PHYSOR 2004 -The Physics of Fuel Cycles and Advanced Nuclear Systems: Global Developments
Chicago, Illinois, April 25-29, 2004, on CD-ROM, American Nuclear Society, Lagrange Park, IL. (2004)

HTR-N Plutonium Cell Burnup Benchmark: Definition, Results & Intercomparison

J.C. Kuijper*[1], N. Cerullo[5], F. Damian[2],
J.L. Kloosterman[4], G. Lomonaco[5], J. Oppe[1],
X. Raepsaet[2], H.J. Ruetten[3]
[1]*NRG, Petten, the Netherlands*
[2]*CEA, Saclay, France*
[3]*FZJ, Juelich, Germany*
[4]*IRI, Delft University of Technology, Delft, the Netherlands*
[5]*Universita di Pisa, Pisa, Italy*

In order to obtain a further validation of several reactor physics code systems to be used for the analysis of High Temperature gas-cooled Reactors (HTR) for plutonium burning applications, a HTR plutonium cell burnup calculational benchmark exercise was defined. For simplicity, the benchmark configuration only consists of a single spherical, 6 cm diameter HTR ("pebble") fuel element containing coated (PuO_2) fuel particles.

The requested calculations concerned the tracking of the multiplication factor, nuclide densities in the fuel particles and other relevant parameters during the irradiation of the fuel element at constant power up to the unusually high burnup of 800 MWd/kgHM. Generally a good agreement is found between the results of 3 out of 4 participants, representing 4 out of 5 code systems. The remaining differences in results between the 3 participants can be largely attributed to differences in the modeling of the reaction paths, which are amplified by the unusually high flux levels typical to this particular benchmark.

KEYWORDS: HIGH TEMPERATURE GAS-COOLED REACTOR, PLUTONIUM BURNING, HTR-N, EUROPEAN UNION FIFTH FRAMEWORK PROGRAM

1. Introduction

In the "HTR-N" and "HTR-N1" projects of the European Fifth Framework Program [1-3] investigations are being made concerning the feasibility of burning plutonium in "High Temperature Gas-Cooled Reactors (HTR)". The capability to reach ultra high burnup (up to 740 MWd/kgHM) with (TRISO/BISO) coated particles containing actinides, which has already been demonstrated in the early seventies, opens the way to burn e.g. military or civil plutonium in a way that no intermediate or further reprocessing is required. In addition the HTR coated particle fuel may already be well suited for final disposal due to the ceramic coating retaining the fission products from the biosphere.

* Corresponding author:
Phone: +31 224 564506, Fax:: +31 224 568490, E-mail: kuijper@nrg-nl.com

A substantial part of the "HTR-N" project is devoted to investigation and intercomparison of the plutonium and actinide burning capabilities of a number of HTR concepts and associated fuel cycles, with emphasis on the use of civil plutonium from spent LWR uranium fuel (*1st generation* Pu) and from spent LWR MOX fuel (*2nd generation* Pu). Two main types of HTRs under investigation are the hexagonal block type reactor with batch-wise reloading and the continuously loaded pebble bed reactor. In conjunction with the reactor types also a number of different fuel types (e.g. Pu-based and Pu/Th-based) and associated fuel cycles are under investigation. Furthermore a study is being conducted on the possibilities of optimisation of a park of symbiotic LWRs and HTRs to obtain a stable or even a decreasing plutonium stockpile.

As the investigations aim at obtaining a -very- high burnup in Pu-fueled HTRs, it was considered appropriate to provide a further validation for the variety of code systems in use by the project partners. Therefore a "HTR Plutonium Cell Burnup Benchmark" was defined by the "Forschungszentrum Juelich (FZJ)" and the "Nuclear Research & Consultancy Group (NRG)" [4]. Calculations for the benchmark were performed by four project partners, viz. the "Commisariat à l'Energie Atomique (CEA)", the "Interfaculty Reactor Institute of the Delft University of Technology (IRI)", NRG and the "Universita di Pisa (UNIPI)", employing their specific code systems in use for HTR reactor physics analysis.

2. Benchmark description

For simplicity the benchmark concerns only a spherical HTR ("pebble") fuel element containing coated fuel particles. The neutronic boundary condition is assumed to be "white", i.e. isotropic reflection from the outer boundary of the pebble. Although this is not entirely representativie for a full scale pebble bed HTR it is expected to serve the purpose as a basis for intercomparison of codes and data in use for reactor physics analysis of an HTR fuel at high burnup. More specifically k_∞ will drop below 1 at high values of the irradiation. This is not considered to be a problem, as in a real pebble bed HTR the fuel element will be surrounded by "driver" fuel at lower burnup so that the criticality of the reactor can be maintained. Furthermore, although the benchmark geometry is taken from the pebble bed type HTR, it is also considered representative for a "compact" type HTR fuel, employed in hexagonal block type HTRs, where the coated fuel particles are contained in a cylindrical matrix.

2.1 Configuration

The main parameters for the spherical HTR fuel element employed in the benchmark are the following:

- Diameter of the fuel element: 6.0 cm
- Diameter of the central fuel zone: 5.0 cm
- Graphite density: 1.75 g/cm^3

The central 5 cm diameter fuel zone contains coated particles, embedded in a graphite matrix. The main paramaters of the coated particles are as follows:

- PuO_2 density in the kernel: 10.4 g/cm^3
- Kernel diameter: 0.24 mm
- Coating layer materials (inner to outer): C / C / SiC / C
- Coating thickness (inner to outer): 95 / 40 / 35 / 40 μm
- Coating density (inner to outer): 1.05 / 1.90 / 3.18 / 1.90 g/cm^3

At the beginning of the irradiation the kernel of the coated particle is pure PuO_2 at the

specified density. The initial isotopic compositions are listed in Table 1. Compositions "A" and "B" are considered representative for *first generation* plutonium, obtained from reprocessed LWR UO_2 fuel. Composition "C" is considered representative for *second generation* plutonium, obtained from reprocessed LWR MOX fuel [5].

Table 1 Isotopic composition of first and second generation plutonium in this benchmark (weight %).

Isotope	**1st generation (original) "A"**	**1st generation (alternative) "B"**	**2nd generation "C"**
^{238}Pu	1	2.59	4.9
^{239}Pu	62	53.85	26.9
^{240}Pu	24	23.66	34.3
^{241}Pu	8	13.13	15.3
^{242}Pu	5	6.78	18.6

2.2 General parameters for the benchmark cases

General parameters for the benchmark are the following:

- Power per fuel element (constant during burnup): 1 kW
- Average temperature of 5 cm central fuel zone (i.e. kernel, coatings and matrix): 800 ^{o}C
- Average temperature of the 0.5 cm graphite outer zone: 750 ^{o}C
- Final burnup: 800 MWd/kgHM

It should be noted that, as the fission power of the fuel element is to be kept constant at 1 kW, and the final fuel burnup is fixed at 800 MWd/kgHM, the required irradiation time changes with the initial heavy metal load of the fuel element. As the plutonium content of a coated particle is fixed, the initial amount of plutonium in the fuel element is controlled by the packing fraction of the coated particles in the matrix..

In total four different benchmark cases were defined:

- **"Case A"**: first generation Pu (composition "A") at 1 gram per fuel element, requiring an irradiation time of 800 full power days to reach 800 MWd/kgHM
- **"Case B"**: first generation Pu (composition "B") at 1 gram per fuel element, requiring an irradiation time of 800 full power days
- **"Case C1"**: second generation Pu (composition "C") at 1.5 gram per fuel element, requiring an irradiation time of 1200 full power days
- **"Case C2"**: second generation Pu (composition "C") at 3 gram per fuel element, requiring an irradiation time of 2400 full power days

2.3 Parameters to be calculated

The burnup history of the fuel at the defined constant power is to be calculated for the selected initial amount and composition of plutonium, *not* using any neutron poison, or any other means, for reactivity control. For a burnup of 0, 100, 400, 600 and 800 MWd/kgHM the following paramaters are to be reported:

- Neutron multiplication (k_∞) of the fuel element [-]
- Isotopic composition of the fuel kernel [10^{24}/cm^3] for the heavy metal and fission product isotopes specified below
- Neutron flux (collapsed to 1 energy group) [s^{-1}cm^{-2}]
- 1-group microscopic absorption (= capture + fission) cross sections for each of the considered isotopes [barn]

- 1-group microscopic fission cross sections for each of the considered heavy metal iscotopes [barn]
- Total fission rate [s^{-1}]

The nuclides to be considered in the isotopic compositions are the following:

- Heavy metal: Pu-238, Pu-239, Pu-240, Pu241, Pu-242, Am-241, Am242m, Am-243, Cm-242, Cm-243, Cm244
- Fission products: Se-79, Rb-87, Sr-90, Zr-93, Mo-93, Nb-94, Tc-99, Pd-107, Sn-126, I-129, Cs-135, Cs-137, Sm-147, Sm-151, Eu-154

It should be noted that the actual calculation of the neutron flux and -spectrum will usually take place at -much- smaller time/burnup intervals, selected by the benchmark participants on the basis of their usual methodology for HTR reactor physics calculations.

3. Code systems and modeling

The participants in the benchmark exercise each used different codes and code systems to perform the requested calculations. In general these code systems employ a sequence of alternating neutron flux/spectrum and burnup/time step calculations. In the following sub-sections a brief description will be given of the code systems used by the benchmark partcipants, together with some details of the modeling of this particular benchmark exercise.

3.1 Code systems used by NRG

At NRG the benchmark calculations were performed by the WIMS8A [6] code system and by the OCTOPUS [7] code system. In the OCTOPUS code system the continuous energy monte carlo particle transport code MCNP version 4C3 [8,9] is combined with a burnup/inventory code, to be selected from ORIGEN-S [10] and FISPACT [11].

The calculations by WIMS8A were performed using nuclear data from the JEF-2.2 based 172-group cross section library supplied with the code, with some extensions by NRG [12]. These extensions mainly concerns additional data for temperature- and background cross section dependent resonance integrals for all actinides already present in the original library.

The collision probability module WPROC of the WIMS8A code was selected for the modeling of the spherical HTR fuel element. This module is used to calculate collision probabilities, both for the subgroup resonance treatment and the 172-group flux/spectrum calculation. As WPROC was designed to model an infinite cylindrical structure containing spherical coated particles, a geometry transformation was applied to model the spherical HTR fuel element: the 5 cm diameter inner fuel zone was modeled as an infinite cylinder with the same mean chord length [13]. This effectively means the conservation of the surface-to-volume ratio of the fuel zone, together with the conservation of the packing fraction of the coated fuel particles in the matrix graphite. The 0.5 cm outer graphite shell is also transormed into a cylindrical shell, hereby preserving the volume ratio between fuel zone and outer graphite shell. By the use of WPROC as collision probability module in the subgroup resonance shielding calculation sequence in WIMS8A, the double heterogeneity of the HTR fuel element is explicitly taken into account. Subgroup resonance treatment was applied for Pu-239, Pu-240, Pu-241 and Pu-242. For all other nuclides in the kernel the resonance shielding was calculated by equivalence theory. This method has been applied succesfully in earlier HTR analyses [14].

The time/burnup steps between the flux/spectrum calculations were originally chosen according to the recommendations in the WIMS8A manual [5]. For “Case A” multiple runs

were performed with smaller time steps, until the k_∞ versus burnup behaviour did not change significantly with a further decrement of the time step. The burnup time step sequence thus obtained was applied for all cases. To reach the requested 800 MWd/kgHM, 230 burnup/time steps (and flux/spectrum calculations) were taken, varying from 0.05 to 4 MWd/kgHM.

In the OCTOPUS [7] calculations the MCNP 4C3 continuous energy particle transport code was used as flux/spectrum calculator employing a JEF-2.2 based point energy cross section library. Interpolation in the square root of the temperature is performed on the point energy cross section tables in the library, to obtain cross sections at the specified temperatures.

The spherical fuel element can be modeled almost exactly in MCNP. The central 5 cm fuel zone is modeled by means of a separate MCNP "universe" that describes a single coated particle with its corresponding fraction of the matrix graphite. A cubic ordering of the coated particles is used as a good approximation to the more realistic stochastic ordering [14,15].

At the beginning of each burnup/time step MCNP performs a k_∞- and flux/spectrum calculation. On the basis of a hyperfine group spectrum (18250 energy groups) and the point energy cross sectons from the MCNP library, 172-group shielded cross sections are calculated for the nuclides in the fuel kernel for which data is available in the MCNP library. The 172-group cross sections are subsequently used to update the cross sections in the nuclear data library of the inventory code, viz. FISPACT or ORIGEN, hereby enabling an improved calculation of the subsequent burnup/time step.

In the OCTOPUS-MCNP-ORIGEN (further abbreviated as "NRG ORIGEN" in the remainder of this paper) and OCTOPUS-MCNP-FISPACT ("NRG FISPACT") calculations the same burnup/time steps between the flux/spectrum calculations were used as in the WIMS8A calculations. The standard deviation for k_∞ is approx. 0.003 in the calculations presented in this paper.

3.2 Code system used by CEA

CEA employed the APOLLO2 transport code [16], which is part of the French code system SAPHYR. The standard 172-group cross section library issued mainly from JEF-2.2 was used for the calculations. The integral form of the Boltzmann equation is solved by the collision probabilty method (1D). The double heterogeneity of the geometry, characterised by the spherical coated fuel particles on one hand and the pebble spherical geometry on the other, is taken into account explicitly in the calculations.

For the calculations the standard depletion chain consists of 24 heavy metal nuclei (up till Cm-248) and 77 fission products. Seven of the pricipal heavy metal nuclei (Pu-238 to Pu-242, Am-241 and Am-243) are self-shielded during the fuel evolution. To reach the requested 800 MWd/kgHM, 42 burnup/time steps were taken, varying between 2 and 25 MWd/kgHM.

3.3 Code system used by IRI

IRI used the SCALE [17] computer code system with a JEF-2.2 based nuclear data library. From the SCALE code system the BONAMI-S code was used for resonance treatment in the unresolved energy range, the NITAWL-S code was used for resonance treatment in the resolved energy region, and the XSDRNPM-S code was used for the cell weighting calculations. The Dancoff factor used in the resonance shielding was calculated by an analytical procedure [18] and took into account the double heterogeneity of the fuel. The actual burnup calculations were done using the ORIGEN-S inventory code [10] and a nuclear data library based on JEF-2.2 and EAF3 [19]. At the beginning of each burnup/time

step the appropriate cross sections of the appropriate nuclides in the ORIGEN-S library were updated on the basis of the shielded values obtained from the XSDRNPM-S calculation. All codes were interconnected via PERL scripts and in-house developed FORTRAN programs.

The whole sequence of cell weighting and burnup/time step calculations was repeated several times to calculate the k_∞ and the composition of the fuel as function of burnup. To reach the requested 800 MWd/kgHM, for "Case B" 10 burnup/time steps were taken, varying between 10 and 100 MWd/kgHM. For "Case C" 48 burnup/time steps of 25 MWd/kgHM were taken.

3.4 Code system used by UNIPI

UNIPI has acquired the MONTEBURNS-1 code system [20] through the OECD/Nuclear Energy Agency Data Bank in Paris, France. This program interconnects the MCNP 4B monte carlo N-particle transport code system [21] and the ORIGEN 2.1 depletion code [22] through the MONTEB utility and a PERL procedure.

MONTEBURNS produces a large number of criticality and burnup results based on various material feed/removal specifications, power(s) and time intervals. MONTEBURNS processe input from the user that specifies the system geometry, inital material compositions, feed/removal specifications, and other code-specific parameters. Various results from MCNP 4B, ORIGEN 2.1 and other calculations are then output successively as the code runs. The principle function of MONTEBURNS is to transfer one-group cross sections from MCNP 4B to ORIGEN 2.1, and to transfer the resulting material compositions (after irradiation and/or decay) from ORIGEN 2.1 to MCNP 4B in a repeated, cyclic fashion. This is quite similar to the operation of OCTOPUS at NRG. However, MONTEBURNS uses a simple predictor-corrector method in this process.

The cross section data used in the MCNP 4B came from libraries supplied with the code, viz. "ZZ-MCJEF22NEA.BOLIB", "ZZ-MCB63NEA.BOLIB" and "ZZ-MCLIB-E6".It should be noted that, in this cross sections set, the temperature is fixed at 1000 K. In the future it is planned to adapt the cross section sets to the appropriate temperature and to repeat the calculations.

In a fashion similar to the OCTOPUS calculations by NRG, the spherical HTR fuel element was modeled almost exactly in MCNP 4B. In the 5 cm central fuel zone the randomly packed coated fuel particles are approximated by a cubic array of particles. To reach the requested 800 MWd/kgHM, 48 burnup/time steps were taken, varying between 16.570 and 21.099 MWd/kgHM for "Case C1". The standard deviation for k_∞ is approx. 0.003 in the calculations presented in this paper.

4 Results & discussion

Employing the code systems described in the previous section, the benchmark participants performed calculations on a number of benchmark cases. In Table 2 an overview is presented of the cases calculated by each of the participants.

As the WIMS8A code, used by NRG, was the only code system by which all benchmark cases were calculated, it's results were selected as the reference solutions for intercomparison purposes. However, this does not mean on beforehand that it is considered as the "best" solution.

The assessment and intercomparison of the results concerns a vast amount of data to be handled. Although this exercise has not been entirely completed yet, in the remainder of this

paper a few highlights will be presented, which are representative for the main trends observed. The main focus in this paper is on "Case C1". Details of all results obtained by the participants, together with those of additional studies, can be found in the respective reports on the benchmark results [23-26].

Table 2 Benchmark cases calculated by each of the participants (present status)

Participant	Code system	Case A 1st gen. Pu 1.0 g	Case B 1st gen. Pu (alt.) 1.0 g	Case C1 2nd gen. Pu 1.5 g	Case C2 2nd gen. Pu 3.0 g
NRG	WIMS8A	+	+	+	+
NRG	"NRG ORIGEN"	+			
NRG	"NRG FISPACT"	+		+	
CEA	APOLLO2		+	+	+
IRI	SCALE		+	+	
UNIPI	MONTEBURNS		+	+	+

4.1 Infinite multiplication factor

In Fig. 1 the k_∞ is shown as function of the burnup for "Case C1" (2nd generation plutonium, initially1.5 g Pu per fuel element). The general shape of the curve, which is characterised by the sharp decrease in reactivity beyond approx. 500 MWd/kgHM, and a slight increase beyond approx. 700 MWd/kgHM, is predicted reasonably well by all particpants. The slight increase of the reactivity beyond 700 MWd/kgHM is connected to the second increase of the Cm-245 density, following a decrease between 550 and 750 MWd/kgHM [23]. It should be noted that the NRG (both WIMS8A – deterministic and "NRG FISPACT" – monte carlo) solutions are particularly close together up to approx. 650 MWd/kgHM. Also the solutions provided by CEA and IRI correspond quite well to those of NRG up to the indicated burnup.

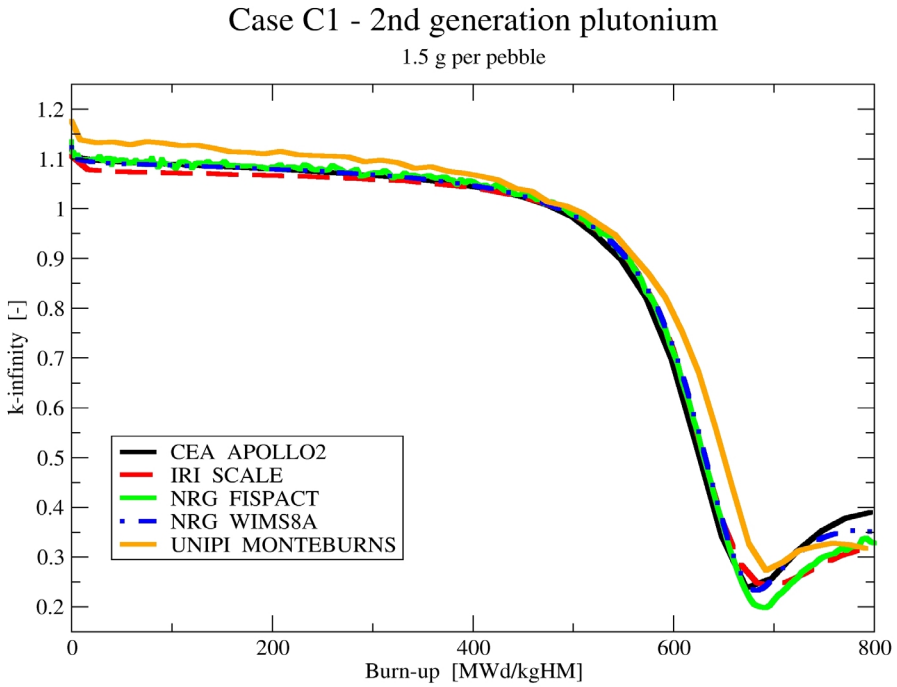

Fig. 1 Infinite multiplication factor as function of burnup (2nd generation Pu, 1.5 g).

In Table 3 some numerical details are given at the burnup levels requested in the benchmark specification. It should be noted that, up to 400 MWd/kgHM the difference between the results of the two NRG methods is of the same order of magnitude as the standard deviation in the OCTOPUS-MCNP-FISPACT k_∞-result (see sub-section 3.1). In Table 4 similar information is presented for "Case B" (1st generation plutonium, alternative composition, initially 1 g per fuel element). Again a good correspondence is observed between the results of NRG (WIMS8A), CEA and IRI up to approx. 600 MWd/kgHM. This trend is also observed in the other benchmark cases.

Table 3 Infinite multiplication factor as function of burnup (2nd generation Pu, 1.5 g). NRG WIMS8A is reference solution. For the other solutions the difference in reactivity Δρ with the reference is given.

Burnup [MWd/kgHM]	NRG WIMS8A k_∞ [-]	CEA Δρ [%]	IRI Δρ [%]	NRG FISPACT Δρ [%]	UNIPI Δρ [%]
0	1.1236	0.32	-1.45	0.93	3.96
100	1.0872	0.16	-1.29	0.03	3.45
400	1.0465	-0.19	-0.44	0.69	1.95
600	0.71899	-7.54	-0.62	-1.74	12.04
800	0.35081	28.76	-27.80	-19.30	-30.41

Table 4 Infinite multiplication factor as function of burnup (1st generation Pu, alternative composition, 1 g). NRG WIMS8A is reference solution. For the other solutions the difference in reactivity Δρ with the reference is given.

Burnup [MWd/kgHM]	NRG WIMS8A k_∞ [-]	CEA Δρ [%]	IRI Δρ [%]	UNIPI Δρ [%]
0	1.3846	0.02	-0.70	4.08
100	1.3104	0.00	-0.44	3.35
400	1.2056	-0.35	0.85	2.47
600	1.0568	-2.47	3.63	0.08
800	0.13404	36.64	353.05	415.24

4.2 Nuclide densities

In Table 5 the density of plutonium isotopes is shown as function of the burnup, again for "Case C1". Also for the Pu nuclide densities a good agreement, mostly within a few percent, is observed between the results of NRG (both WIMS8A and "NRG FISPACT"), CEA and IRI up to a burnup of approx. 600 MWd/kgHM. The differences with the UNIPI results are generally larger for Pu-239 to Pu-241, and approx. increasing with burnup.

For the other actinide and fission product nuclides the observed differences between the results of different partners are of the same order of magnitude.

4.3 One-group cross sections

The effective (shielded) cross section, collapsed to a single energy group, provides a measure of the ability of the code system to calculate the correct (self- and mutual) shielding effect in a changing nuclide mixture. In Table 6 the one-group microscopic absorption cross section of 5 plutonium isotopes is given as function of burnup for "Case"C1".

For the one-group efective cross sections of the plutonium isotopes a good agreement, mostly within a few percent, is observed between the results of NRG (both WIMS8A and "NRG FISPACT"), CEA and IRI for the entire burnup range, over which the magnitude of the

effective cross section changes considerably. The observed differences with the UNIPI results are generally larger.

For the other actinide and fission product nuclides, and also for the one-group fission cross sections, the observed differences between the results of different partners are of the same order of magnitude.

Table 5 Nuclide densities of Pu-238 to Pu-242 as function of burnup (2nd generation Pu, 1.5 g). NRG WIMS8A is reference solution. For the other solutions the relative difference with the reference is given.

Nuclide	Burnup [MWd/kgHM]	Density NRG WIMS8A [10^{24}cm^{-3}]	Diff. CEA [%]	Diff. IRI [%]	Diff. NRG FISPACT [%]	Diff. UNIPI [%]
Pu-238	0	1.14E-03	0	-0.06	0	-0.13
Pu-238	100	1.07E-03	0.13	-0.17	0.05	-2.32
Pu-238	400	8.73E-04	-0.13	-1.36	-0.58	-20.75
Pu-238	600	5.37E-04	-3.03	-5	-4.24	-42
Pu-238	800	4.99E-07	10.04	46.15	-33.17	-31.37
Pu-239	0	6.22E-03	0	-0.01	0	-0.01
Pu-239	100	4.16E-03	-1.67	-1.24	-1.48	11.46
Pu-239	400	6.18E-04	-10.7	-5.77	-7.41	82.51
Pu-239	600	7.39E-05	-6.38	-5.69	-2.1	206.93
Pu-239	800	6.29E-08	7.86	44.39	-29.82	158.27
Pu-240	0	7.90E-03	-0.01	-0.01	0	-0.04
Pu-240	100	6.66E-03	1.07	0.76	1.1	3.4
Pu-240	400	2.87E-03	0.41	-1.11	1.42	9.74
Pu-240	600	5.77E-04	-5.44	-13.11	-0.71	52.81
Pu-240	800	2.50E-06	20.57	12.69	-1.79	3.19
Pu-241	0	3.51E-03	0	0	0	0.09
Pu-241	100	4.12E-03	-0.22	-0.31	-0.57	-6.32
Pu-241	400	2.98E-03	-1.37	-0.87	-1.97	-3.71
Pu-241	600	4.37E-04	-10.59	-9.82	-8.37	78.86
Pu-241	800	5.78E-07	17.62	16.9	-7.38	25.98
Pu-242	0	4.25E-03	0	0	0	-0.13
Pu-242	100	4.22E-03	0	-0.8	-0.07	0.57
Pu-242	400	4.65E-03	0.53	-2.84	-0.12	-0.76
Pu-242	600	4.95E-03	0.56	-5.08	-0.55	-2.27
Pu-242	800	9.50E-04	18.43	35.87	-12.49	70.42

4.4 General observations

From the results obtained by the different benchmark participants using different code systems it is generally seen that the results of NRG, IRI and CEA are close together up to a burnup of approx. 600 MWd/kgHM. At higher values of the burnup the differences in calculated nuclide densities, and consequently in k_∞, are increasing considerably, not only between those of different partners, but also between the three calculational routes employed by NRG. Additional studies [23] show that these differences can be largely attributed to:

- differences in the set of heavy metal and fission product nuclides taken into account in the burnup calculation;
- differences in the reactions taken into account explicitly in the burnup calculation. In the WIMS8A reaction schemes, e.g. the Am-243 (n,γ) reaction directly leads to Cm-244, hereby ignoring a possible interaction of a neutron with Am-244. Also the α-decay of

Cm-245 is missing in the WIMS8A reaction scheme. in "NRG ORIGEN" on the other hand these reactions are modeled explicitly;

- different values of the Am-241 capture branching ratio.

Under usual circumstances (i.e. flux and burnup levels) these differences will not lead to large differences in results. However, in this particular benchmark both the final burnup and the flux levels are very high. E.g. in "Case C1" the flux increases from approx. $1.85 \cdot 10^{14}$ $cm^{-2}s^{-1}$ at zero burnup to approx. $7 \cdot 10^{15}$ $cm^{-2}s^{-1}$ at 800 MWd/kgHM [23], due to the constant power level during irradiation. This greatly amplifies the influence of the differences mentioned above. In a real HTR this kind of unusually high flux levels are not expected.

Continued investigations are required to explain the differences between the results of UNIPI and the other benchmark participants.

Table 6 One-group effective microscopic absorption cross section of Pu-238 to Pu-242 as function of burnup (2nd generation Pu, 1.5 g). NRG WIMS8A is reference solution. For the other solutions the relative difference with the reference is given.

Nuclide	Burnup [MWd/kgHM]	σ_{abs} NRG WIMS8A [barn]	Diff. CEA [%]	Diff. IRI [%]	Diff. NRG FISPACT [%]	Diff. UNIPI [%]
Pu-238	0	2.35E+01	-2.01	-0.43	-0.73	72.35
Pu-238	100	2.52E+01	-1.2	0.38	0.71	74.27
Pu-238	400	4.51E+01	0.75	0.46	3.81	86.87
Pu-238	600	1.08E+02	1.71	-0.56	4.87	85.5
Pu-238	800	1.67E+02	-0.02	-0.92	3.88	134.33
Pu-239	0	1.57E+02	4.36	3.44	4.27	-4.25
Pu-239	100	1.80E+02	4.58	3.8	3.85	-9.58
Pu-239	400	3.67E+02	3.65	2.6	2.88	-28.2
Pu-239	600	8.74E+02	3.88	4.7	1.75	-43.69
Pu-239	800	1.32E+03	2.22	0.33	0.55	-37
Pu-240	0	1.08E+02	-1.65	-0.46	-1.16	-3.53
Pu-240	100	1.17E+02	-1.42	0.09	-1.72	-4.48
Pu-240	400	1.74E+02	0.02	3.05	0.06	-2.71
Pu-240	600	2.54E+02	3.84	5.8	-1.71	4.84
Pu-240	800	2.30E+02	-0.91	2.49	-4.17	28.07
Pu-241	0	1.33E+02	-1.23	-1.38	-0.04	15.11
Pu-241	100	1.47E+02	-0.44	-0.39	0.58	12.66
Pu-241	400	2.76E+02	2.46	1.24	3.32	2.6
Pu-241	600	6.58E+02	3	2.43	3.34	-10.79
Pu-241	800	1.01E+03	1.32	-0.1	2.28	6.03
Pu-242	0	3.57E+01	-1.47	8.93	-1.35	-2.6
Pu-242	100	3.50E+01	-0.9	9.98	1.1	-3.33
Pu-242	400	3.04E+01	-0.61	11.24	2.19	3.05
Pu-242	600	2.07E+01	-2.34	6.53	-0.52	27.13
Pu-242	800	1.43E+01	-2.45	1.75	-0.46	54.75

5 Summary & Conclusions

Some results have been presented from calculations on the "HTR Plutonium Cell Burnup Benchmark", as obtained by different benchmark particpants using different code systems. Generally a good agreement, up to a burnup of approx. 600 MWd/kgHM, is found between the results of 3 out of 4 particpants, representing 4 out of 5 code systems. The remaining

differences in results between the 3 particpants can be largely attributed to differences in modeling of reaction paths in the different code systems, which are amplified by the unusually high flux levels typical to this particular benchmark exercise.

Acknowledgements

The work presented in this paper was partly funded by the European Union Fifth Framework Program, under contracts no. FIKI-CT-2000-00020 ("HTR-N") and FIKI-CT-2001-00169 ("HTR-N1").

References

1) "HTR-N – High-Temperature Reactor Physics and Fuel Cycle Studies", European Union Fifth Framework Program contract no. FIKI-CT-2000-00020 (2000).
2) "HTR-N1 – High-Temperature Reactor Physics, Waste and Fuel Cycle Studies", European Union Fifth Framework Program contract no. FIKI-CT-2001-00169 (2001).
3) W. von Lensa et al. "European Programme on High Temperature Reactor Nuclear Physics, Waste and Fuel Cycle Studies", Proc. ICAPP, Cordoba, Spain (2003).
4) H.J. Ruetten and J.C. Kuijper, "Plutonium (1st and 2nd generation cell burnup benchmark specification", Report 20780/03.52483/C, HTR-N1 project support document no. HTR-N1-02/06-S-3.1.1, NRG, Petten, the Netherlands (2002).
5) J.B.M. de Haas and J.C. Kuijper, "Feasibility of burning first and second generation plutonium in pebble bed HTRs", Proc. Advances in Nuclear Fuel Management III (ANFM 2003), Hilton Head Island, South Carolina, USA, October 5-8, 2003, American Nuclear Society, LaGrange Park, IL, USA (2003).
6) "WIMS - A Modular Scheme for Neutronics Calculations - User Guide for Version 8", Report ANSWERS/WIMS(99)9, ANSWERS Software Service (1999).
7) J. Oppe, "OCTOPUS_TNG Reference Guide", Report 20780/03.54103/C, NRG, Petten, the Netherlands (2003).
8) J.F. Briesmeister, "MCNP - A General Monte Carlo N-Particle Transport Code, Version 4C", Technical Report LA-13709, Los Alamos National Laboratory, USA (2000).
9) J.S. Hendricks, "MCNP4C3", Report X-5:RN(U)-JSH-01-17, Los Alamos National Laboratory, USA (2001).
10) O.W. Hermann and R.M. Westfall, "ORIGEN-S - SCALE system module to calculate fuel depletion, actinide transmutation, fission product buildupand decay, and associated radiation source terms", Oak Ridge National Laboratory, USA (1989).
11) R.A. Forest and J.-Ch. Sublet, "FISPACT 4 User Manual", EASY Documentation Series UKAEA FUS 287 (1995).
12) J. Oppe, "WIMS datagram library uitbreiding (*WIMS datagram library extension*, in Dutch)", Report 20780/02.48983 FAI/JO/AB, NRG, Petten, the Netherlands (2002).
13) K.M. Case, F. de Hoffmann and G. Placzek, "Introduction to the theory of neutron diffusion", Vol. 1, U.S. A.E.C. Report, Los Alamos National Laboratory, Los Alamos, New Mexico, USA (1953).
14) J.C. Kuijper *et al.*, "Reactor Physics Calculations on the Dutch Small HTR Concept", IAEA Technical Committee Meeting on High Temperature Gas Cooled Reactor Development, Johannesburg, Republic of South Africa, IAEA-TECDOC-988, November 13–15 (1996).
15) E.E. Bende, "Plutonium burning in a Pebble-Bed Type High Temperature Nuclear Reactor", Ph.D thesis, Delft University of Technology, Delft, the Netherlands, Nuclear

Research and Consultancy Group, Petten, the Netherlands, ISBN 90-9013168-X (1999).
16) R. Sanchez, A. Hebert, Z. Stankovski, M. Coste, S. Loubiere, C. van der Gucht and I. Smijarevic, "APOLLO2 Twelve Years Later", Proc. Mathematics and Computation, Reactor Physics and Environmental Analysis in Nuclear Applications, Madrid (1999).
17) "SCALE 4.2 - Modular code system for performing standardized computer analyses for licensing evaluations", Oak Ridge Natonal Laboratory, Tennessee, USA (1994).
18) E.E. Bende, A. Hogenbirk, J.L. Kloosterman and H. van Dam, "Analytical calculation of the average Dancoff factor for a fuel kernel in a pebble-bed type high-temperature reactor", Nucl. Sci. Eng., **133**, 1 (1999).
19) J.E. Hoogenboom and J.L. Kloosterman, "Generation and validation of ORIGEN-S libraries for depletion and transmutation calculations based on JEF-2.2 and EAF3 basic data", Nuclear engineering and Design, **170**, 107 (1997).
20) D.I. Poston and H.R. Trellue, "User's manual, Version 2.0 for MONTEBURNS Version 1.0", Report LA-UR-99-4999 PSR-0455/01, Los Alamos National Laboratory, USA (1999).
21) "MCNP 4B: Monte Carlo N-Particle Transport Code System", Los Alamos National Laboratory, New Mexico, USA, Edited by RSIC (1997).
22) "ORIGEN 2.1 Isotope Generation and Depletion Code Matrix Exponential Method", Oak Ridge National Laboratory, Tennessee, USA (1996).
23) J. Oppe and J.C. Kuijper, "Plutonium HTR Cell Burnup Benchmark - Several Calculation Methods and Ther Results", Report 20780/03.55862/P, NRG, Petten, the Netherlands (2004).
24) F. Damian and X. Raepsaet, "CEA's contribution to plutonuium cell burnup benchmark problem", HTR-N1 project document HTR-N1-03/04-S-3.1.1-2, CEA, Saclay, France (2003).
25) J.L. Kloosterman, "IRI Results for the Plutonium Cell Burnup Benchmark", Report IRI-131-2003-004, HTR-N1 project support document HTR-N1-03/05-S-3.1.1-3, IRI, Delft University of Technology, Delft, the Netherlands (2003).
26) D. Buffalino, N. Cerullo, G. Lomonaco, "HTR-N1 plutonium burnup benchmark - Results obtained by UNIPI using MONTEBURNS code", Report RL 969(02), HTR-N1 project support document HTR-N1-02/08-S-3.1.1-1_4, University of Pisa, Pisa, Italy (2002).