Analysis of an OECD/NEA High-Temperature Reactor Benchmark

J G Hosking[1], T D Newton[1], O Köberl[2], P Morris[3], S Goluoglu[4], T Tombakoglu[5], U Colak[5] & E Sartori[6]

[1]*Serco Assurance, Winfrith Technology Centre, Dorchester, DT2 8DH, UK*
[2] *CEA-Cadarache, 13108 Saint Paul Lez Durance, France*
[3]*Nexia Solutions, UK*
[4]*Nuclear Science & Technology Division, ORNL, Oak Ridge, TN 37831-6170, USA*
[5]*Nuclear Engineering Department, Hacettepe University, Turkey*
[6]*OECD NEA Data Bank, 92130 Issy-les-Moulineaux, France*

Abstract

This paper describes analyses of the OECD/NEA HTR benchmark organized by the 'Working Party on the Scientific Issues of Reactor Systems (WPRS)', formerly the 'Working Party on the Physics of Plutonium Fuels and Innovative Fuel Cycles'. The benchmark was specifically designed to provide inter-comparisons for plutonium and thorium fuels when used in HTR systems. Calculations considering uranium fuel have also been included in the benchmark, in order to identify any increased uncertainties when using plutonium or thorium fuels. The benchmark consists of five phases, which include cell and whole-core calculations.

Analysis of the benchmark has been performed by a number of international participants, who have used a range of deterministic and Monte Carlo code schemes. For each of the benchmark phases, neutronics parameters have been evaluated. Comparisons are made between the results of the benchmark participants, as well as comparisons between the predictions of the deterministic calculations and those from detailed Monte Carlo calculations.

KEYWORDS: OECD, NEA, HTR, URANIUM, PLUTONIUM, THORIUM

1. Introduction

The Organization for Economic Co-operation and Development/Nuclear Energy Agency (OECD/NEA) high-temperature reactor (HTR) benchmark organized by the 'Working Party on the Scientific Issues of Reactor Systems (WPRS)', formerly the 'Working Party on the Physics of Plutonium Fuels and Innovative Fuel Cycles', consists of five phases. These are

1: Uranium fuel: Cell Calculation
2: Plutonium fuel: Cell Calculation
3: Plutonium fuel: Whole-Core Calculation
4: Uranium fuel: Whole-Core Calculation
5: Thorium/Uranium fuel (Th232/U233): Cell Calculation

For each phase of the benchmark, calculated values for neutron multiplication factors (k-infinity or k-effective) are presented. For the plutonium core phase, results indicating estimates of xenon worth at start-of-life are also provided.

2. Overview of the Benchmark Specification

This section provides an overview of the benchmark specification. A detailed description is given in Reference 1.

The cell calculations consider an infinite array of pebbles. Each pebble has a diameter of 6cm and a central 5cm diameter sphere containing a matrix to support the fuel particles. In each case, 15,000 fuel particles were included in every pebble. Each pebble was contained within a cubic cell with side of length 6cm. The volume between the exterior of the pebble and edge of the cubic cell was filled with helium coolant. Reflective boundary conditions were used. Use of a cubic cell with reflective boundary conditions ensured that the boundary treatment would be equivalent in deterministic and Monte Carlo calculations. If a spherical boundary condition were used, there may have been discrepancies between the boundary treatments applied in the deterministic and Monte Carlo methods. Whilst deterministic calculations generally use white boundary conditions when modeling spherical systems, Monte Carlo methods typically employ an isotropic flux boundary condition. Since there is helium present at the edge of the cell being modeled here, the boundary flux will, however, be anisotropic.

The assumed core design includes most of the main design features expected in a typical HTR core. It is not optimized for a particular fuel type, since a range of fuels are studied in the benchmark.

3. Code Schemes and Nuclear Data Used by Benchmark Participants

Table 1 includes details of the participants of HTR benchmark, as well as the code schemes and nuclear data they have used in their calculations.

Table 1: Code Schemes and Nuclear Data Used by Benchmark Participants

Participant	Organization	Code Schemes	Nuclear Data
A	Serco Assurance, UK	Deterministic – WIMS9 (Ref. 2) Monte Carlo – MONK (Ref 3)	Based on JEF2.2
B	CEA, France	Deterministic – APOLLO2 (Ref. 4) Monte Carlo – TRIPOLI4 (Ref. 6)	Based on JEF2.2 (Ref. 5)
C	Haceteppe University, Turkey	Monte Carlo - MCNP-4B	Based on ENDF-B/VI
D	Haceteppe University, Turkey	Monte Carlo - MCNP-4B + BURN-HUNEM to calculate depletion	Based on ENDF-B/VI
E	Nexia Solutions, UK	Deterministic - VSOP-99	Based on ENDF/B-V and JEF1
F	ORNL, USA	Deterministic – XSDRNPM within SCALE (Ref. 7) Monte Carlo – KENO V.a within SCALE (Ref. 7)	Based on ENDF/B-V

4. Deterministic Methods Used in the Calculations

The section outlines some of the deterministic methods employed by the benchmark

participants for aspects of their HTR calculations.

4.1 Resonance Shielding and Double Heterogeneity

Participant A has used the subgroup treatment within WIMS9 to calculate resonance shielding. The use of the subgroup treatment allows the effects of the double heterogeneity in the geometry to be accounted for directly in the resonance shielding of the cross-sections. The double heterogeneity treatment used in WIMS9 is based upon the assumptions of J.R. Askew.

Participant B has generated self-shielded cross sections using the 'all resonances' TR model of the APOLLO2 code (Reference 8), where it is assumed that the scattering is isotropic in the centre-of-mass reference frame and the nuclei are heavy. An advantage of the TR model is that no assumptions regarding the resonance shape are required.

Participant F has calculated self-shielded cross sections using the CENTRM/PMC/CHOPS modules of the SCALE code system.

Participant A's treatment of double heterogeneity for deriving neutron fluxes is the same as that used for the derivation of the subgroup fluxes.

The APOLLO2 double heterogeneity treatment used by participant B is based on assumptions made by J.R. Askew. The main principle of participant B's method is to apply the escape probability for a single absorbing particle. The collision probabilities are calculated with the flat flux approximation and the slowing down within the particles is neglected.

Participant F has treated double-heterogeneity by first calculating the flux disadvantage factors for the grains and then using these factors to create the homogenized grain/matrix mixture cross sections. The homogenized cross sections are used on second pass to create the final resonance-shielded cross sections that represent the fuel pebbles.

4.2 Number of Energy Groups

For the cell calculations, Participant A has used a 172 energy-group scheme. The whole-core calculations of Participant A have been performed using a condensed 10-group scheme. Corrections are applied to account for the energy-group condensation.

For all phases of the benchmark, Participant B has performed calculations using a 172 energy-group scheme. Furthermore, whole-core transport calculations have been performed with various condensed energy-group schemes (8, 13 and 26 groups).

Participant F has used a 238-group scheme.

5. Results

5.1 Phase 1: Uranium fuel: Cell calculation

Table 2: Phase 1 – Results from Monte Carlo Calculations

PARAMETER	UNITS	A	C	D	F	Mean	St. Dev.
k_{inf} with zero buckling and at T=293.6K	-	1.5222 ±100 pcm	1.50697	1.5107	1.50770 ±43 pcm	1.51150	618pcm
k_{inf} with zero buckling and at T=1000K	-	1.4329 ± 100 pcm	-	-	1.40889 ±47 pcm	1.42090	1698pcm

Table 3: Phase 1 – Results from Deterministic Calculations

PARAMETER	UNITS	A	F	Mean	St. Dev.
k_{inf} with zero buckling and at T=293.6K	-	1.51785	1.50748	1.51267	733pcm
k_{inf} with zero buckling and at T=1000K	-	1.42668	1.40773	1.41721	1340pcm

In general, there is reasonable agreement between the participants' Monte Carlo predictions of k-infinity at 293.6K. Participant A's prediction of k-infinity is higher than the predictions from other participants. This may be a result of Participant A using JEF2.2 data, whereas participants C, D and F use data based on ENDF evaluations. There is a difference (1.5107 – 1.50697 = 373pcm) between the Monte Carlo k-infinity predictions of participants C and D, despite them both using MCNP and ENDF-B/VI data. This difference could be attributed to participants C and D making different modeling assumptions.

Participant A's and Participant F's Monte Carlo predictions of k-infinity at 1000K are in greater difference than the equivalent values at 293.6K. After increasing the temperature from 293.6K to 1000K, Participant A predicts a decrease in k-infinity of 8930pcm (1.5222 – 1.4329), whereas Participant F predicts a decrease in k-infinity of 9881pcm (1.50770 – 1.40889). The ~9% discrepancy between these results could be attributed to differences in nuclear data and calculation methods.

The deterministic results from Participant A and Participant F are in reasonable agreement with the equivalent Monte Carlo results provided by these participants.

5.2 Phase 2: Plutonium fuel: Cell calculation

Table 4: Phase 2- Results from Monte Carlo Calculations

PARAMETER	UNITS	A	C	D	F	Mean	St. Dev.
k_{inf} with zero buckling and at T=293.6K	-	1.4657 ±100 pcm	1.44418	1.4575	1.47717± 34 pcm	1.46114	1389pcm
k_{inf} with zero buckling and at T=1000K	-	1.3928 ± 100 pcm	-	-	1.39218± 38 pcm	1.39249	44pcm

Table 5: Phase 2 – Results from Deterministic Calculations

PARAMETER	UNITS	A	F	Mean	St. Dev.
k_{inf} with zero buckling and at T=293.6K	-	1.46181	1.47656	1.46919	1043pcm
k_{inf} with zero buckling and at T=1000K		1.38911	1.39241	1.39076	233pcm

At 293.6K, the Monte Carlo predictions of k-infinity differ more significantly than the equivalent values calculated for a uranium-fuelled system in Phase 1. There is a large difference between the results of participants C and D and those from Participant F. Since the Phase 1 results from these participants were in good agreement, it is unlikely that this discrepancy in the Phase 2 results may be caused by calculation method differences. It could therefore be a consequence of differences in the nuclear data in ENDF-B/VI (used by participants C and D) and ENDF-B/V (used by participant F).

There is close agreement between Participant A's and Participant F's Monte Carlo predictions of k-infinity at 1000K. However, since the results from these participants differ at 293.6K, the predictions of the k-infinity change following an increase in temperature are inconsistent. Participant A predicts a decrease in k-infinity of 7290pcm (1.4657 – 1.3928) after increasing the temperature from 293.6K to 1000K, whereas Participant F predicts a decrease of 8499pcm (1.47717 – 1.39218).

The deterministic results from Participant A and Participant F are in reasonable agreement with the equivalent Monte Carlo results provided by those participants.

5.3 Phase 3: Plutonium fuel: Whole-Core calculation

Table 6: Phase 3 – Results from Monte Carlo Calculations

PARAMETER	UNITS	A	B	C	D	F	Mean	St. Dev.
Core k-effective at 293.6K	-	1.3494 ±100 pcm	1.35714 ±50 pcm	1.35302	1.347	1.36127 ± 50 pcm	1.35357	576pcm
Core k-effective at 1000K	-	1.2998 ±100 pcm	1.31111 ±50 pcm	1.30577	1.318	1.29879 ±42 pcm	1.30669	803pcm
Core k-effective at an irradiation of 1500 MWd/te	-	-	-	-	1.294	-	-	-

Table 7: Phase 3 – Results from Deterministic Calculations

PARAMETER	UNITS	A	B	E	Mean	St. Dev.
Core k-effective at 293.6K	-	1.34624	1.35075	1.29827	1.33175	2908pcm
Core k-effective at 1000K	-	1.29494	1.29820	1.26230	1.28515	1985pcm
Core k-effective at an irradiation of 1500 MWd/te	-	1.28435	1.27818	1.24099	1.26784	2346pcm

The mean calculated Monte Carlo core k-effective of all participants at 293.6K is 1.35357 with a standard deviation between results of ±576pcm. The outlying results are from Participant D (-657pcm from the mean) and Participant F (+770pcm from the mean).

The difference between Participant A's Monte Carlo and deterministic results for the core k-effective at 293.6K is 316 ± 100pcm, and that for Participant B is 639 ± 50pcm. This is relatively good agreement considering the stochastic nature of the pebble arrangement. The deterministic results from Participant E are significantly lower than those from participants A and B. These differences may, in part, be due to using ENDF/B-5 relative to JEF2.2 nuclear data.

For the Monte Carlo calculations, the k-effective decrease following an increase in temperature to 1000K is 4960pcm from Participant A, 4603pcm from Participant B, 2900pcm, 4725pcm from Participant C, 2900pcm from Participant D and 6248pcm from Participant F. The deterministic calculations of participants A, B and E respectively give values of the k-effective decrease as 5130pcm, 5255pcm and 3597pcm.

Participants A, B and E have included deterministic evaluations of the reduction in k-effective following irradiation to 1500MWd/te (this reduction includes the effect of xenon poisoning). Participant A calculates this reduction in k-effective as 1059pcm, Participant B calculates it as 2002pcm and Participant E calculates it as 2131pcm. Participant D's Monte Carlo estimate of the same parameter is 2400pcm.

5.4 Phase 4: Uranium fuel: Whole-Core calculation

Table 8: Phase 4 – Results from Monte Carlo Calculations

PARAMETER	UNITS	A	B	F	Mean	St. Dev.
Core k-effective at 293.6K	-	1.3697 ± 100 pcm	1.38208 ± 50 pcm	1.36881± 48pcm	1.37353	742pcm
Core k-effective at 1000K	-	1.2863 ± 100 pcm	1.30557± 50 pcm	1.27599± 46pcm	1.28929	1501pcm

Table 9: Phase 4 – Results from Deterministic Calculations

PARAMETER	UNITS	A	B	E	Mean	St. Dev.
Core k-effective at 293.6K	-	1.36818	1.37663	1.35018	1.36500	1351pcm
Core k-effective at 1000K	-	1.28443	1.29460	1.27078	1.28327	1195pcm

There is good agreement (1.3697 – 1.36881 = 89pcm) between Participant A's and Participant F's Monte Carlo predictions of k-effective at 293.6K, although their Monte Carlo results differ more significantly at 1000K (1.2863 – 1.27599 = 1031pcm). The difference at 1000K may be a result of Participant A using JEF2.2 data, where Participant F is using ENDF-B/V data. The Monte Carlo results of Participant A and Participant B differ by more than 1000pcm at both 293.6K and 1000K. Because Participant A and Participant B both use JEF2.2 data, these discrepancies are likely to be a result of differences in calculation methods or modeling approaches for these whole-core calculations.

Participant A's Monte Carlo and deterministic results are in good agreement at 293.6K (1.3697 – 1.36818 = 152pcm) and at 1000K (1.2863 – 1.28443 = 187pcm). There are larger differences between the Monte Carlo and deterministic results from Participant B (545pcm at 293.6K and 1097pcm at 1000K). As in the plutonium whole-core calculation in Phase 3, the deterministic results from Participant E are lower than those from participants A and B. However, in these Phase 4 calculations, the differences between Participant E's deterministic results and those from participants A and B are significantly smaller than in the Phase 3 plutonium whole-core calculations.

5.5 Phase 5: Thorium/Uranium fuel: Cell calculation

Table 10: Phase 5 – Results from Monte Carlo Calculations

PARAMETER	UNITS	A	F	Mean	St. Dev.
k_{inf} with zero buckling and at T=293.6K	-	1.4618 ± 20 pcm	1.46470 ± 34 pcm	1.46325	205pcm
k_{inf} with zero buckling and at T=1000K	-	-	1.46127 ± 26 pcm	-	-

Table 11: Phase 5 – Results from Deterministic Calculations

PARAMETER	UNITS	A	B	F	Mean	St. Dev.
k_{inf} with zero buckling and at T=293.6K	-	1.46066	1.46269	1.4645	1.46262	192pcm
k_{inf} with zero buckling and at T=1000K	-	-	1.46276	1.46163	1.46150	134pcm

The Monte Carlo estimates of k-infinity at 293.6K from Participant A and Participant F are in reasonable agreement (1.46470 – 1.4617 = 300pcm). At 293.6K, there is good agreement between the equivalent deterministic and Monte Carlo calculations from participants A and F. Participant B's deterministic result at 293.6K is consistent with the deterministic results from participants A and F.

Participant A has not provided results for k-infinity at 1000K because, although the WIMS and MONK libraries contain temperature-dependent data for Th232, they do not contain temperature-dependent data for U233.

Participant B's and Participant F's results show differing trends in the change in k-infinity following an increase in temperature. Participant B calculates a small increase in k-infinity, whereas Participant F calculates a decrease in k-infinity.

Participant B has noted that, in the APOLLO2 calculations, the U233 fission, U233 absorption and Th232 absorption one-group cross-sections all decrease with increasing temperature. In APOLLO2, this leads to an apparent compensating effect between the nuclide reaction rates as the temperature increases, meaning the effective change in k-infinity is positive and relatively small.

6. Conclusions

A benchmark inter-comparison of results has been made for a series of cell and whole core configurations relevant to uranium, plutonium and thorium fuelled pebble bed modular reactors.

Contributions to the benchmark have been made by six organizations Serco Assurance (UK), CEA (France), Nuclear Engineering Department Hacettepe University (Turkey), Nuclear Engineering Department Hacettepe University (Turkey), Nexia Solutions (UK) (formerly BNFL R&T, UK) and Nuclear Science & Technology Division ORNL (USA).

According to the participant, ENDF/B-V, ENDF/B-VI and JEF2.2 nuclear data have been applied in both Monte Carlo and deterministic analyses of the benchmark.

Generally, participants using the same nuclear data report similar results, however, there are some differences, particularly, in relation to the fuel temperature coefficients and the whole core xenon fission product poisoning effect.

There is also evidence of good agreement between Monte Carlo and deterministic solutions for some of the participants, despite the difficultly of modeling the stochastic nature of the HTR fuel geometry.

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References

1) G. Hosking and T. D. Newton , Proposed Benchmark Specification for an HTR fuelled with Reactor Grade Plutonium (or Reactor Grade Pu/Th and U/Th), NEA/NSC/DOC(2003)22, 2003
2) T. D. Newton and J. L. Hutton , The Next Generation WIMS Lattice Code: WIMS9, PHYSOR 2002, Seoul, Korea, October 2002
3) J. L. Hutton , Advanced Monte Carlo Features, PHYSOR 1996, Japan, September 1996
4) A. Herbert et al.,APOLLO2: Notice D'Utilisation Version 2.4, CEA report, SERMA/LENR/RT/98-2478/A, 1998
5) C. Andrieux, Notice d'identification des bibliothèques CEA93.V6 à 172 et 99 groupes, CEA report, SERMA/LENR/RT/99-2724/A, 1999
6) J.P. Both, Y. Pénéliau, The Monte Carlo Code TRIPOLI-4 and its first benchmark interpretations International Conference on the Physics of Reactors PHYSOR 1996, Mito, Ibaraki, Japan, 1996
7) SCALE: A Modular Code Scheme for Performing Standardized Computer Analysis for Licensing Evaluations, ORNL/TM-2005/39 Version 5, Volumes I-III, April 2005. Available from the Radiation Safety Information Computational Center at Oak Ridge National Laboratory as CCC-725
8) M. Coste et al., Self-Shielding Calculations by APOLLO2 Code for Fuel Pins with a Temperature Distribution, International Conference on Mathematical Methods and Supercomputing for Nuclear Applications, Saratoga Springs, New York, October 5-9 1997