP input / output file hyperlinks are:

Origen ARP\PWR_P14.inp – Input file;

Origen ARP\PWR_P14.out – Output File;

Figure II.1 represents main (composition) screen of the OrigenARP GUI.

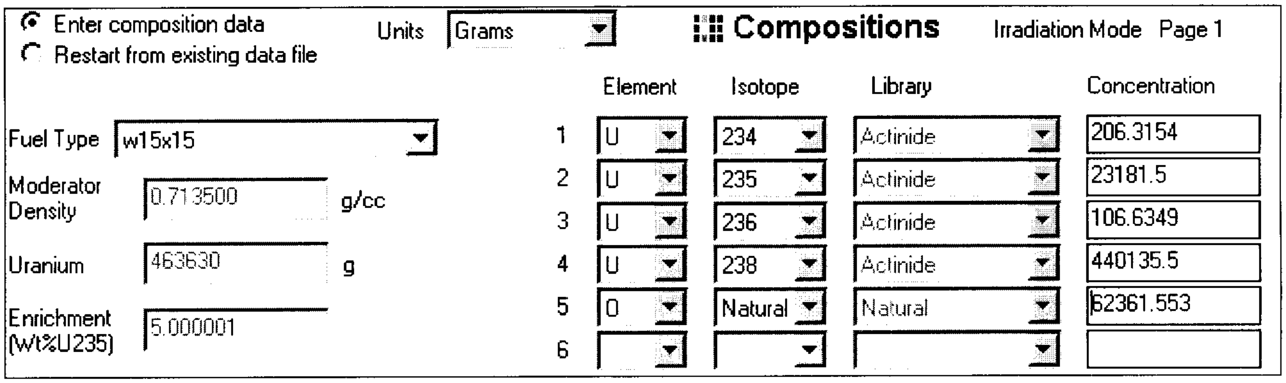

Figure II.1. Main screen of the OrigenARP GUI.

Neutron nuclide densities are recalculated from original OrigenARP output by converting them for MCNP input for each time step: 100, 500, 2 000, 10 000 and 100 000 years (see SN September 2007 Radiolysis.xls, sheet "Neutron Nuclides Densities").

Photon nuclide densities are recalculated from original OrigenARP output by converting them for MCNP input only for one time step - 500 years (see SN September 2007 Radiolysis.xls, sheet "Photon Nuclides Densities"), so all photon calculation cases uses the same material composition.

Neutron spectra for each time step adapted for 44 group library have been extracted from OrigenARP output file as is (see SN September 2007 Radiolysis.xls, Sheet "Neutron Spectra") and presents at the Table II.1.

Photon spectra for each time step adapted for 44 group photon library are extracted from OrigenARP output file as is (see SN September 2007 Radiolysis.xls, Sheet "Gamma Spectra") and presents at the Table II.2.

No new entries on this page

Table II.1. Total neutron spectra for basis = 0.46363 MTU neutrons/sec/basis

grp	Start	End	100 Years	500 Years	2000 Years	10,000 Years	100,000 Years
	MeV	MeV	n/sec/basis	n/sec/basis	n/sec/basis	n/sec/basis	n/sec/basis
1	1.00E-11	3.00E-09	5.137E-05	4.468E-05	3.602E-05	1.181E-05	7.537E-07
2	3.00E-09	7.50E-09	4.330E-05	3.187E-05	2.574E-05	8.548E-06	6.446E-07
3	7.50E-09	1.00E-08	2.264E-05	1.506E-05	1.217E-05	4.079E-06	3.400E-07
4	1.00E-08	2.53E-08	1.447E-04	8.317E-05	6.737E-05	2.301E-05	2.317E-06
5	2.53E-08	3.00E-08	4.828E-05	2.502E-05	2.031E-05	7.052E-06	8.192E-07
6	3.00E-08	4.00E-08	1.092E-04	5.404E-05	4.390E-05	1.537E-05	1.896E-06
7	4.00E-08	5.00E-08	1.178E-04	5.570E-05	4.529E-05	1.598E-05	2.089E-06
8	5.00E-08	7.00E-08	2.598E-04	1.174E-04	9.555E-05	3.400E-05	4.700E-06
9	7.00E-08	1.00E-07	4.445E-04	1.919E-04	1.563E-04	5.610E-05	8.197E-06
10	1.00E-07	1.50E-07	8.683E-04	3.602E-04	2.937E-04	1.063E-04	1.631E-05
11	1.50E-07	2.00E-07	1.019E-03	4.191E-04	3.440E-04	1.309E-04	1.992E-05
12	2.00E-07	2.25E-07	5.565E-04	2.261E-04	1.856E-04	7.080E-05	1.092E-05
13	2.25E-07	2.50E-07	5.853E-04	2.361E-04	1.938E-04	7.388E-05	1.149E-05
14	2.50E-07	2.75E-07	6.127E-04	2.458E-04	2.017E-04	7.684E-05	1.203E-05
15	2.75E-07	3.25E-07	1.303E-03	5.191E-04	4.260E-04	1.621E-04	2.558E-05
16	3.25E-07	3.50E-07	6.883E-04	2.727E-04	2.238E-04	8.508E-05	1.352E-05
17	3.50E-07	3.75E-07	7.117E-04	2.811E-04	2.307E-04	8.765E-05	1.398E-05
18	3.75E-07	4.00E-07	7.344E-04	2.893E-04	2.373E-04	9.013E-05	1.442E-05
19	4.00E-07	6.25E-07	7.533E-03	2.938E-03	2.410E-03	9.131E-04	1.479E-04
20	6.25E-07	1.00E-06	1.567E-02	6.038E-03	4.950E-03	1.868E-03	3.073E-04
21	1.00E-06	1.77E-06	4.169E-02	1.591E-02	1.304E-02	4.902E-03	8.170E-04
22	1.77E-06	3.00E-06	8.709E-02	3.305E-02	2.706E-02	1.014E-02	1.704E-03
23	3.00E-06	4.75E-06	1.577E-01	5.963E-02	4.882E-02	1.824E-02	3.080E-03
24	4.75E-06	6.00E-06	1.327E-01	5.009E-02	4.100E-02	1.530E-02	2.590E-03
25	6.00E-06	8.10E-06	2.550E-01	9.614E-02	7.869E-02	2.932E-02	4.975E-03
26	8.10E-06	1.00E-05	2.614E-01	9.845E-02	8.057E-02	2.999E-02	5.097E-03
27	1.00E-05	3.00E-05	4.047E+00	1.519E+00	1.243E+00	4.617E-01	7.876E-02
28	3.00E-05	1.00E-04	2.616E+01	9.807E+00	7.834E+00	2.896E+00	4.950E-01
29	1.00E-04	5.50E-04	3.712E+02	1.386E+02	1.115E+02	4.120E+01	7.035E+00
30	5.50E-04	3.00E-03	4.713E+03	1.758E+03	1.418E+03	5.241E+02	8.948E+01
31	3.00E-03	1.70E-02	6.382E+04	2.381E+04	1.915E+04	7.081E+03	1.208E+03
32	1.70E-02	2.50E-02	5.384E+04	2.008E+04	1.613E+04	5.967E+03	1.018E+03
33	2.50E-02	1.00E-01	8.365E+05	3.122E+05	2.513E+05	9.297E+04	1.585E+04
34	1.00E-01	4.00E-01	6.016E+06	2.246E+06	1.813E+06	6.706E+05	1.142E+05
35	4.00E-01	9.00E-01	1.308E+07	4.872E+06	3.934E+06	1.453E+06	2.466E+05
36	9.00E-01	1.40E+00	1.311E+07	4.858E+06	3.906E+06	1.441E+06	2.419E+05
37	1.40E+00	1.85E+00	1.068E+07	3.929E+06	3.107E+06	1.146E+06	1.892E+05
38	1.85E+00	2.35E+00	1.042E+07	3.795E+06	2.913E+06	1.076E+06	1.734E+05
39	2.35E+00	2.48E+00	2.313E+06	8.360E+05	6.280E+05	2.321E+05	3.676E+04
40	2.48E+00	3.00E+00	8.331E+06	2.987E+06	2.217E+06	8.172E+05	1.280E+05
41	3.00E+00	4.80E+00	1.426E+07	5.043E+06	3.872E+06	1.407E+06	2.168E+05
42	4.80E+00	6.43E+00	3.714E+06	1.295E+06	1.053E+06	3.771E+05	5.453E+04
43	6.43E+00	8.19E+00	1.158E+06	3.922E+05	3.190E+05	1.129E+05	1.512E+04
44	8.19E+00	2.00E+01	3.903E+05	1.265E+05	1.027E+05	3.579E+04	4.292E+03
		Total	**8.44316E+07**	**3.07377E+07**	**2.41528E+07**	**8.87528E+06**	**1.43898E+06**

Table II.2. Total Photon Spectra for basis = 0.46363 MTU [photons/sec/basis]

grp	Start MeV	End MeV	100 Years p/sec/basis	500 Years p/sec/basis	2000 Years p/sec/basis	10000 Years p/sec/basis	100000 Years p/sec/basis
1	1.00000E-02	2.00000E-02	1.34600E+14	2.51900E+13	5.32600E+12	1.74200E+12	1.64100E+11
2	2.00000E-02	3.00000E-02	4.51400E+13	3.95200E+12	4.63500E+11	7.21100E+10	2.62500E+10
3	3.00000E-02	4.50000E-02	5.39900E+13	2.96800E+11	1.58600E+11	7.34700E+10	1.50900E+10
4	4.50000E-02	6.00000E-02	6.55500E+13	2.35800E+13	2.17600E+12	2.80300E+10	1.02200E+10
5	6.00000E-02	7.00000E-02	1.00100E+13	3.67900E+10	3.09000E+10	1.67000E+10	4.91800E+09
6	7.00000E-02	7.50000E-02	5.71700E+12	1.41200E+12	1.22600E+12	5.78600E+11	5.40800E+09
7	7.50000E-02	1.00000E-01	1.67800E+13	2.40200E+11	2.03900E+11	1.14100E+11	4.53500E+10
8	1.00000E-01	1.50000E-01	1.78800E+13	1.29300E+12	1.11100E+12	5.28700E+11	1.12300E+10
9	1.50000E-01	2.00000E-01	1.07300E+13	1.45800E+10	1.24200E+10	7.98400E+09	7.22100E+09
10	2.00000E-01	3.00000E-01	8.88900E+12	6.17800E+11	5.37000E+11	2.58100E+11	2.41700E+10
11	3.00000E-01	4.00000E-01	5.88400E+12	8.37000E+10	7.84500E+10	4.97100E+10	3.93500E+10
12	4.00000E-01	4.50000E-01	1.72800E+12	2.30400E+10	2.29000E+10	2.17700E+10	1.57200E+10
13	4.50000E-01	5.10000E-01	1.65500E+12	5.31100E+08	3.98200E+08	3.81100E+08	1.43200E+09
14	5.10000E-01	5.12000E-01	1.17100E+09	2.45200E+06	5.73400E+05	4.73400E+06	3.62500E+07
15	5.12000E-01	6.00000E-01	7.28800E+11	6.28300E+08	5.72100E+08	6.06500E+08	8.79000E+08
16	6.00000E-01	7.00000E-01	3.54200E+14	8.25000E+10	4.77300E+10	4.80000E+10	4.84700E+10
17	7.00000E-01	8.00000E-01	7.11500E+11	2.38900E+09	2.21800E+09	2.55800E+09	5.35400E+09
18	8.00000E-01	1.00000E+00	7.66100E+11	1.32700E+09	1.23200E+09	1.53700E+09	3.89000E+09
19	1.00000E+00	1.20000E+00	3.37200E+11	6.44600E+08	6.82700E+08	1.82500E+09	1.02800E+10
20	1.20000E+00	1.33000E+00	1.54800E+11	1.04700E+08	1.36800E+08	6.30000E+08	4.34300E+09
21	1.33000E+00	1.44000E+00	4.30700E+10	7.40400E+06	5.16900E+07	6.05200E+08	4.70200E+09
22	1.44000E+00	1.50000E+00	1.39700E+10	8.86600E+07	8.75200E+07	8.83200E+07	9.07500E+07
23	1.50000E+00	1.57000E+00	1.27200E+10	2.94800E+06	1.83200E+07	2.14200E+08	1.83700E+09
24	1.57000E+00	1.66000E+00	1.78200E+10	2.16500E+06	1.15900E+07	1.34900E+08	1.04700E+09
25	1.66000E+00	1.80000E+00	1.03800E+10	1.80100E+07	1.23400E+08	1.39000E+09	1.07900E+10
26	1.80000E+00	2.00000E+00	4.72200E+09	3.17700E+06	1.92900E+07	2.12700E+08	1.64400E+09
27	2.00000E+00	2.15000E+00	8.10600E+08	5.55000E+05	8.74500E+06	1.06000E+08	8.25300E+08
28	2.15000E+00	2.35000E+00	1.84100E+07	7.03700E+06	3.48000E+07	3.71400E+08	2.88000E+09
29	2.35000E+00	2.50000E+00	3.08600E+06	5.24300E+05	9.08200E+06	1.10100E+08	8.57900E+08
30	2.50000E+00	3.00000E+00	2.85700E+08	8.31900E+06	3.26500E+06	1.01900E+07	7.20800E+07
31	3.00000E+00	3.50000E+00	5.14800E+06	1.78200E+06	1.64500E+06	2.93200E+06	1.86200E+07
32	3.50000E+00	4.00000E+00	2.98300E+06	1.02600E+06	8.39900E+05	3.22700E+05	6.57000E+04
33	4.00000E+00	4.50000E+00	1.72800E+06	5.94500E+05	4.86900E+05	1.87100E+05	3.80900E+04
34	4.50000E+00	5.00000E+00	1.00100E+06	3.44500E+05	2.82200E+05	1.08400E+05	2.20800E+04
35	5.00000E+00	5.50000E+00	5.80400E+05	1.99700E+05	1.63600E+05	6.28600E+04	1.28000E+04
36	5.50000E+00	6.00000E+00	3.36400E+05	1.15700E+05	9.48600E+04	3.64400E+04	7.42300E+03
37	6.00000E+00	6.50000E+00	1.95000E+05	6.70700E+04	5.50000E+04	2.11300E+04	4.30400E+03
38	6.50000E+00	7.00000E+00	1.13000E+05	3.88800E+04	3.18900E+04	1.22500E+04	2.49500E+03
39	7.00000E+00	7.50000E+00	6.55100E+04	2.25400E+04	1.84900E+04	7.10100E+03	1.44700E+03
40	7.50000E+00	8.00000E+00	3.79800E+04	1.30600E+04	1.07200E+04	4.11700E+03	8.38900E+02
41	8.00000E+00	1.00000E+01	4.48400E+04	1.54300E+04	1.26600E+04	4.86300E+03	9.90900E+02
42	1.00000E+01	1.20000E+01	2.31700E+03	7.97200E+02	6.54400E+02	2.51400E+02	5.12300E+01
43	1.20000E+01	1.40000E+01	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
44	1.40000E+01	2.00000E+01	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
		Total:	7.35556E+14	5.68282E+13	1.14000E+13	3.55006E+12	4.68476E+11

See SN September 2007 Radiolysis.xls, Sheet "Gamma Spectra"

No new entries on this page

III. MCNP Calculational Cases

Refined MCNP model is created for investigation of radiolytic generation of nitric acid and other species inside 21-PWR TAD WP within air-water vapor volume.

III.1. MCNP Input Data

Fuel is smeared in volume of a dry assembly with external volume sources in each of them (different set of cases for neutron and gamma transport).
Tables III.1, III.2 reflect MCNP case codes and their main parameters. Table III.3 consists of hyperlinks on MCNP input/output files.

Tables III.1 Common MCNP Input Parameters

Fuel Basket Plate:	11 mm Neutronit A978 analogous to 304B6 with 75%% B-10 and B-11	
Casc:	TAD canister	
Assembly:	Smeared Dry	
Filled With	Air + H2O	
BurnUp	78.25864508	GWd/MTU

Tables III.2. MCNP Case Codes

	Physics: (N/G)	Years of Decay	H2O in Air	Absorber Plates
	P	Y	H	AP
				11 mm Neutronit A978 analogous to 304B6 with 75%% B-10 and B-11
PN_Y100_H0_APB11	N	100	0	B11
PN_Y500_H0_APB11	N	500	0	B11
PN_Y2000_H0_APB11	N	2000	0	B11
PN_Y10000_H0_APB11	N	10000	0	B11
PN_Y100000_H0_APB11	N	100000	0	B11
PG_Y100_H0_APB11	G	100	0	B11
PG_Y500_H0_APB11	G	500	0	B11
PG_Y2000_H0_APB11	G	2000	0	B11
PG_Y10000_H0_APB11	G	10000	0	B11
PG_Y100000_H0_APB11	G	100000	0	B11

Tables III.3. MCNP Input/Output file hyperlinks

MCNP Case Codes	MCNP Input	MCNP Output
PN_Y100_H0_APB11	MCNP\Neutron\PN_Y100_H0_APB11.inp	MCNP\Neutron\PN_Y100_H0_APB11.out
PN_Y500_H0_APB11	MCNP\Neutron\PN_Y500_H0_APB11.inp	MCNP\Neutron\PN_Y500_H0_APB11.out
PN_Y2000_H0_APB11	MCNP\Neutron\PN_Y2000_H0_APB11.inp	MCNP\Neutron\PN_Y2000_H0_APB11.out
PN_Y10000_H0_APB11	MCNP\Neutron\PN_Y10000_H0_APB11.inp	MCNP\Neutron\PN_Y10000_H0_APB11.out

PN_Y100000_H0_APB11	MCNP\Neutron\PN_Y100000_H0_APB11.inp	MCNP\Neutron\PN_Y100000_H0_APB11.out
PG_Y100_H0_APB11	MCNP\Gamma\PG_Y100_H0_APB11.inp	MCNP\Gamma\PG_Y100_H0_APB11.out
PG_Y500_H0_APB11	MCNP\Gamma\PG_Y500_H0_APB11.inp	MCNP\Gamma\PG_Y500_H0_APB11.out
PG_Y2000_H0_APB11	MCNP\Gamma\PG_Y2000_H0_APB11.inp	MCNP\Gamma\PG_Y2000_H0_APB11.out
PG_Y10000_H0_APB11	MCNP\Gamma\PG_Y10000_H0_APB11.inp	MCNP\Gamma\PG_Y10000_H0_APB11.out
PG_Y100000_H0_APB11	MCNP\Gamma\PG_Y100000_H0_APB11.inp	MCNP\Gamma\PG_Y100000_H0_APB11.out

No new entries on this page

III.2. MCNP Input Data Geometry

Figures III.2.1 - III.2.3 below show MCNP cases geometry and location of the cell #1 – the cell where radiolysis processes in moist air environments lead to the fixation of nitrogen as NO_2. Vapor density and absorbed dose rate calculations are performed in the cell #1 as the most valuable cell for radiolysis processes.

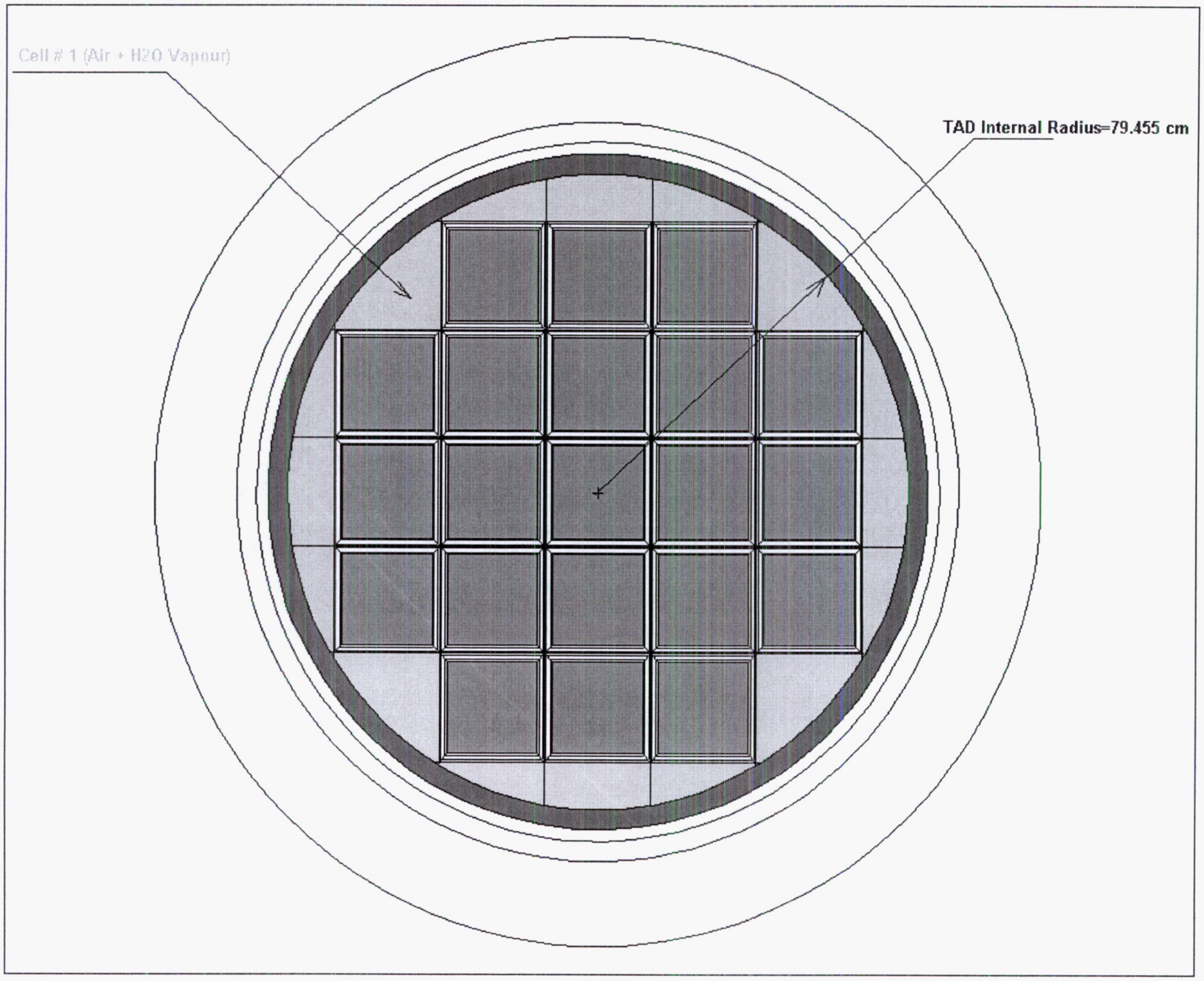

Figure III.2.1. PWR-21 Radial Geometry

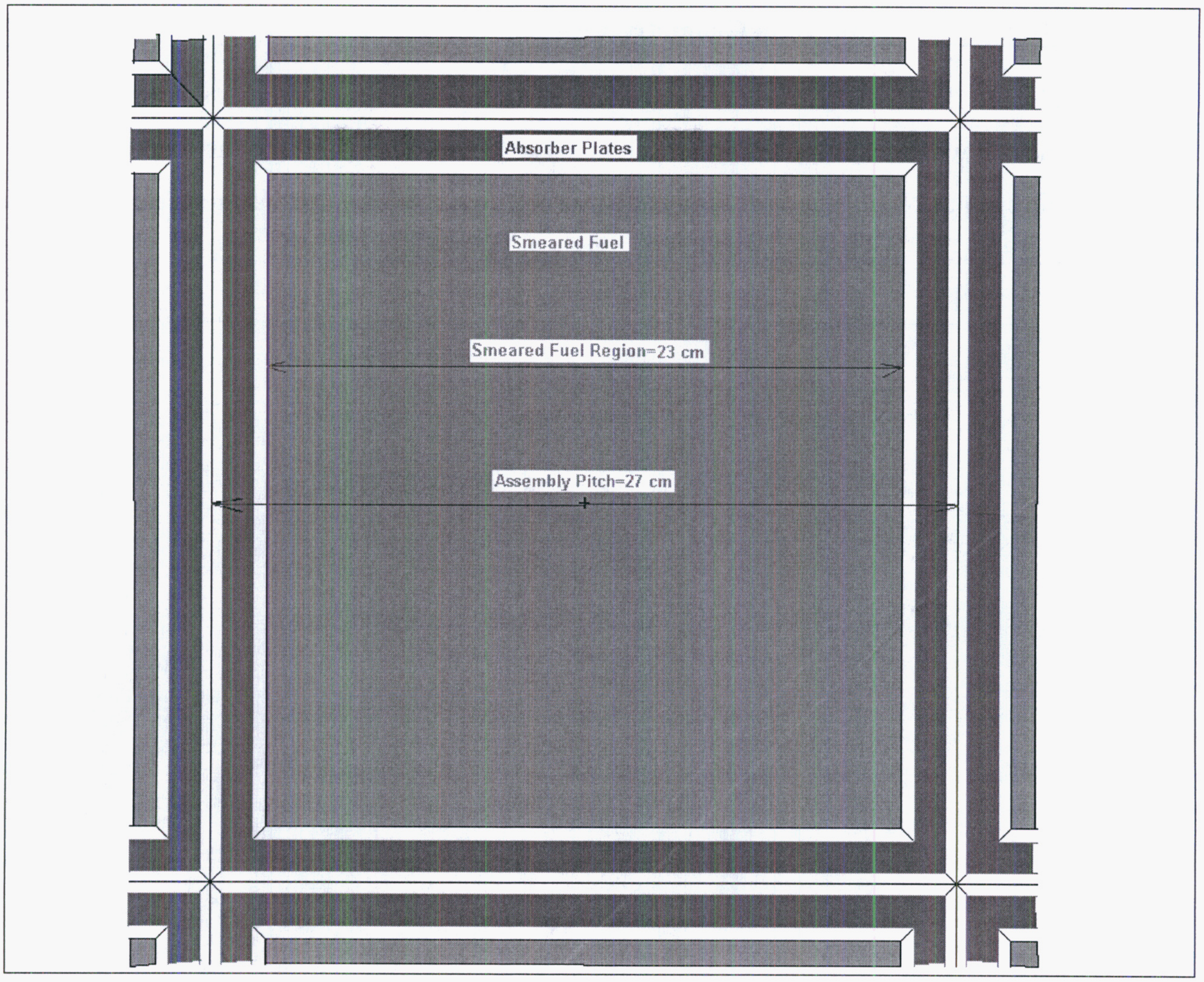

Figure III.2.2. Assembly Radial Geometry

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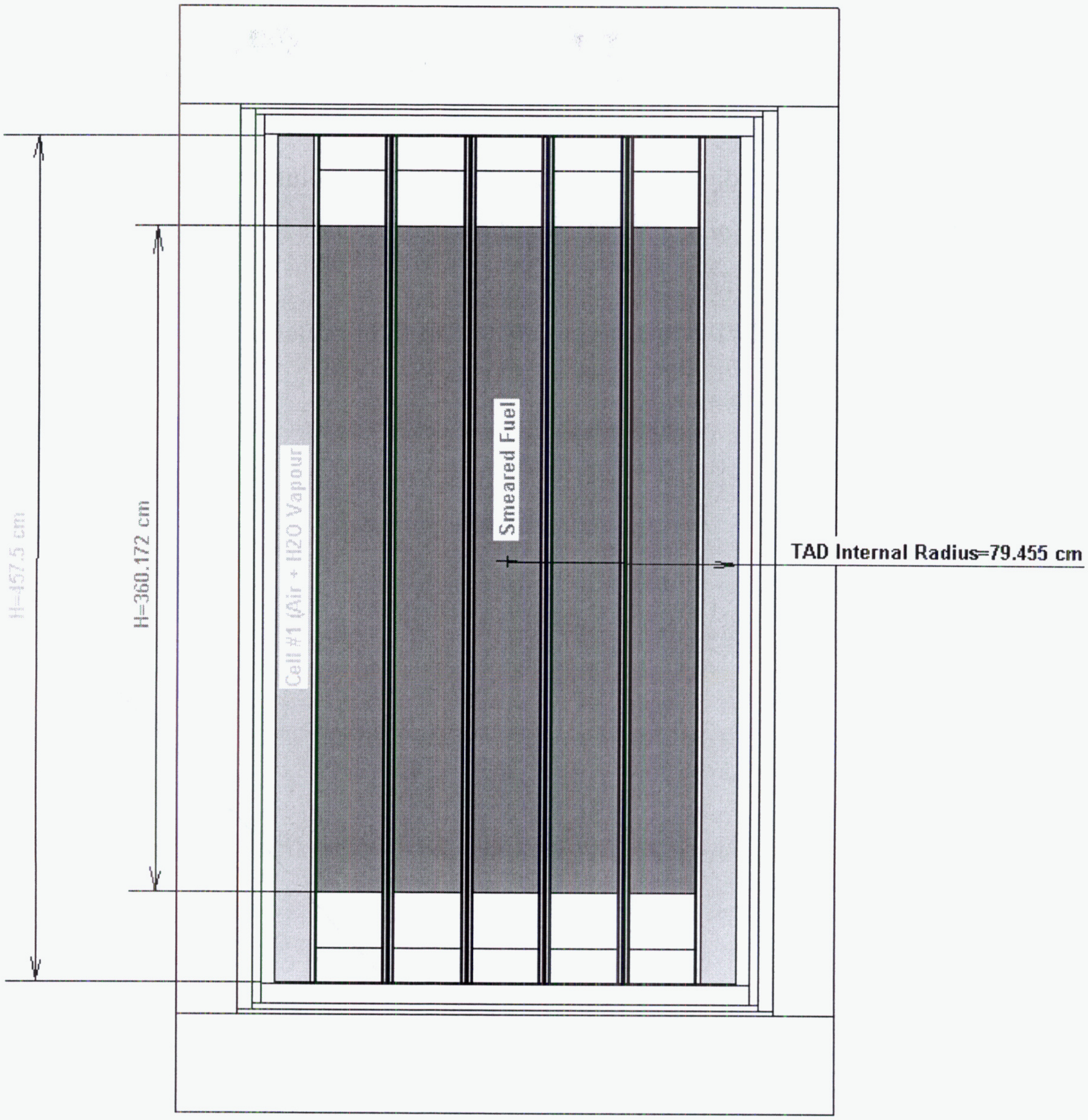

Figure III.2.3. PWR-21 Axial Geometry

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III.3. MCNP Cell Parameters

MCNP cell parameters are extracted from MCNP output and present at the Table II.3.1.
Total Assemblies Volume = 7.00388E+06 cm^3 = Summ(Cell#1011 : Cell#1053) - see SN September 2007 Radiolysis.xls, sheet "MCNP Cells Volumes"
Out of Assemblies Volume = calculated volume of Cell #1 - Total Assemblies Volume =
9.07368E+06 - 7.00388E+06 = 206981 cm^3
Volume of the cell #1 is used as an input in all future calculations.

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Table III.3.1. MCNP Cell Parameters

Cell	atom density	gram density	Input volume	calculated volume	Mass
1	**2.15408E-03**	**2.21868E-02**	**2.06981E+06**		**4.59225E+04**
1011	2.15408E-03	2.21868E-02		3.33518E+05	7.39969E+03
1012	2.15408E-03	2.21868E-02		3.33518E+05	7.39969E+03
1013	2.15408E-03	2.21868E-02		3.33518E+05	7.39969E+03
1021	2.15408E-03	2.21868E-02		3.33518E+05	7.39969E+03
1022	2.15408E-03	2.21868E-02		3.33518E+05	7.39969E+03
1023	2.15408E-03	2.21868E-02		3.33518E+05	7.39969E+03
1024	2.15408E-03	2.21868E-02		3.33518E+05	7.39969E+03
1025	2.15408E-03	2.21868E-02		3.33518E+05	7.39969E+03
1031	2.15408E-03	2.21868E-02		3.33518E+05	7.39969E+03
1032	2.15408E-03	2.21868E-02		3.33518E+05	7.39969E+03
1033	2.15408E-03	2.21868E-02		3.33518E+05	7.39969E+03
1034	2.15408E-03	2.21868E-02		3.33518E+05	7.39969E+03
1035	2.15408E-03	2.21868E-02		3.33518E+05	7.39969E+03
1041	2.15408E-03	2.21868E-02		3.33518E+05	7.39969E+03
1042	2.15408E-03	2.21868E-02		3.33518E+05	7.39969E+03
1043	2.15408E-03	2.21868E-02		3.33518E+05	7.39969E+03
1044	2.15408E-03	2.21868E-02		3.33518E+05	7.39969E+03
1045	2.15408E-03	2.21868E-02		3.33518E+05	7.39969E+03
1051	2.15408E-03	2.21868E-02		3.33518E+05	7.39969E+03
1052	2.15408E-03	2.21868E-02		3.33518E+05	7.39969E+03
1053	2.15408E-03	2.21868E-02		3.33518E+05	7.39969E+03
3	2.35422E-02	3.44986E+00		1.90531E+05	6.57305E+05
4	8.58620E-02	7.81992E+00		5.37562E+03	4.20369E+04
5	8.58620E-02	7.81992E+00		5.37562E+03	4.20369E+04
6	8.58620E-02	7.81992E+00		5.37562E+03	4.20369E+04
7	8.58620E-02	7.81992E+00		5.37562E+03	4.20369E+04
801	8.87710E-02	7.74452E+00		1.26316E+04	9.78255E+04
901	8.87710E-02	7.74452E+00		1.26316E+04	9.78255E+04
101	8.87710E-02	7.74452E+00		1.26316E+04	9.78255E+04
111	8.87710E-02	7.74452E+00		1.26316E+04	9.78255E+04
8	2.15408E-03	2.21868E-02		4.88015E+03	1.08275E+02
9	2.15408E-03	2.21868E-02		4.88015E+03	1.08275E+02
10	2.15408E-03	2.21868E-02		4.88015E+03	1.08275E+02
11	2.15E-03	2.22E-02		4.88E+03	1.08E+02
12	9.87E-02	1.78E+00		1.60E+04	2.84E+04
13	2.15E-03	2.22E-02		9.74E+03	2.16E+02
14	9.87E-02	1.78E+00		1.60E+04	2.84E+04
15	2.15E-03	2.22E-02		9.74E+03	2.16E+02
120	2.15E-03	2.22E-02		9.92E+03	2.20E+02
121	2.15E-03	2.22E-02		9.92E+03	2.20E+02
122	8.70E-02	7.96E+00		1.18E+06	9.40E+06
123	8.70E-02	7.96E+00		2.46E+05	1.96E+06
124	8.70E-02	7.96E+00		2.46E+05	1.96E+06
125	2.15E-03	2.22E-02		7.21E+04	1.60E+03
126	2.15E-03	2.22E-02		7.21E+04	1.60E+03
127	2.15E-03	2.22E-02		7.79E+05	1.73E+04

128	8.51E-02	8.69E+00	1.37E+06	1.19E+07
129	8.51E-02	8.69E+00	5.37E+04	4.67E+05
130	8.51E-02	8.69E+00	5.37E+04	4.67E+05
131	2.15E-03	2.22E-02	6.71E+06	1.49E+05
132	2.15E-03	2.22E-02	2.17E+06	4.81E+04
133	2.15E-03	2.22E-02	2.17E+06	4.81E+04
134	0.00E+00	0.00E+00	0.00E+00	0.00E+00

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IV. Waste package drift wall temperatures and vapor pressures and densities

Data on relative humidity are obtained, examined and analyzed to figure out vapor densities in the cell #1. WP and drift wall temperatures are available from TPA output. All calculations are performed and presented in SN September 2007 Radiolysis.xls, sheet “Drift wall temperature” and “Radiolysis Results” and Tables IV.1, IV.2 to determine water vapor parameters for MCNP model input.

Tables IV.1 Drift Wall Temperatures

Time[yr]	0.5	Mean
...		
8.56430E+01	1.46320E+02	1.46560E+02
8.99580E+01	1.46120E+02	1.46360E+02
9.43740E+01	1.45730E+02	1.45970E+02
9.88940E+01	1.45200E+02	1.45430E+02
1.03520E+02	1.40570E+02	1.40790E+02
1.08250E+02	1.38910E+02	1.39130E+02
...		
4.48250E+02	1.17840E+02	1.17980E+02
4.61060E+02	1.17450E+02	1.17590E+02
4.74160E+02	1.17060E+02	1.17200E+02
4.87570E+02	1.16610E+02	1.16750E+02
5.01300E+02	1.16110E+02	1.16250E+02
5.15350E+02	1.15590E+02	1.15730E+02
...		
1.85430E+03	7.99960E+01	8.01100E+01
1.90000E+03	7.91490E+01	7.92620E+01
1.94680E+03	7.83050E+01	7.84180E+01
1.99470E+03	7.74770E+01	7.75900E+01
2.04370E+03	7.66960E+01	7.68090E+01
2.09390E+03	7.59460E+01	7.60590E+01
...		
9.76900E+03	4.56260E+01	4.56950E+01
1.00000E+04	4.53450E+01	4.54140E+01
1.04500E+04	4.47640E+01	4.48310E+01
...		
1.00000E+05	2.51610E+01	2.51670E+01

Interpolation to 100 Years:

0.5	Mean
1.44093E+02	1.44321E+02

Interpolation to 500 Years:

0.5	Mean
1.16157E+02	1.16297E+02

Interpolation to 2000 Years:

0.5	Mean
7.73925E+01	7.75055E+01

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Tables IV.2 Drift Wall Temperatures and Corresponding Water Vapor Pressures and Densities

Time	Drift Wall temperature	X	Vapour Pressure*	Vapour Density**
Years	centigrades	x = 1.0 - (t+273.0)/647.3	Pa==n/m^2	g/cm^3
100	144.0930437	0.35564183	4.03886E+05	0.020795827
500	116.1573416	0.398799102	1.74788E+05	0.009645758
2,000	77.39252449	0.458686043	4.23425E+04	0.002595206
10,000	45.345	0.508195582	9.69178E+03	0.000653816
100,000	25.161	0.539377414	3.17352E+03	0.000228581

*Vapor Pressure= 221.2E+5 *exp((vpa * x +vpb * x**(1.5) + vpc * x**3 +vpd * x**6)/ (1 - x))
Vpa = - 7.76451;
Vpb = 1.45838;
Vpc = - 2.7758;
Vpd = - 1.23303;

** Vapor Density= $P * \mu / R / T$;
Where:
μ = 17.8559 (for H_2O)
R = 831,441 ± 0,00026 [J/(mole*K)]

(See SN September 2007 Radiolysis.xls, Sheet "Radiolise Results")

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V. Cells Absorbed Energies and Nitrogen Dioxide Production

Nitric acid is assumed to be the principal corrosive radiolytic chemical specie and is produced in an irradiated air-water vapor system when the hydroxyl radicals generated from the water vapor convert nitrogen dioxides, that are formed by the radiolytic reaction between nitrogen and oxygen, to nitric acids.

The **"G"** value represents the number of molecules of a chemical species produced per **100 eV** of

absorbed radiation energy in the volume containing the irradiated environment.

Measurements of the **"G"** factor for production of **nitrogen dioxide** (one-to-one production ratio for nitric acid) from mixed neutron-gamma radiation range from approximately **0.5 to 2.5** molecules/100 eV of absorbed energy (Reed and Van Konynenburg 1991). Present calculation assumed that the **"G"** factor for production of nitrogen dioxide is equal 1 (one molecule nitrogen dioxide and as a result one molecule of nitric acid per 100 eV of absorbed radiation energy)

All intermediate results are presented in the **SN September 2007 Radiolysis.xls**, Sheet:" Radiolysis Results", Cells: AB42:AB246 – Gamma; Cells: AJ42:AJ246 – Neutrons.

Table V.1 and V.2 represent Neutron and Gamma Radiation Power Calculation Results in cell #1 which are the input for Nitrogen Dioxide Production calculations presented in Table V.3 and V.4.

Table V.5 shows nitrogen dioxide accumulation from gamma radiation in cell #1 under assumption that no acid removal mechanisms present.

Nitrogen dioxide production power chart for gamma and neutron radiation depends on time step smoothed and represented at the Fig. V.1. Spline interpolation of the MCNP results is done to perform correct temporal integration and is presented in Figure V.1.

Spline approximation is performed by C# FunWork software (see solution at the FunWork_2005\FunWork\FunWork.sln and results at the FunWork_2005\FunWork\bin\Debug\Ln_G_Sec_SplineApproximation and FunWork_2005\FunWork\bin\Debug\Ln_G_Sec_Neutron_SplineApproximation)

Numerical integration is performed and verified in **SN September 2007 Radiolysis.xls**, Sheet:" Radiolysis Results", Cells: V41:AR646. Results of integration are presented at the Fig.V.2.

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Table V.1 Cell #1 Neutron Radiation Rate Calculation Results

Down Years	Neutron Spectrum Particles/ sec/basis	Assemblies	MCNP Case	MCNP F6 Tally:Neutron MeV/ g/Particle	Error	Neutron Radiation Rate per Gram of Weight MeV/g/sec
100	8.44316E+07	21	PN_Y100_H0_APB11	1.20909E-06	0.0063	2.14379E+0
500	3.07377E+07	21	PN_Y500_H0_APB11	1.15635E-06	0.0062	7.46414E+0
2000	2.41528E+07	21	PN_Y2000_H0_APB11	9.33076E-07	0.0062	4.73265E+0
10000	8.87528E+06	21	PN_Y10000_H0_APB11	5.54051E-07	0.0063	1.03264E+0
100000	1.43898E+06	21	PN_Y100000_H0_APB11	3.20950E-07	0.0051	9.69862E+0

Table V.2 Cell #1 Photon Radiation Rate Calculation Results

Down Years	Gamma Spectrum Particles/ sec/basis	Assemblies	MCNP Case	MCNP F6 Tally:Gamma MeV/ g/Particle	Relative Error	Photon Radiation Rat per Gram of Weight MeV/g/sec
100	7.35556E+14	21	PG_Y100_H0_APB11	1.21864E-09	0.0092	1.88239E+
500	5.68282E+13	21	PG_Y500_H0_APB11	6.67947E-12	0.0849	7.97122E+
2000	1.14E+13	21	PG_Y2000_H0_APB11	2.06937E-11	0.0477	4.95408E+
10000	3.55006E+12	21	PG_Y10000_H0_APB11	7.34349E-11	0.0322	5.47467E+
100000	4.68476E+11	21	PG_Y100000_H0_APB11	1.41971E-09	0.0106	1.39671E+

Table V.3 Nitric Acid Production in Cell #1 from Neutron Radiation

Down	Neutron Radiation Rate per Gram of Weight*	Vapour Density**	G-Factor for production of nitric acid	Nitric Acid Production in Cell #1 from Neutron Radiation		
Years	MeV/g/sec	g/cm^3	Moleculs/MeV	Moleculs/ cm^3/sec	Moleculs/sec	g/Year
100	2.14379E+03	2.07958E-02	10000	4.45819E+05	9.22302E+11	3.01932E-03
500	7.46414E+02	9.64576E-03	10000	7.19973E+04	1.48947E+11	4.87603E-04
2000	4.73265E+02	2.59521E-03	10000	1.22822E+04	2.54092E+10	8.31814E-05
10000	1.03264E+02	6.53816E-04	10000	6.75160E+02	1.39676E+09	4.57253E-06
100000	9.69862E+00	2.28581E-04	10000	2.21692E+01	4.58632E+07	1.50141E-07

* See Table 17 "Cell #1 Neutron Radiation Rate Power Calculation Results"
** See Table 16 "Drift Wall Temperatures and Calculated Vapour Pressures and Densities"

Table V.4 Nitric Acid Production in Cell #1 from Gamma Radiation

Down	Gamma Radiation Rate per Gram of Weight*	Vapor Density**	G-Factor for production of nitric acid	Nitric Acid Production in Cell #1 from Gamma Radiation		
Years	MeV/g/sec	g/cm^3	Moleculs/MeV	Moleculs/ cm^3/sec	Moleculs/sec	g/Year

100	1.88239E+07	2.07958E-02	10000	3.91460E+09	8.09844E+15	2.65117E+01
500	7.97122E+03	9.64576E-03	10000	7.68885E+05	1.59065E+12	5.20729E-03
2000	4.95408E+03	2.59521E-03	10000	1.28569E+05	2.65980E+11	8.70733E-04
10000	5.47467E+03	6.53816E-04	10000	3.57943E+04	7.40505E+10	2.42417E-04
100000	1.39671E+04	2.28581E-04	10000	3.19261E+04	6.60482E+10	2.16220E-04

* See Table 18 "Cell #1 Photon Radiation Rate Calculation Results"
** See Table 16 "Drift Wall Temperatures and Calculated Vapor Pressures and Densities"

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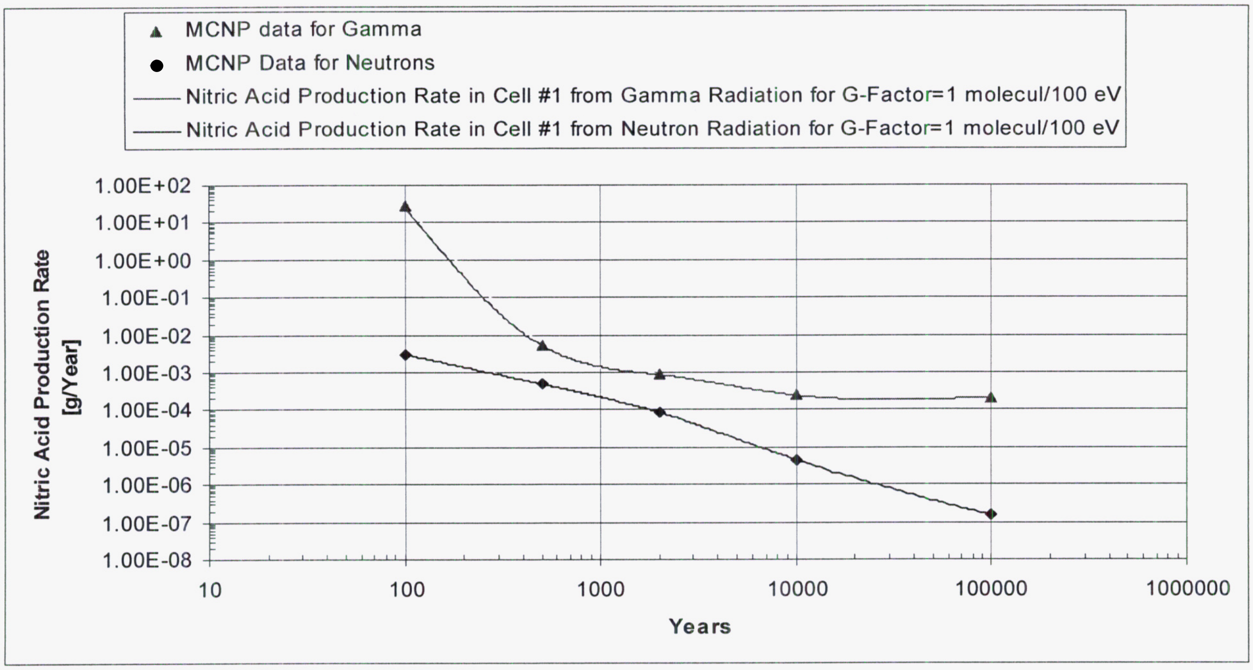

Figure V.1 Nitric Acid Production Rate

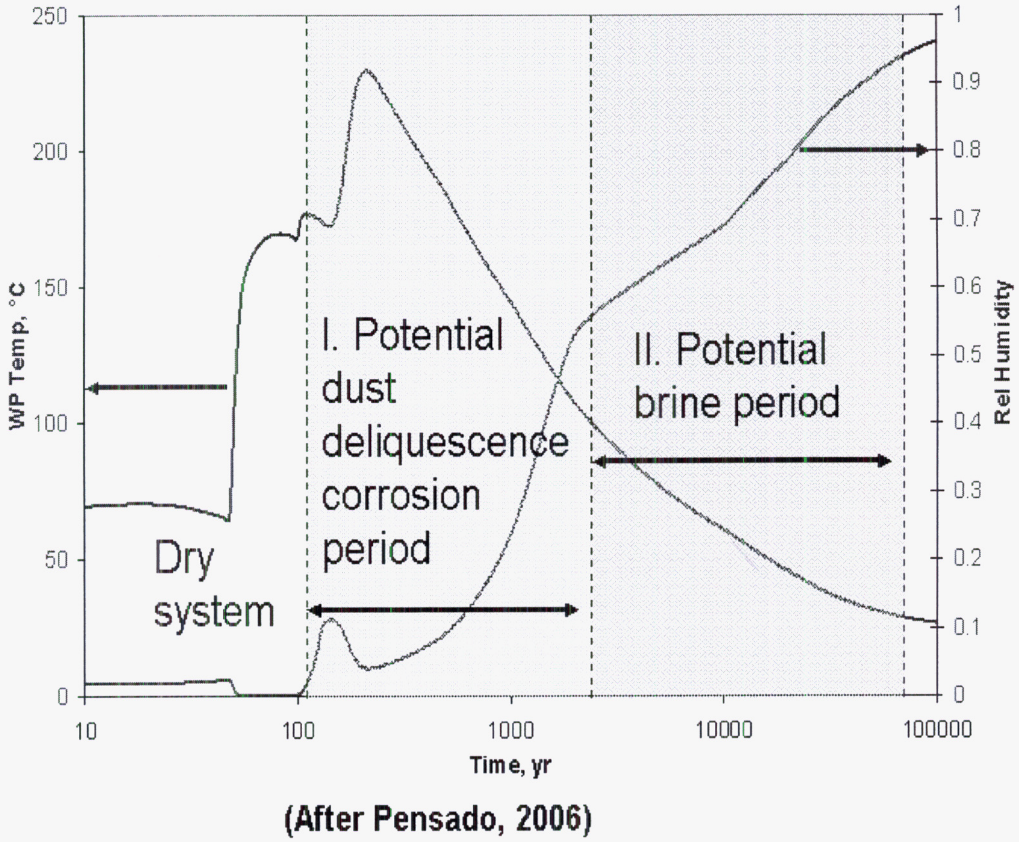

Figure V.1b Repository Thermal Periods (Pensado, 2006)

Table V.5 Nitric Acid Accumulation from Gamma Radiation in Cell #1
Under Assumption that No Acid Removal Mechanisms Present

Down Years	Gamma Radiation Rate per Gram of Weight* MeV/g/sec	G-Factor for production of nitric acid Moleculs/MeV	Nitric Acid Production in Cell #1 from Gamma Radiation gram
100	1.88239E+07	10000	0
500	7.97122E+03	10000	499.9
2000	4.95408E+03	10000	502.1
10000	5.47467E+03	10000	505.4
100000	1.39671E+04	10000	523.1

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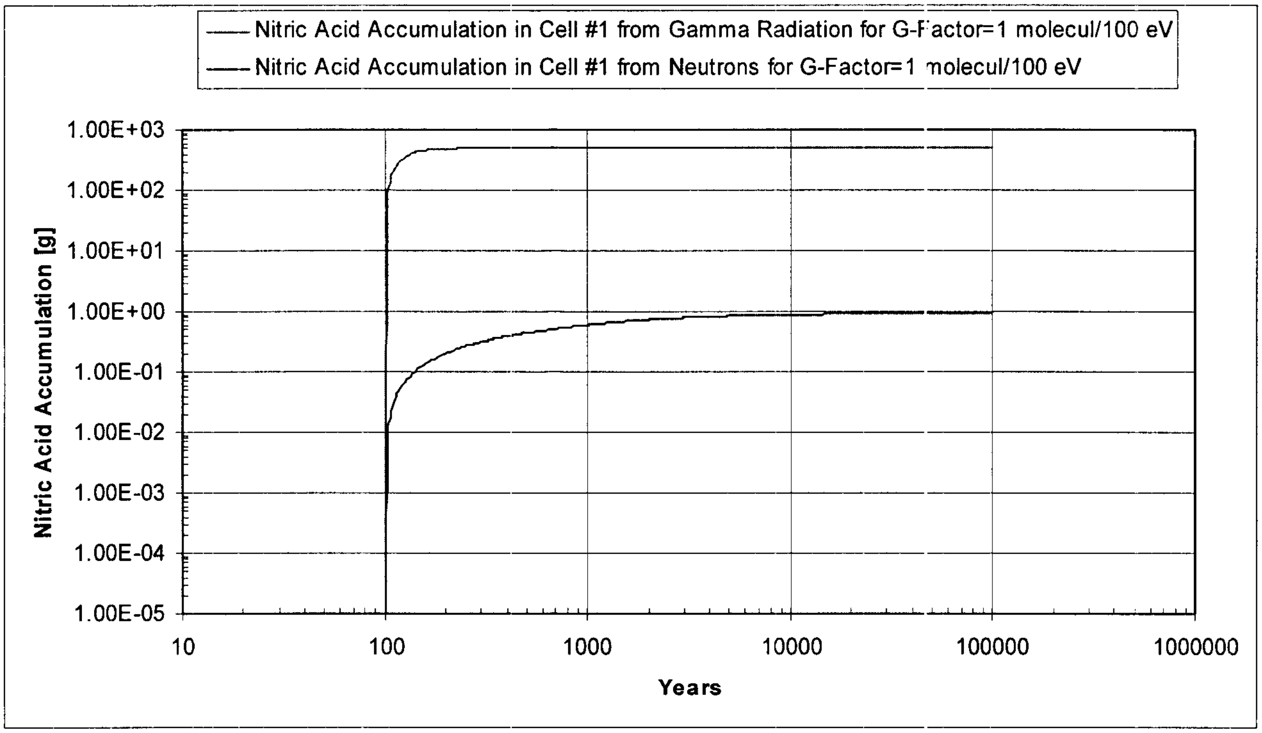

Figure V.2 Nitric Acid Accumulation under assumption that no acid removal mechanisms present

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VI. Verification of results

Results are checked by comparing with the RADCOG version 02.17 outputs and with the output data from "Radiolytic Specie Generation from Internal Waste Package Criticality", Document Identifier: CAL-EBS-NU-000017 REV 00, Page 32, Table 6.2.

RADCOG testing calculations:

PWR 21 simplified geometry is represented by twenty one fuel assemblies that irradiate air-vapor volume inside "TAD Internal" 3D Element (see Figures VI.1, VI.2). Absorbed energy calculation results for gamma sources with different energies listed at the Tables VI.1, VI.2. All results are produced for the Air/H_2O vapor density **2.19958E-02** g/cm^3 which represents 100-year case.

RADCOG Input / Output file hyperlinks are:

PWR 21\PWR-21 Simplified Model Radiolisis.hpr

PWR 21\PWR-21 Simplified Model Radiolisis DosesResults 1000_000.xls

Correspondence MCNP Input / Output file hyperlinks are:

PWR 21\PWR-21 Simplified Model Radiolisis.inp

PWR 21\PWR-21 Simplified Model Radiolisis.out

Tables VI.1 RadCog and MCNP Absorbed Energy Calculations Results for a 4 MeV Mono-energetic Isotropic Volume Source

RADCOG	MCNP	Difference
100,000 chords	1,000,000 particles	
Mev/g/particle	Mev/g/particle	%
8.64E-08	8.65E-08	0
2.66E-07	2.59E-07	-3
2.79E-07	2.76E-07	-1
2.59E-07	2.61E-07	1
2.62E-07	2.59E-07	-1
3.00E-07	2.98E-07	-1
3.11E-07	3.06E-07	-2
3.01E-07	2.98E-07	-1
2.66E-07	2.59E-07	-3
2.77E-07	2.72E-07	-2
3.11E-07	3.07E-07	-1
3.13E-07	3.08E-07	-1
3.02E-07	3.06E-07	1

2.75E-07	2.75E-07	0
2.57E-07	2.61E-07	2
3.01E-07	3.01E-07	0
3.12E-07	3.10E-07	0
2.96E-07	2.99E-07	1
2.59E-07	2.59E-07	0
2.66E-07	2.60E-07	-2
2.77E-07	2.77E-07	0
2.58E-07	2.61E-07	1

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Tables VI.2 RADCOG and MCNP Absorbed Dose Calculations Results for Radionuclide Decay Gamma Source for 100 Years From OrigenARP Output

RADCOG 1,000,000 chords			MCNP 10,000,000 particles		
Computer time = 10.78 minutes			Computer time = 15.53 minutes		
3-D Element:	Mev/g/particle:	Stat. Error(%):	Cell#	Mev/g/particle:	Stat. Error(%):
TAD Internal	3.67E-09	0.43	2	4.15E-09	0.17
As_11	2.46E-08	0.53	3	2.3E-08	0.23
As_12	2.48E-08	0.52	4	2.36E-08	0.23
As_13	2.45E-08	0.53	5	2.31E-08	0.23
As_21	2.48E-08	0.52	6	2.31E-08	0.23
As_22	2.56E-08	0.51	7	2.44E-08	0.23
As_23	2.57E-08	0.51	8	2.45E-08	0.23
As_24	2.57E-08	0.51	9	2.43E-08	0.23
As_25	2.48E-08	0.52	10	2.31E-08	0.23
As_31	2.52E-08	0.52	11	2.35E-08	0.23
As_32	2.59E-08	0.51	12	2.45E-08	0.23
As_33	2.59E-08	0.51	13	2.44E-08	0.23
As_34	2.58E-08	0.51	14	2.45E-08	0.23
As_35	2.45E-08	0.53	15	2.36E-08	0.23
As_41	2.43E-08	0.53	16	2.31E-08	0.23
As_42	2.56E-08	0.51	17	2.44E-08	0.23
As_43	2.57E-08	0.51	18	2.44E-08	0.23
As_44	2.55E-08	0.51	19	2.44E-08	0.23
As_45	2.43E-08	0.53	20	2.3E-08	0.23
As_51	2.45E-08	0.53	21	2.31E-08	0.23
As_52	2.47E-08	0.52	22	2.36E-08	0.23
As_53	2.44E-08	0.53	23	2.31E-08	0.23

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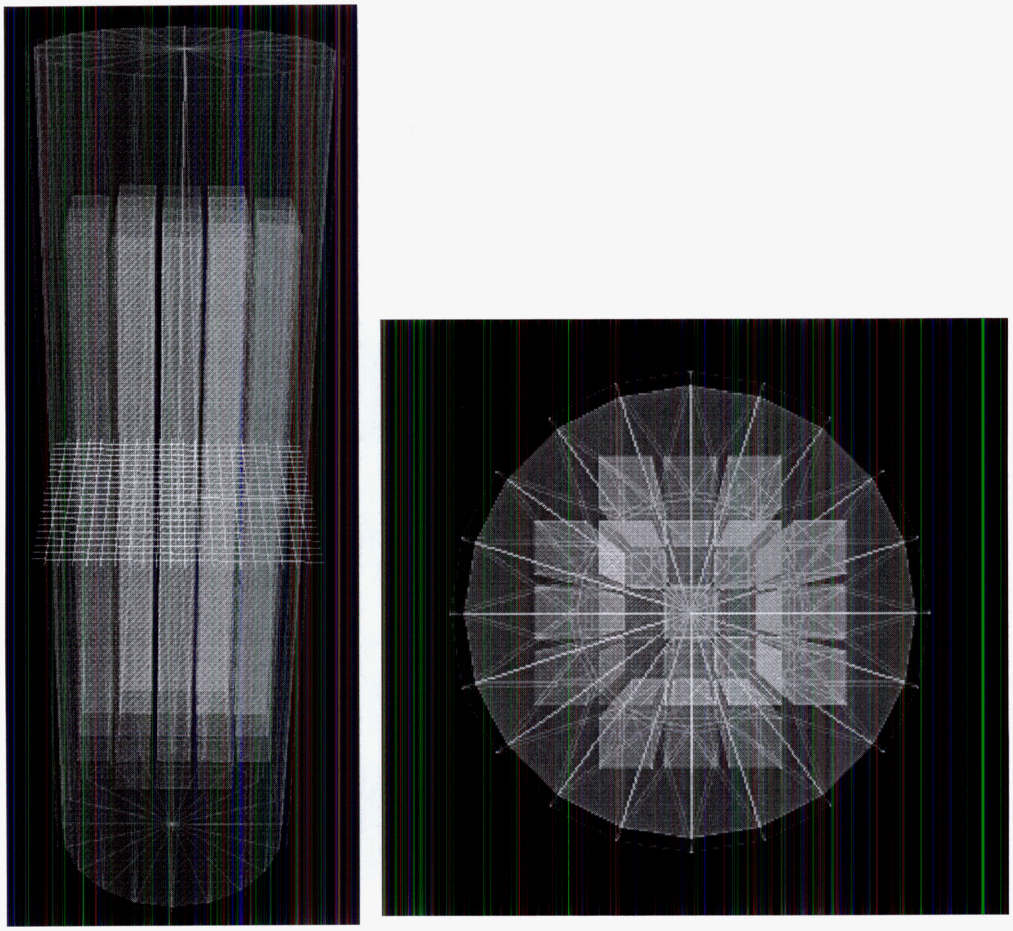

Figures VI.1 PWR-21 TAD WP Simplified Geometry as Represented in RADCOG Model

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- TAD External
  - TAD Internal
    - As_11
    - As_12
    - As_13
    - As_21
    - As_22
    - As_23
    - As_24
    - As_25
    - As_31
    - As_32
    - As_33
    - As_34
    - As_35
    - As_41
    - As_42
    - As_43
    - As_44
    - As_45
    - As_51
    - As_52
    - As_53

Figures VI.2 PWR-21 TAD WP Simplified Geometry 3D Elements and Their Hierarchy in RADCOG model

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Comparisons of the results with data from "Radiolytic Specie Generation from Internal Waste Package Criticality"

In Tables VI.3 presents gamma radiation decay powers and corresponding nitric acid production in the Cell #1 in assuming a constant gamma radiation decay rate over 90,000 years. Data has been presented only for comparison purposes.

According Tables VI.3, row #1, 7.5 moles of HNO3 produced over 90,000 years at 0.4597 rad/hr from radionuclide decay. For 4 rad/hr it would be approximately 65 moles – 3 times more then shown in "*Radiolytic Specie Generation from Internal Waste Package Criticality*"

Tables VI.3 Nitric Acid Production in the Cell #1 Estimation in Assuming of a Constant Gamma Radiation Decay Power Over 90,000 years

Down	Gamma Radiation Decay Power for Cell #1		NO2	NNO3	
Years	MeV/g/sec	rad/hr	gram produced over 90,000 years	gram produced over 90,000 years	moles produced over 90,000 years*
500	7971.2	0.4597	342	468	7.5
2000	4954.1	0.2857	57.2	78.3	1.25
10000	5474.7	0.31576	15.9	21.8	0.349
100000	13967.1	0.80559	14.2	19.5	0.311

* *"The 74-mole quantity of HNO3 from the hypothetical static criticality calculation compares toapproximately 20moles of* HNO_3 *produced over 90,000 years at < 4 rad/hr from radionuclide decay (BSC 2001b, Section 6)."*

See "*Radiolytic Specie Generation from Internal Waste Package Criticality*", Document Identifier: CAL-EBS-NU-000017 REV 00, Page 31

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CONCLUSIONS

The rate of nitric acid radiolytic production by decay radiation is the highest for earlier years when the radiation rates are higher; the rate drops exponentially with time.

The time point of 100 years was selected as the onset of the dust deliquescence corrosion period (Pensado, 2006, page 5). The nitric acid production rate is presented in Figure V.1. The production rate is found to be about 26.5 grams per year per waste package at the year 100. After this onset the rate drops exponentially to about 5 milligrams per year by the year 500. The cumulative data presented in Figure V.2 should be taken cautiously because the cumulative amount of acid is determined mostly by the selection of the initial time point (i.e. 100 years in this calculation). The later the onset time point of acid accumulation the lower the accumulation plateau is on the plot in Figure V.2.

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01/02/08 (AK)(OP)

The total energy deposited in cell #1 increases after 2000 years. The possible cause is the modification of gamma spectrum. In order to investigate why the increase occurs, some gamma spectrum normalizations were made combined with DCF(E) graphical representation.

#11/22/07

Performed set of calculations to support explanation of increasing of the total energy deposited in a cell after 2000 years of cooling time;

$$Dose \approx \int_E \Sigma(E)\overline{\Phi}_V(E)dE$$

Where

Dose (Gy/sec) – Dose in the Cell #1;

$\Sigma(E)$ - Photon Flux-to-Dose Rate Conversion Factor (Gy/sec)/(p/cm^2-s);

$\overline{\Phi}_V(E)$ - Average Photon Spectrum in the Cell #1 (p/cm^2-s/MeV);

Because $\overline{\Phi}_V(E)$ mostly depends on the Source Spectrum and because Spectrum in the Cell #1 does NOT depend on vapor density (it's too small to absorb photons significantly), Dose in the cell #1 will depend mostly on "hardness" of the photon spectrum in the cell #1 that depends on the photon source.

$\Sigma(E)$ - Photon Flux-to-Dose Rate Conversion Factor – depends on the Energy also, so the high-energetic photons will weigh more.

Figures 11/22/07-1, 11/22/07-2 and 11/22/07-2 present photon spectra and Photon Flux-to-Dose Rate Conversion Factor and can explain, why after 2000 years dose in the cell #1 increases.

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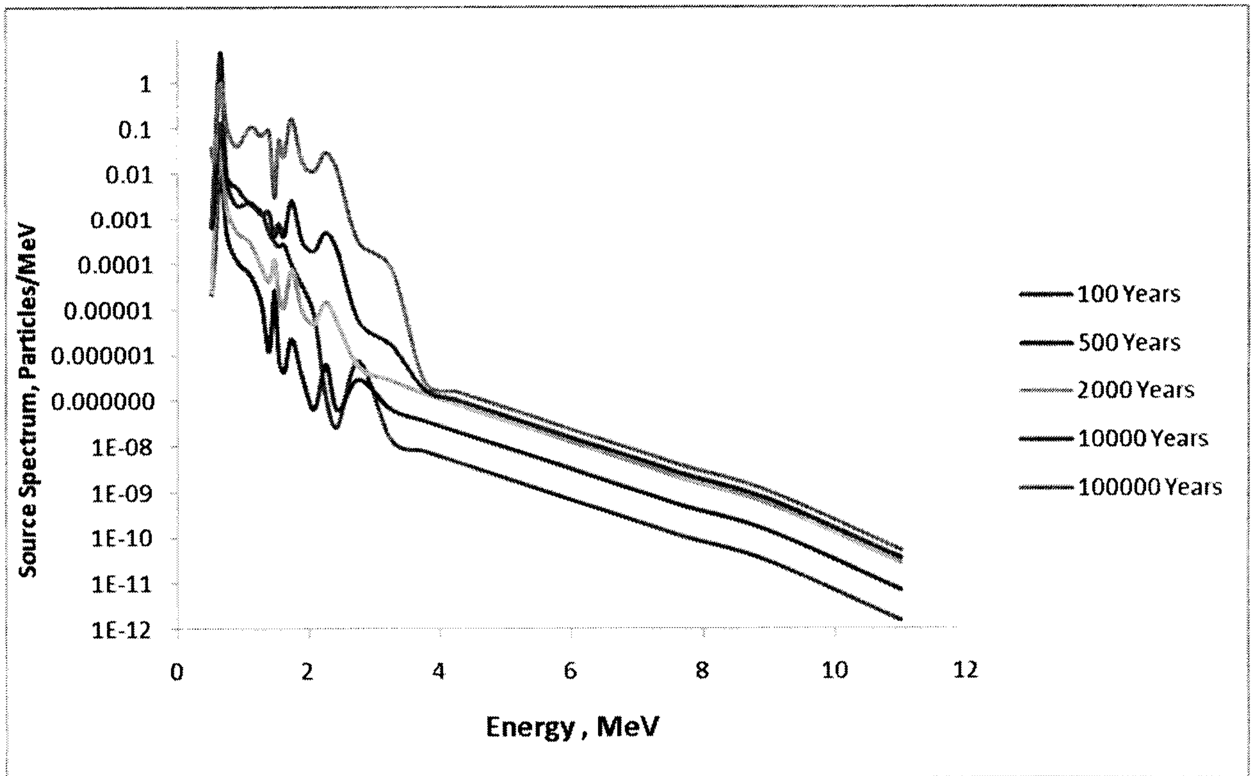
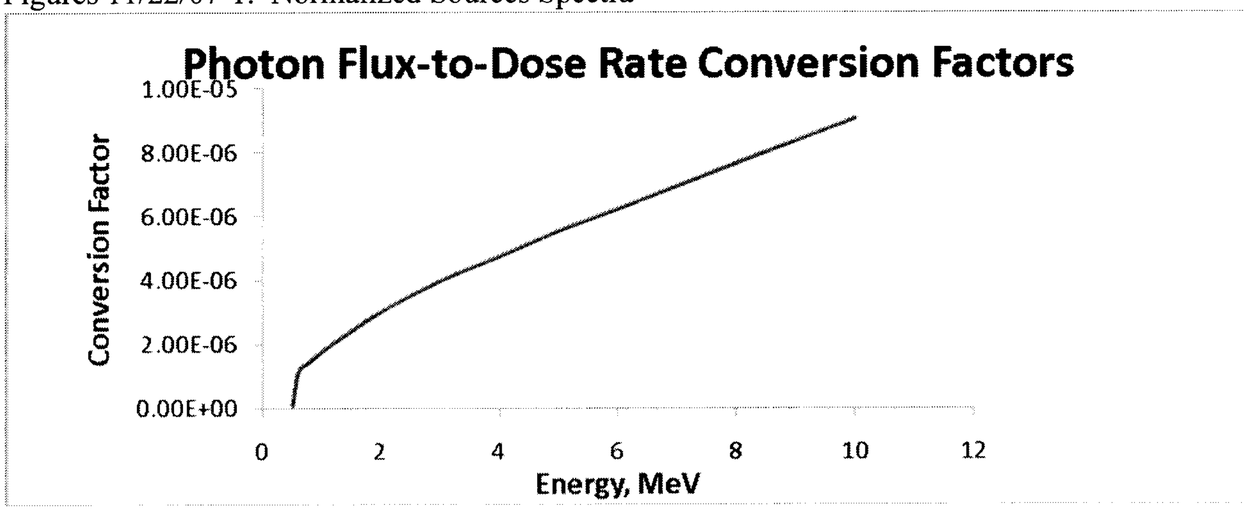
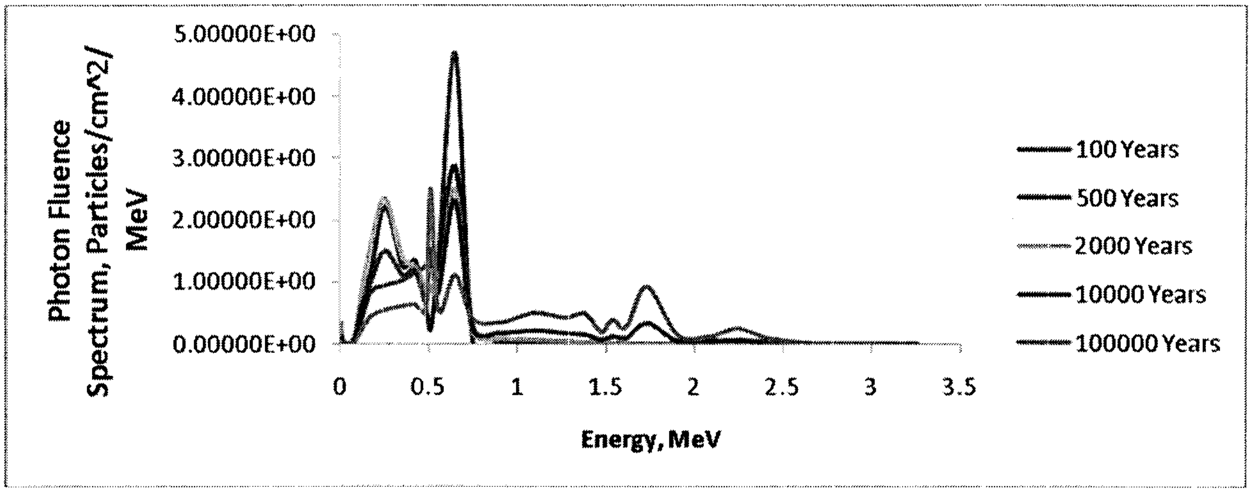


Figures 11/22/07-1. Normalized Sources Spectra



Figures 11/22/07-2. Photon Flux-to-Dose Rate Conversion Factors



Figures 11/22/07-3. Normalized Spectra in the Cell #1

Conclusion: Gamma spectrum hardens with time. This hardening causes increase of deposited energy since DCF increases with E.

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01/03/08 (AK)(OP)

Peroxide (H_2O_2) production was calculated on the external surface of the WP in thin water film.
Source of energy: gamma rays from maximum CSNF.
Medium: 0.67 mm water film.
Peroxide production G factor is assumed=0.68 molecule per 100 eV of absorbed gamma energy.

Cell 1310 (water film on WP surface) Absorbed Energies and Peroxide Production

The "G" value represents the number of molecules of a chemical species produced per 100 eV of absorbed radiation energy in the volume containing the irradiated environment. In present calculations assumed that the **"G"** factor for production of Peroxide is equal 0.68 molecule per 100 eV of absorbed radiation energy
All intermediate results are presented in the SN December 2007 Radiolysis.xlsx,

Sheet:" Radiolysis Results - Peroxid"

Table 12/26/07-1 represent Gamma Radiation Power Calculation Results in cell #1310 which are the input for Peroxide Production calculations presented in Table 12/26/07-2 Table 12/26/07-3 shows Peroxide accumulation from gamma radiation in cell #1310 under assumption that no acid removal mechanisms present.
Nitrogen dioxide production power chart for gamma radiation depends on time step smoothed and represented at the Fig 12/26/07-1 Spline interpolation of the MCNP results has been done to perform correct integrating over time and presents at the Figure 12/26/07-2.

Spline approximation has been performed by C# FunWork software (see "Report …"

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Table 12/26/07-1. Cell #1310 Photon Radiation Rate Calculation Results

Down	Years	100	500	2000	10000	100000
Gamma Spectrum	Particles/sec/basis	7.356E+14	5.683E+13	1.140E+13	3.550E+12	4.685E+11
# Assemblies		21	21	21	21	21
MCNP F6 Tally:Gamma	MeV/g/Particle	1.858E-12	1.091E-14	4.038E-14	3.495E-13	1.520E-11
Relative Error		2.800E-02	4.245E-01	2.169E-01	9.170E-02	2.440E-02
Statistic	Particles	6.607E+07	7.725E+07	7.228E+07	6.795E+07	1.818E+07
Gamma	MeV/g/sec	2.870E+04	1.302E+01	9.668E+00	2.605E+01	1.495E+02
Radiation Power	Gy/sec	4.598E-06	2.086E-09	1.549E-09	4.174E-09	2.396E-08
per Gram of	Gy/hr	1.655E-02	7.510E-06	5.576E-06	1.503E-05	8.62E-05
Weight*	rad/hr	1.655E+00	7.510E-04	0.000558	0.001503	0.008625

Table 12/26/07-1 Peroxide Production in Cell #1310 from Gamma Radiation

Down Years	Gamma Radiation Power rad/hr	G-Factor for production of Peroxide Moleculs per 100 eV	Peroxide Production in Cell #1310 from Gamma Radiation g/Year
100	1.655134	0.68	6.58570E-03
500	0.000751	0.68	2.98812E-06
2000	0.000558	0.68	2.21878E-06
10000	0.001503	0.68	5.97898E-06
100000	0.008625	0.68	3.43177E-05

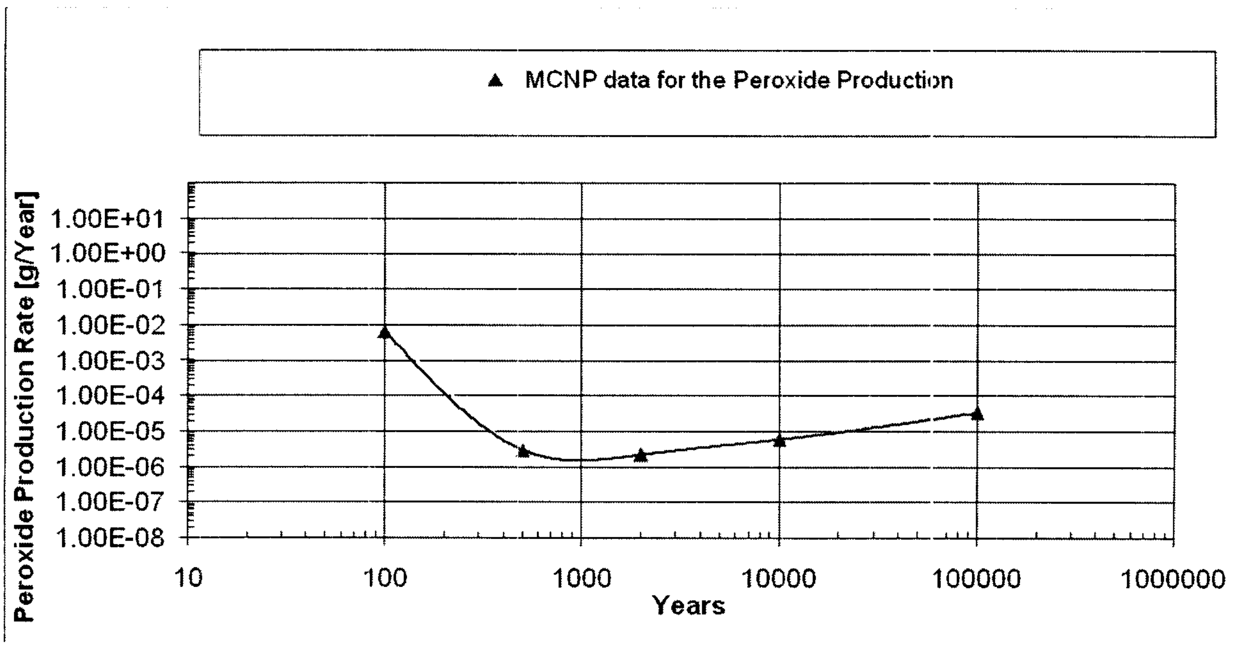

Figure 12/26/07-1. Peroxide Production Rate

Table 12/26/07-1 Peroxide Accumulation from Gamma Radiation in Cell #1310 Under Assumption that No Acid Removal Mechanisms Present

Down Years	Gamma Radiation Power rad/hr	G-Factor for production of nitrogen dioxide Moleculs per 100 eV	Peroxide Production g
100	1.692883	0.68	0
500	0.000754	0.68	0.134911
2000	0.000559	0.68	0.137651
10000	0.002347	0.68	0.172177
100000	0.008471	0.68	2.039827

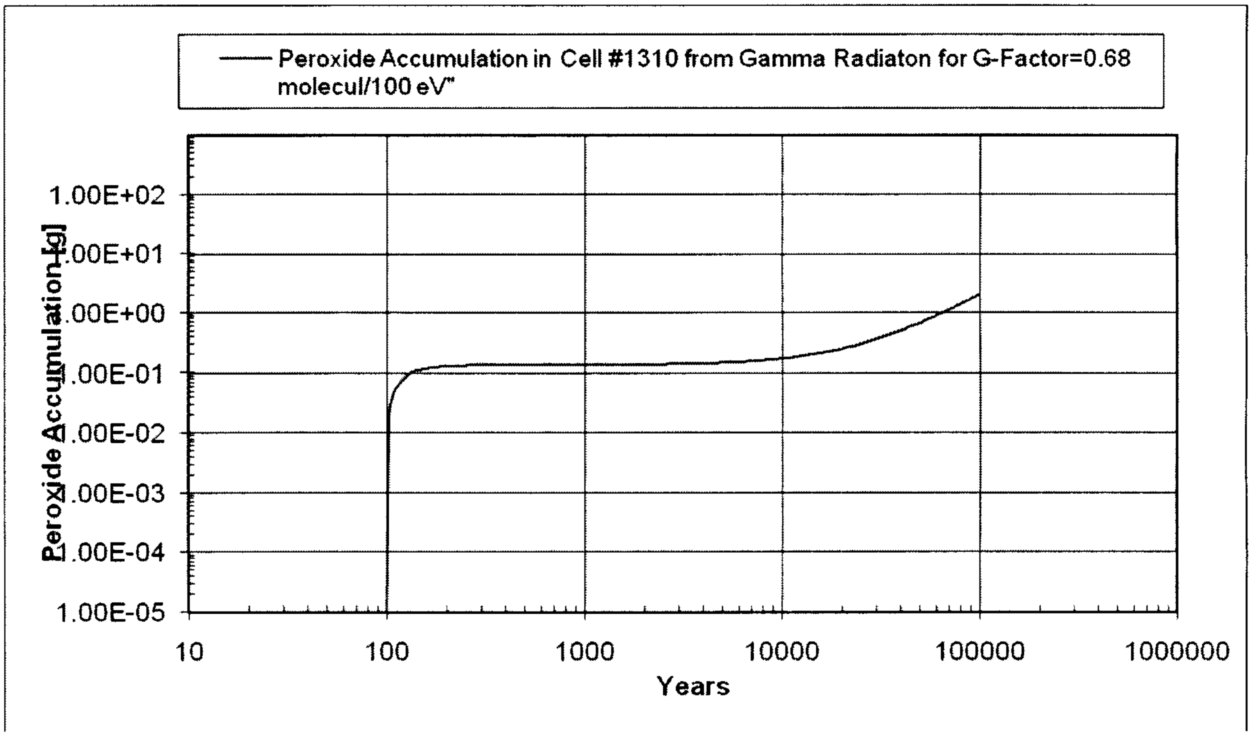

Figure 12/26/07-2 Peroxide Accumulation under assumption that no acid removal mechanisms present

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#12292007 #12302007

Investigation of increasing of deposited gamma energy after 2000 years

Performed set of calculations to support explanation of increasing of the total energy deposited in a cell after 2000 years of cooling time;

$$Dose \approx \int_E \Sigma(E)\overline{\Phi}_V(E)dE$$

Where

Dose (Gy/sec) – Dose in the Cell #1;

$\Sigma(E)$ - Photon Flux-to-Dose Rate Conversion Factor (Gy/sec)/(p/cm^2-s);

$\overline{\Phi}_V(E)$ - Average Photon Spectrum in the Cell #1 (p/cm^2-s/MeV);

Because $\overline{\Phi}_V(E)$ mostly depends on the Source Spectrum and because Spectrum in the Cell #1 does NOT depend on vapor density (it's too small to absorb photons significantly), Dose in the cell #1 will depend mostly on "hardness" of the photon spectrum in the cell #1 that depends on the photon source.

$\Sigma(E)$ - Photon Flux-to-Dose Rate Conversion Factor – depends on the Energy also, so the high-energetic photons will weigh more.

Figures 11/22/07-1, 11/22/07-2 and 11/22/07-2 present photon spectra and Photon Flux-to-Dose Rate Conversion Factor and can explain, why after 2000 years dose in the cell #1 increases.

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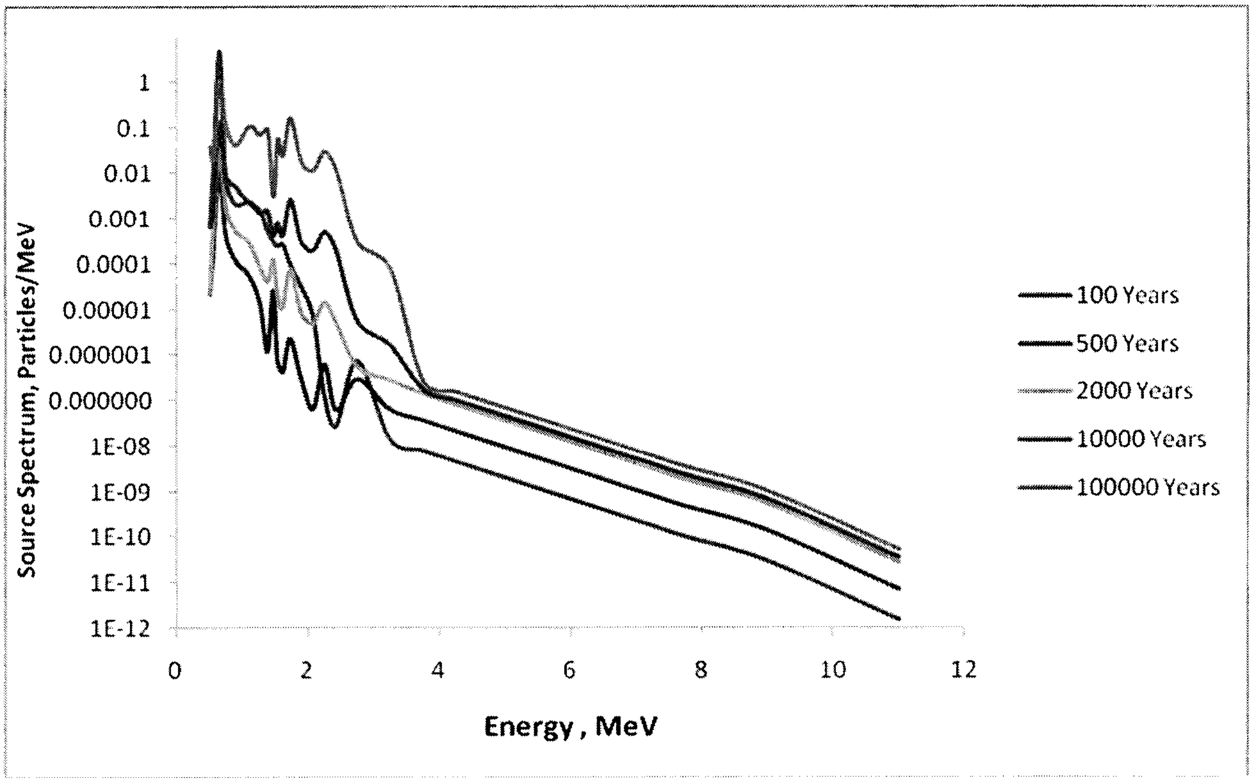
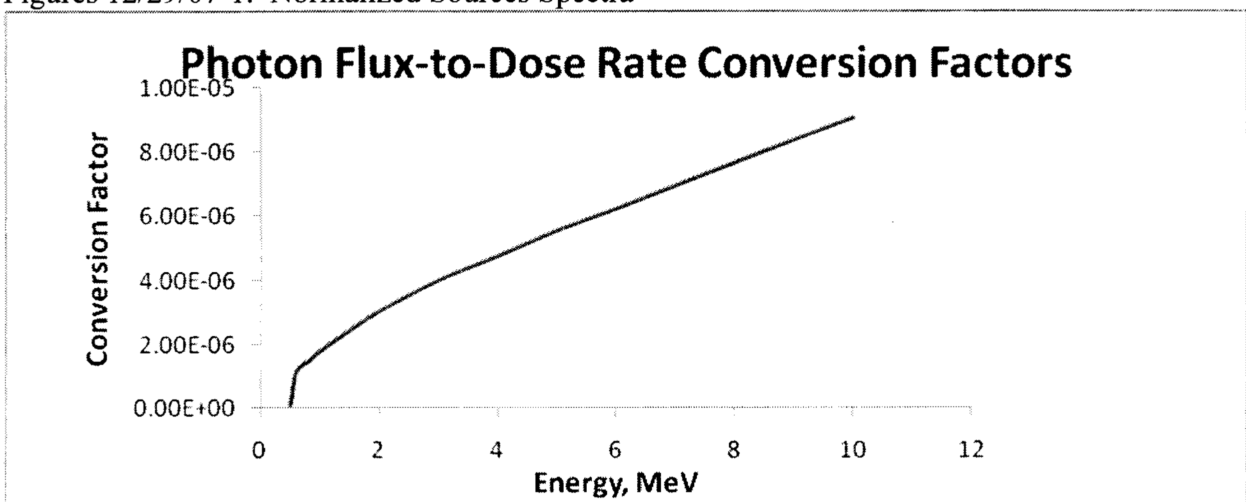
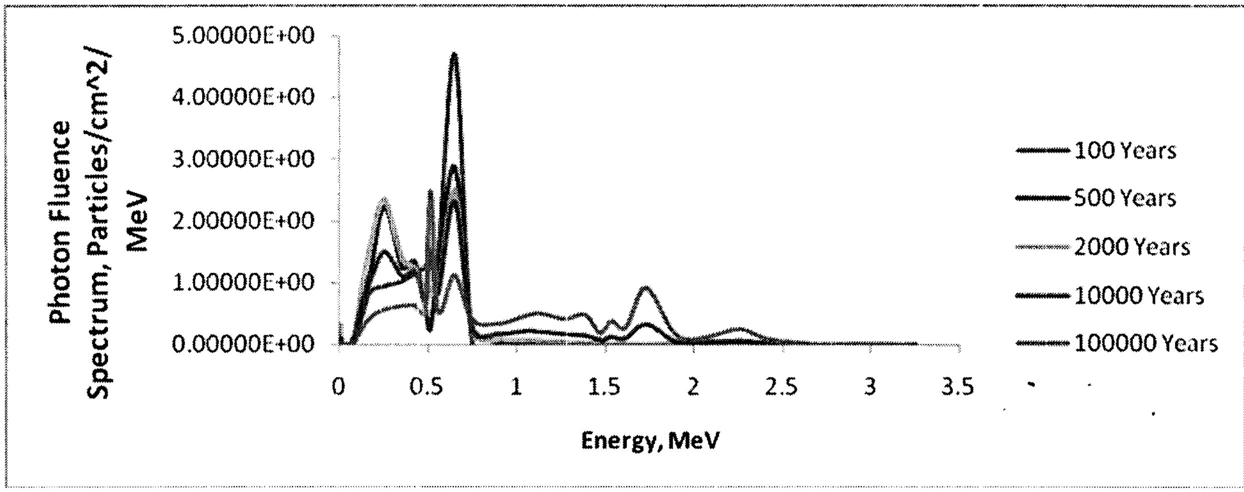


Figures 12/29/07-1. Normalized Sources Spectra



Figures 12/29/07-2. Photon Flux-to-Dose Rate Conversion Factors



Figures 12/30/07. Normalized Spectra in the Cell #1

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02/01/2008 (AK)(OP)
Results for nitric acid generation were compared with DOE results from "Bechtel SAIC. Gamma and Neutron Radiolysis in the 21-PWR Waste Package from Ten to One Million Years. 000-00C-DSU0-00700-000-00A. 2004."
report.
Comparison results are compiled in DOE Comparing Results.xls spreadsheet and also in

Notebook closed – no further entries
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ADDITIONAL INFORMATION FOR SCIENTIFIC NOTEBOOK NO. 897E

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