

**INTERNATIONAL STUDIES ON BURNUP CREDIT CRITICALITY SAFETY
BY AN OECD/NEA WORKING GROUP**

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ABSTRACT

The results and conclusions from a six-year study by an international benchmarking group in the comparison of computational methods for evaluating burnup credit in criticality safety analyses is presented. Approximately 20 participants from 12 countries have provided results for most problems. Four detailed benchmark problems for pressurized-water-reactor fuel have been completed. Results from work being finalized, addressing burnup credit for boiling-water-reactor fuel, are discussed, as well as planned activities for additional benchmarks, including mixed-oxide fuels, and other activities.

I. INTRODUCTION

The Organization for Economic Cooperation and Development's Nuclear Energy Agency (OECD/NEA) has sponsored criticality safety benchmark groups for more than a decade. These groups have addressed criticality safety issues of storage, dissolution and transportation of nuclear materials. In 1991, the benchmark group elected to pursue a study of burnup credit criticality benchmarks.

The main objective of the burnup credit group is to demonstrate that the available criticality safety calculational tools are appropriate for application to burned fuel systems and that a reasonable safety margin can be established. We describe the suite of burnup credit criticality benchmarks that was established by the OECD/NEA Burnup Credit Criticality Benchmark Group. The benchmarks have been selected to allow a comparison of results among participants using a wide variety of calculational tools and nuclear data libraries. The nature of the burnup credit problem requires that the capability to

calculate both spent fuel composition and reactivity be demonstrated. The benchmark problems were selected to investigate code performance over a variety of physics issues associated with burnup credit: relative performance of fission products and actinides with respect to the multiplication factor (k) for pressurized-water reactors (PWRs); trends in k and isotopic composition with burnup and enrichment for PWRs; effects of axially distributed burnup in PWRs; more recent problems have focused on similar considerations for boiling-water reactors (BWRs) and mixed-oxide (MOX) fuels. It is important to note that the focus of the working group is the comparison of the results submitted by each participant to assess the capability of commonly used code systems, not to quantify the physical phenomena investigated in the comparisons or to make recommendations for licensing action. Participants used a wide variety of codes and methods based on transport and diffusion theory, using Sn, nodal and Monte Carlo techniques. Nuclear data (both cross-section and decay data) were taken from a variety of sources - multiple versions of the Evaluated Nuclear Data Files (ENDF/B), the Japan Evaluated Nuclear Data Libraries (JENDL), the Joint Evaluated Files (JEF), and the United Kingdom Nuclear Data Libraries (UKNDL). Both multigroup and continuous-energy cross-section data were used in the study. Table I is a summary of the benchmark problems addressed by the group, noting both the primary objective and current status of each.

The following sections provide brief descriptions of each of the benchmark problems and a summary of results. Since the objective of the benchmark group has been, thus far, to assess code capabilities, the results are most often presented as the standard deviation (2σ) among participants. The group has not attempted to make a safety

Table I. Summary of Benchmark Problems Addressed by OECD/NEA Criticality Safety Benchmark Group.

Benchmark	Primary Objective	Status
Phase I-A	Examine effects of seven major actinides and 15 major fission products for an infinite array of PWR rods. Isotopic composition specified at 3.6 wt % U-235 at 0, 30, 40 GWd/MTU and at 1- and 5-year cooled.	Completed 13 cases. Ref. 1
Phase I-B	Compare computed nuclide concentrations for depletion in a simple PWR pin-cell model, comparison to actual measurements at three burnups (27.34, 37.12, and 44.34 GWd/MTU). Comparisons made for 12 major actinides and 15 fission products for each burnup case.	Completed three cases. Ref. 2
Phase II-A	Examine effects of axially distributed burnup in an array of PWR pins as a function of initial enrichment, burnup and cooling time. Effects of fission products independently examined. Isotopic compositions specified.	Completed 26 cases. Ref. 3
Phase II-B	Repeat study of Phase II-A in a 3-D geometry representative of a conceptual burnup credit transportation container. Isotopic compositions specified.	Completed nine basic cases and two accident configurations. Ref. 4
Phase II-C	Complementary study on the sensitivities due to different axial burnup profiles across the full range of burnups	Proposed
Phase III-A	Investigate the effects of moderator void distribution in addition to burnup profile, initial enrichment, burnup and cooling-time sensitivities for an array of BWR pins. Isotopic compositions specified.	Report for 22 cases being finalized
Phase III-B	Compare computed nuclide concentrations for depletion in a BWR pin-cell model.	Draft results in review
Phase IV	Investigate burnup credit for MOX spent fuel	In progress

case for licensing nor has there been an attempt to provide bounding values on the observed trends or physical phenomena (e.g., the effect of axially distributed burnup). Specific or suspected sources of discrepancies are discussed. Based on 2σ results, some areas for future study are identified.

II. PHASE I AND PHASE II: PRESSURIZED-WATER-REACTOR STUDIES

The burnup covered in these studies ranges from fresh fuel to 50 GWd/t and cooling periods from 1–5 years and different enrichments in the fuel. Studies included Phase I, which looked at the calculated multiplication factor for an infinite lattice of PWR pins and the prediction of isotopic composition of spent PWR fuel under simplified conditions, to permit the greatest participation among members. Phase II addressed the study of axially

distributed burnup in PWRs. The results for Phase I are covered in detail in Ref. 1 and 2 and were summarized in Ref. 5. As such, only a brief description of the Phase I problem specifications are given here.

A. Phase I-A: Multiplication Factors-PWR Infinite Lattice Studies (1D)

This benchmark consists of 13 cases. Each case is an eigenvalue calculation of a simple infinite lattice of PWR fuel rods. The investigated parameters were burnup, cooling time and combinations of nuclides in the fuel region. The groupings of nuclides include four subgroups: major actinides (U-234, 235, 236, and 238; Pu-239, 240 and 241); minor actinides (Pu-238 and 242; Am-241 and 243; Np-237); major fission products (Mo-95; Tc-99; Ru-101; Rh-103; Ag-109; Cs-133; Sm-147, 149, 150, 151 and 152; Nd-143 and 145; Eu-153; and Gd-155) and minor

fission products (all others available to participant). The fuel compositions for each case by nuclide were provided as part of the problem specification so that the results could be focused on the calculation of (impacts on) the multiplication factor. In total, 25 sets of results were submitted from 19 institutes in 11 countries. Phase I-A is perhaps the most detailed of the benchmark problems in terms of types of data collected and analyzed. Participants were asked to provide the following: codes used, nuclear data libraries, and energy grouping of libraries (group structure or continuous energy); calculated multiplication factor; neutron spectrum in water; neutron spectrum in fuel; absorption rates for all major and minor actinides, major fission products and oxygen; and production rates and neutrons per fission for all major and minor actinides. The results are briefly summarized below.

The results suggest that the largest component of uncertainty originates from the minor fission products. For cases including major fission products, the standard deviation (2σ) values are smaller than for the case of fresh fuel. The agreement among participants for the cases without fission products is significantly better than the fresh fuel and burned fuel with fission product cases. No trends in the standard deviation among participants were observed with either burnup or cooling time. Trends in the multiplication factors with burnup and cooling time were as expected; k decreases as both burnup and cooling time increase. The larger 2σ value for the fresh fuel case was expected based on known biases that decrease with fuel depletion. Fourteen participants provided neutron spectra in both the fuel and water. The number of energy groups varied from 27 to 247, and the maximum energy boundaries varied from 8.2 MeV to 20 MeV. Results based on continuous-energy data were converted for mutual comparison. The spectra were in quite good agreement. The effects of Pu resonances were clearly seen at approximately 0.3 and 1.0 eV in the fuel region and smaller effects at these energies were observed in the moderator region. Seventeen participants supplied the requested reaction rate data. Both the absorption rates and production rates were normalized to unity for comparison. A comparison of absorption rates revealed differences of 0.4–0.7% of the total absorption rate for U-238, U-235 and Pu-239. The production rates for these nuclides revealed observed differences among participants of 0.6 to 0.8% of the total production rate. Differences were also observed in the calculated values of neutrons per fission for these nuclides; however, there were some discrepancies among participants in the definition of this parameter, so the results are inconclusive. Smaller differences in absorption rates (less than 0.1% of the total absorption rate) were observed for Pu-240, Pu-241, Gd-155, Nd-143, Rh-103, Sm-149, Sm-151 and Tc-99.

B. Phase I-B: Spent Fuel Compositions, PWR Fuel

The purpose of this calculational benchmark problem was to compare computed nuclide concentrations for depletion in a simple pin-cell model. The detailed problem description and results are given in Ref. 2. This benchmark consists of three cases, each with a different burnup. The specific power and boron concentrations for each cycle and cumulative burnup were given in the problem description. Initial isotopic compositions for both the fuel and the moderator were given. Participants were requested to report calculated compositions for the 12 actinides and 15 fission products named in Phase I-A. A total of 21 sets of results were submitted by 16 organizations from 11 countries. Unlike Phase I-A, trends in the standard deviation with burnup are evident in this study. For many nuclides this trend is relatively small; however, the trend of increasing standard deviation with increasing burnup appears to be significant for U-235. A list of nuclides for which further study and comparison of additional information (such as fission product yield data, thermal cross sections, etc.) would be warranted is as follows: Pu-239, Gd-155, U-235, Pu-241, Pu-240, Sm-151, and Sm-149, as these have the largest integral effect on k . Of these nuclides, only Gd-155 and Sm-149 exceed both the 10% standard deviation and a $\Delta k/\% \Delta N$ of 0.01%.

C. Phase II-A: Multiplication Factors-Distributed Burnup Studies (2-D)

The configuration considered in this benchmark problem was a laterally infinite array of PWR fuel assemblies with the following characteristics: initial enrichment equals to 3.6 or 4.5 wt %; fuel radius equals to 0.412 cm and array pitch equals to 1.33 cm, which leads to a moderation ratio $V_{\text{mod}}/V_{\text{ox}} = 2.0$; different burnups were considered (0, 10, 30 or 50 GWd/MTU) and two cooling times, 1 or 5 years; axially, a symmetrical configuration was adopted including 9 fuel regions (total height = 365.7 cm); and an upper and lower plug and water reflector (30 cm). Specific isotopic compositions were specified for each fuel region and conditions. Cases were analyzed for the axially distributed burnup as well as a uniform burnup assumption equal to the assembly average burnup. The axial burnup profiles used were symmetric about the midplane. As in Phase I-A, the effects of major actinides and fission products were also investigated. Participants were asked to provide calculated multiplication factors and fission densities by axial zone for three cases. In total, 22 results for the 26 configurations were calculated by 18 different participants from 10 countries.

Details of the problem specification and results for this benchmark, presented in Refs. 3 and 5, are discussed

here. No significant trends in the agreement among participants (2σ values) were observed with initial enrichment or burnup. As in Phase I-A, the inclusion of fission products results in a greater deviation among participants (larger 2σ values). No clear trends were observed with the inclusion of the axially distributed burnup, although cases with both high burnup (greater than 10 GWd/MTU) and with fission products have some indications of increasing 2σ when axially distributed burnup is considered. At higher burnup (50 GWd/MTU with and without fission products) there is a suggestion of a trend in 2σ with cooling time. Overall, the most interesting result in this benchmark is that the largest discrepancy (2σ) among participants is still seen for the fresh fuel cases. The "end effect" was defined as the difference in the multiplication factors between the corresponding cases with and without an axial burnup distribution. Tendencies were observed in the multiplication factors that indicate an increase in end effect with increasing burnup. It is very important to note that the end effect is calculated as the difference of two close values and, therefore, has large calculated standard deviations, from 25% to greater than 100% of the value calculated for the end effect (in most cases approximately 75%). Although these tendencies are believed to be representative in general, the effects of both neutron leakage and axial asymmetry of material composition (which was not considered here) may make a considerable difference in the magnitude of the end effect. The fission density data provided by the participants was found to be in relatively good agreement. The data illustrate the importance of the end regions: approximately 70% of the total fissions occurred in the upper 40 cm of the fuel (representing approximately 22% of the total fuel volume). Therefore, adequate modeling and convergence at the fuel ends are essential to obtaining reliable eigenvalues for highly irradiated spent fuel systems.

D. Phase II-B: Multiplication Factors-Distributed Burnup Studies (3-D)

In this benchmark problem, a realistic configuration of 21 PWR spent fuel assemblies in a stainless steel transport cask was evaluated. A borated stainless steel basket centered in the flask separates the assemblies. The basket (5 × 5 array with the four corner positions removed) was fully flooded with water. Nine basic cases and two additional accident configurations were considered with the following varying parameters: burnup (fresh fuel, 30 and 50 GWd/MTU), fuel composition (actinides only and actinides with 15 fission products), axial burnup discretization (1 or 9 zones). In all, 14 participants from 7 countries submitted partial or complete results (multiplication factors, reaction rates).

Good agreement was found between participants for calculated k . The dispersion of results, characterized by 2σ (where σ is the ratio between the standard deviation and the average value) ranged from 0.5 to 1.1% for irradiated fuels and was equal to 1.3% for fresh fuel (see Table II). The reactivity effect of axial burnup profile for basic cases was similar to that obtained in Phase II-A: less than 1,000 pcm (percent per mil, $10^{-5} \Delta k/k$ for cases with burnup less than or equal to 30 GWd/MTU or for cases without fission products and about -4,000 pcm for 50 GWd/MTU burnup and composition including fission products. However, two accident cases highlighted that the reactivity effect of axial burnup discretization depends on the configuration studied. For the accident conditions defined for this benchmark, the axially averaged flat distribution was found to be a nonconservative approximation even for low burnups (10 GWd/MTU) and without fission products; the reactivity effect of burnup profile reached -14,000 pcm for 50 GWd/MTU burnup including fission products. Clearly, the use of axially homogeneous fuel compositions may be unsuitable for cases where there are significant axial heterogeneities.

The calculation of fission fractions and densities was also investigated. The comparison of fission distributions indicates problems of eigenfunction convergence for cases indicating increasing dispersion among participant results (higher values of 2σ); for cases including fission products this behavior is reversed. In Phase II-B the results with fission products have *smaller* 2σ values than those cases with no fission products. Consistent with earlier results the highest value of 2σ is for the fresh fuel case. Overall, the agreement among participants is better for Phase II-B than in the Phase II-A benchmark.

III. PHASE III: BOILING-WATER-REACTOR STUDIES

Benchmark calculations for irradiated BWR fuels started from 1996 as a new series, Phase III. The main features of BWRs important in criticality analyses that differ substantially from PWRs are the moderator void distribution in the core and the complicated composition of a fuel assembly. The Phase III-A Benchmarks compare the results of criticality calculations of irradiated BWR fuels in storage facilities or transportation casks. Phase III-B, which is in progress, will compare prediction capability of depletion codes for irradiated BWR fuels.

A. Phase III-A: Criticality Calculations of BWR Spent Fuel in Storage and Transportation

An infinite array of BWR fuel assemblies, modeled on STEP-II-type assemblies, was specified for the criticality

Table II. Phase II-B Results - Average Multiplication Factors (Ref. 4).

Case	Initial enrichment (wt %)	Burnup GWd/MTU	Cooling time (years)	Fission products	Burnup profile	k (2 σ)
1	4.5	Fresh	N/A	N/A	N/A	1.1257 (0.013)
2	4.5	30	5	Yes	No	0.8934 (0.007)
3	4.5	30	5	No	No	0.9716 (0.010)
4	4.5	30	5	Yes	Yes	0.8953 (0.010)
5	4.5	30	5	No	Yes	0.9647 (0.011)
6	4.5	50	5	Yes	No	0.7641 (0.005)
7	4.5	50	5	No	No	0.8737 (0.007)
8	4.5	50	5	Yes	Yes	0.7933 (0.008)
9	4.5	50	5	No	Yes	0.8791 (0.010)

benchmark calculations. Each fuel assembly consisted of an 8×8 fuel rod array, in which a thick (3.2-cm diameter) water rod is centered, all surrounded by a channel box which is surrounded by an 8.5-mm-thick water reflector. The reflective boundary condition is imposed outside a 15.24-cm^2 cell of a fuel assembly. All fuel rods are assumed to be identical. The mean uranium concentration of fresh fuel rods, including the top and bottom blanket regions, is assumed to be 3.5 wt %. The total length of the fuel rods including the blanket regions is about 370 cm. The fuel rod is divided into 9 regions, and the irradiated fuel composition in each region was given in the problem specification. Twenty-two cases were proposed where burnup varies from 0 to 40 GWd/MTU, fission products are included in some cases, an axial burnup distribution is considered in some cases, an axial void distribution is used in some cases (40 and 70% uniform void cases are considered) and cooling times of 1 and 5 years are specified. In total, 21 results were submitted from 17 institutions in 9 countries. Participation was also categorized by the evaluated nuclear data of the main actinides that formed the bases of the calculations: 9 results were based on ENDF, 9 were on JEF, 2 were on JENDL, and 2 used data from UKNDL.

The detailed results for this benchmark problem have been reviewed and approved by the Working Group and are expected to be published in the last quarter of 1998 in a report similar to Ref. 3. Overall, the relative dispersion from the average multiplication factor calculated by all participants was within $\pm 1\% \Delta k/k$. Summary results for participant-average k-effective that have been used to determine trending with axial burnup profile, void distribution, cooling time, and fission products are given in Table III. Axial profiles of fractional fission rates (only

requested for 5 of 22 cases) were found to be within 7% for most cases. The end effect defined as the difference of k with and without burnup profiles, has a similar tendency as the PWR cases; however, it appeared less pronounced (i.e., up to $1\% \Delta k$). Constant uniform void ratios, 40% and 70%, were applied. The 70% case overestimates k when the burnup profile is disregarded. Consistent with the PWR cases, k effective decreases as the cooling time increases from 1–5 years.

B. Phase III-B: Spent Fuel Compositions, BWR Fuel

This benchmark was developed to investigate the ability of evaluation tools to calculate the isotopic composition of irradiated BWR fuel. Unlike the problem specification for Phase III-A, the geometry of the BWR fuel assembly was not simplified for this benchmark. The fuel assembly consists of fuel rods at five different initial enrichments and with and without Gd. The initial isotopic composition of each rod and explicit geometry descriptions were specified. As in the Phase III-A specification, the void fraction is varied, cases are evaluated at 0, 40 and 70% uniform void fractions. Number densities for the 12 actinides and 15 fission products of Phase I-A are requested for each of 9 fuel pins in a $1/8$ assembly model. The average composition of each of the 5 fuel-rod types and assembly-average compositions are requested. The calculated burnup for each of the 9 fuel pins is also requested. Participants are also asked to provide neutron multiplication factors for burnups of: 0, 0.2, 10, 20, 30, 40, 50 GWd/MTU for each of the three void fraction cases together with the burnup at which k reaches a maximum value. The Working Group began evaluating this benchmark problem in late 1997. Draft results have been compiled and are under review by the working group.

Table III. Phase III-A Results - Multiplication Factor Trends Based on Average Participant Results (All cases for 3.5 wt % U-235).

Burnup GWd/MTU	Cooling time (years)	Fission products	Burnup profile	Void profile	Average k
20	1	Yes	Yes	Yes	1.194
20	5	Yes	Yes	Yes	1.182
30	1	Yes	Yes	Yes	1.111
30	5	Yes	Yes	Yes	1.091
40	1	Yes	Yes	Yes	1.027
40	5	Yes	Yes	Yes	0.998
40	5	Yes	No	Yes	0.989
40	5	No	No	No	1.104
40	5	Yes	No	40% (uniform)	0.958
40	5	Yes	No	70% (uniform)	0.998
40	5	No	No	40% (uniform)	1.072
40	5	No	No	70% (uniform)	1.114
40	5	No	Yes	Yes	1.100

IV. PHASE IV: MIXED-OXIDE STUDIES

Phase IV-A: This problem specification includes a simple PWR MOX pincell to be evaluated for three initial MOX fuels representing (1) good-quality Pu, (2) weapons-disposition Pu, and (3) poor-quality (multirecycle) Pu. Participants were asked to calculate the infinite multiplication factor for various combinations of burnup, cooling time, and irradiated fuel representations (e.g., major/all actinides, fission products). To date, 16 sets of preliminary results have been received from 10 organizations representing 6 countries. A significant spread is noted in the results, even for fresh MOX fuel. The rate of change of k-infinity with burnup is strongly dependent upon the initial Pu content and composition in fresh MOX. The inclusion of Cm produces a positive contribution to reactivity (up to 1.5% for poor-quality Pu). The initial results are being compiled for review by the Working Group.

Phase IV-B has been proposed to investigate calculational accuracy of predictions of nuclide concentrations in spent MOX fuels. The details of the problem specification are being finalized for review and acceptance by the Working Group at the next meeting (Spring 1999).

V. FUTURE WORK

The Benchmark Working Group is continuing to pursue studies with BWR fuel (Phase III benchmark) and

MOX fuel (Phase IV benchmark). In support of the burnup credit studies a Spent Fuel Isotopic Composition Database (SFCOMPCO, Refs. 6, 7), has been developed, containing data collected from 13 LWRs, including 7 PWRs and 6 BWRs in Europe, the USA and Japan. SFCOMPO contains data collected from 13 LWRs, including 7 PWRs and 6 BWRs in Europe, the USA and Japan. Over the past year, axial burnup profiles from 2 Japanese reactors have been added to the database. The database will be maintained by adding new data as they become available, revising old data as necessary, and providing recommendations for criticality evaluations. This database is unique and provides a valuable resource for the evaluation of burnup credit. It is planned to also include data for measured axial profiles.

The Group, in addition, reviews criticality benchmark experiments that are applicable to burnup credit. Several activities have involved experiments that are applicable to burnup credit. Refs. 8-13 describe several of these ongoing or planned experiments.

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