Nuclear Science Committee

Burn-up Credit Criticality Studies

Benchmark Analyses for Pressurised Water Reactors

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Burn-up Credit Criticality Studies

Benchmark Analyses for Pressurised Water Reactors
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Foreword

The purpose of this report is to organise detailed information on the physics and analysis of burn-up credit and criticality strategies. The information presented here is intended to aid in establishing safety arguments for nuclear material storage, transportation, and reprocessing of irradiated LWR fuel. This information will also attempt to establish practical rules and identify applicable tools when appropriate. The report offers a discussion of any issues encountered when performing the international comparison problems.

The NEA Expert Group on Burn-up Credit Criticality (EGBUC) has done extensive research on the subject and has made recommendations on various burn-up topics. The EGBUC was set up to examine burn-up credit as applied to criticality safety in the transportation, storage and treatment of spent fuel for a wide range of fuel types and reactors. Under the guidance of the Working Party on Nuclear Criticality Safety, the major assignments of the expert group include:

- carrying out international comparison exercises and benchmarks to assess the ability of code systems to predict the reactivity of spent nuclear fuel systems, including comparison with experimental data as available;
- investigating the physics and predictability of burn-up credit based on the specification and comparison of calculational benchmark problems;
- publishing the results for the benefit of criticality safety community, so that the work may be used to help establish suitable safety margins.

More information on this expert group can be found at: https://www.oecd-nea.org/science/wpncs/buc/. The scope of this report covers systems containing irradiated uranium oxide (UOX) and Mixed Oxide (MOX) fuel for Pressurised Water Reactors (PWRs) only.

Various burn-up credit topic summaries have been contributed by members of the EGBUC. Collections of reports on burn-up credit benchmarks performed by the EGBUC have also been incorporated into this benchmark study and are listed in the bibliography section. The full benchmark reports have been published separately and can be found at the website of the EGBUC: https://www.oecd-nea.org/science/wpncs/buc/.

For the present report, a list of appendices has been compiled and is accessible through the following links:

- Appendix A
- Appendix B
- Appendix C
- Appendix D
- Appendix E
- Appendix F
- Appendix G
- Appendix H
- Appendix I
- Appendix J
Acknowledgements

The NEA Secretariat would like to thank all EGBUC participants for their many contributions over the years to the different benchmark studies undertaken. Special thanks are extended to Michaele Brady-Raap for chairing the Expert Group on Burn-up Credit Criticality and for her many years of leadership in this field.
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<tr>
<td>ADSNF</td>
<td>Assay data for spent nuclear fuel</td>
</tr>
<tr>
<td>AMCT</td>
<td>Advanced Monte Carlo Techniques</td>
</tr>
<tr>
<td>ANL</td>
<td>Argonne National Laboratory</td>
</tr>
<tr>
<td>BNFL</td>
<td>British Nuclear Fuels Limited</td>
</tr>
<tr>
<td>BOC</td>
<td>Beginning of cycle</td>
</tr>
<tr>
<td>BUC</td>
<td>Burn-up credit</td>
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<tr>
<td>BWR</td>
<td>Boiling Water Reactor</td>
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<tr>
<td>CR</td>
<td>Control rod</td>
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<tr>
<td>CRC</td>
<td>Commercial reactor criticals</td>
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<tr>
<td>CSA</td>
<td>Criticality safety analysis</td>
</tr>
<tr>
<td>CSI</td>
<td>Criticality safety index</td>
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<tr>
<td>CSNI</td>
<td>Committee on Safety of Nuclear Installations</td>
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<tr>
<td>DOE</td>
<td>Department of Energy</td>
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<tr>
<td>EGBUC</td>
<td>Expert Group on Burn-up Credit Criticality</td>
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<tr>
<td>EOC</td>
<td>End of cycle</td>
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<tr>
<td>EPRI</td>
<td>Electric Power Research Institute</td>
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<tr>
<td>FP</td>
<td>Fission Products</td>
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<td>GNF</td>
<td>Global nuclear fuel</td>
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<tr>
<td>HTC</td>
<td>Haut taux de combustion</td>
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<tr>
<td>IAEA</td>
<td>International Atomic Energy Agency</td>
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<tr>
<td>ICF</td>
<td>Isotopic correction factors</td>
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<tr>
<td>ICSBEP</td>
<td>International Criticality Safety Benchmark Evaluation Project</td>
</tr>
<tr>
<td>IRPhE</td>
<td>International Reactor Physics Experiment Evaluation</td>
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<tr>
<td>JAERI</td>
<td>Japanese Atomic Energy Research Institute</td>
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<tr>
<td>JEFF</td>
<td>Joint Evaluated Fission and Fusion Nuclear Data Library</td>
</tr>
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<td>JENDL</td>
<td>Japanese Evaluated Neutron Data Library</td>
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<tr>
<td>Abbreviation</td>
<td>Description</td>
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<td>-------------------------------------------------------</td>
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<tr>
<td>LC</td>
<td>Loading curve</td>
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<td>LEU</td>
<td>Low Enriched Uranium</td>
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<td>LWR</td>
<td>Light Water Reactor</td>
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<tr>
<td>MDAS</td>
<td>Multi-detector analysis system</td>
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<td>MOX</td>
<td>Mixed oxide</td>
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<td>NDA</td>
<td>Nuclear Decommissioning Authority</td>
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<td>Oak Ridge National Laboratory</td>
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<td>PBC</td>
<td>Partial boron credit</td>
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<td>PIE</td>
<td>Post-irradiation examination</td>
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<td>PWR</td>
<td>Pressurised water reactors</td>
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<td>SCALE</td>
<td>Standardised cask-analysis for licensing evaluation</td>
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<td>SFCOMPO</td>
<td>Spent Fuel Isotopic Composition Database</td>
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<td>SNF</td>
<td>Spent Nuclear Fuel</td>
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<tr>
<td>TRSD</td>
<td>Two-times Relative Standard Deviation</td>
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<tr>
<td>UOX</td>
<td>Uranium oxide</td>
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<tr>
<td>US</td>
<td>United States</td>
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<tr>
<td>VVER</td>
<td>Russian Pressurised Reactor Design</td>
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<tr>
<td>WPNCS</td>
<td>Working Party on Nuclear Criticality Safety</td>
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<td>YMP</td>
<td>Yucca Mountain Project</td>
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1. UOX PWR Summary

Jens Christian Neuber

1.1 Introduction

Burn-Up Credit (BUC) Criticality Safety Analysis (CSA) of Spent/Irradiated Nuclear Fuel (S/INF) management systems consists in implementation of two key steps:

- estimation of the S/INF isotopic composition by means of a depletion calculation code;
- criticality analysis for evaluating the loading criterion which indicates the minimum burn-up necessary for S/INF with a specific initial isotopic composition to be loaded in the S/INF management system of interest.\(^1\)

Application of BUC to a S/INF system of interest includes a third key step:

- quantification of the S/INF burn-up and check whether the loading criterion is met.

This issue, however, is beyond the scope of the working agenda of the NEA Expert Group on BUC Criticality Safety (EGBUC), (see [1-4]\(^2\)).

To perform a depletion analysis the following needs to be defined:

- the fuel characteristics;
- the fuel depletion conditions (reactor operation conditions) and;
- the cooling time.

A criticality safety analysis of a S/INF management system designed for burn-up credit typically comprises the following main steps:

- isotopic selection and validation;
- validation of the criticality calculation code applied;
- evaluation of the reactivity effects of axial and horizontal burn-up profiles;
- estimation of the loading criterion;

---

1. Instead of indicating the minimum required burn-up a loading criterion may specify the limiting value of an observable which is related to the minimum required burn-up. (The limiting value of the related observable may be the maximum allowable value as it is the case for instance if the fissile content serves as the related observable. In that case one has however to observe also the mass ratios of the fissile isotopes because these ratios affect the neutron spectrum of the management system of interest.)

2. Note that on page 22 of [4] the burn-up confirmation requirements laid down in the German burn-up credit criticality safety standards DIN 25471 and DIN 25712 [5,6] are misinterpreted: The requirement that a misloading event has to be excluded as a design basis event by applying the double contingency principle directly to the misloading event does not imply that no burn-up measurement is required [3,7].
• analysis of abnormal and accident conditions, if applicable; for the post-closure phase of a final repository: analysis of scenarios modelling impacts of possible future changes in climate and geological conditions on the SNF waste packages.

In the report at hand the attention is focused on BUC applications to handling, transport, storage and reprocessing of spent/irradiated uranium-dioxid (UO₂) fuel assemblies of western PWR types. The fuel depletion conditions (reactor operation conditions) are therefore characterised by the following parameters:

• specific power and operating history;
• fuel temperature;
• moderator temperature and related density;
• concentration of soluble boron in the moderator (cycle-specific boron let-down curves);
• use of fixed neutron absorbers in form of:
  – control rods;
  – burnable poison rods, axial power shaping rods;
• use of fuel assemblies with integral burnable absorbers in the form of:
  – Gd or Er bearing fuel rods or;
  – IFBA fuel rods (rods containing pellets with burnable absorber coating, e.g. ⁴⁰B coating);
• presence of MOX fuel assemblies in the core.

The NEA EGBUC Burn-up Credit Criticality Benchmark reports [8-14] addressed to applications of burn-up credit to S/INF from UO₂ fuel assemblies of western PWR types present benchmarks for the two key steps of BUC CSA:

• benchmarks for the estimation of S/INF isotopic compositions for predefined fuel characteristics, depletion conditions, and cooling times, [9,13];
• theoretical benchmarks for the estimation of reactivity effects due to burn-up for given S/INF isotopic compositions related to different depletion conditions, burn-up values, cooling times, and axial burn-up profiles, using:
  – different isotopic selection approaches (such as the “actinides-only” BUC approach and the “actinides-plus-the major fission products” BUC approach);
  – different S/INF configurations (pin-cell configurations, arrangement of fuel assemblies of different types in casks designed for SNF transport or storage); and
  – [8], and [10-14].
• theoretical benchmarks combining the estimation of S/INF compositions for predefined fuel characteristics, depletion conditions and cooling times with the analysis of the reactivity changes due to burn-up using different isotopic selection approaches, (see [9,13] in Appendix A).

The BUC Criticality Benchmark reports [8] and [10-14] do not give any predefined theoretical benchmark solutions. The procedure usually taken by the NEA EGBUC is as follows:
• A calculational task is formulated (e.g. a depletion analysis) and all the parameters needed for solving the task are specified.

• Experts in depletion and criticality analysis from different organisations (institutes, companies, etc.) supporting the work of the NEA EGBUC provide solutions of the task obtained by means of the codes and nuclear data libraries usually used for such analysis. The EGBUC thus obtains statistics of different solutions reflecting the variety of codes and nuclear data libraries used in BUC CSA, [8-14].

• Evaluation of these statistics provides the benchmark solutions presented in the reports [8-14]. In most cases these benchmark solutions are simply derived by averaging the respective individual results obtained from the participating organisations.

Thus, these benchmark solutions are random outcomes which are generally different from best estimates\(^3\). These solutions are nevertheless representative since they are based on results obtained by means of that codes and libraries which are usually used in BUC CSA. The deviations of these results from the benchmark solutions derived from these results, reflect the uncertainties characteristic of performing BUC calculations by means of the available tools.

The biases of the benchmark solutions arising from the biases of the results from which the benchmark solutions are derived remain unknown in the case of theoretical benchmarks. This problem will inevitably occur when a theoretical benchmark solution is used. The bias of such a solution can only be estimated by comparison of the results from which the solution is derived with measured data. As always in physics, measurement is crucial to validation\(^4\).

The calculational tasks formulated in [8-14] include variations of depletion parameters, burn-up values, and cooling times as well as variations of the shape of axial burn-up profiles in order to study the effect of these parameters on the S/INF reactivity \(\rho\). In addition, isotopic number densities \(N_i\) are varied to gain sensitivity coefficients by isotope \(i\), \(\partial\rho/\partial N_i\), for different burn-up values and cooling times as well as under different depletion conditions and under different S/INF configurations as well [9] in Appendix A, and [13]\(^5\). The tasks given in [8] include the calculation of neutron spectra for different burn-up values, different cooling times and different isotopic selections to study the impact of the changes in the fuel’s isotopic composition on the neutron spectrum. In addition, isotopic reaction rates for absorption and production and, in conjunction with the production rates, the number of neutrons per fission of the individual actinides are calculated in order, as stated in [8], to help in identifying possible causes of discrepancy involved in the used calculational tools, i.e. in the nuclear data and the calculation codes.

Due to limited resources, the NEA EGBUC is not able to study the effects on the S/INF reactivity for all BUC-relevant parameters separately. However, much of this work has been performed by experts who were or still are members of the EGBUC; and the results have been published in the proceedings of several conferences and workshops [16-29], in BUC training course materials [30-32] as well as in ORNL and NUREG reports [33-47]. These results will

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\(^3\) An estimate is the numerical value yielded by an estimator for a particular set of observations. An estimator is a function of the observations that makes it possible to obtain an estimate from the observations. A best estimate is understood to be obtained by applying an efficient estimator, i.e. an estimator yielding the minimum variance bound for the set of observations, [15] in Section 1.7.4.

\(^4\) In this report validation is defined as the process of determining the degree to which a model or simulation is an accurate representation of the real world from the perspective of the intended uses of the model or simulation.

\(^5\) It should be remembered that sensitivity coefficients, such as \(\partial\rho/\partial N_i\), are spectrum-dependent.
be taken into account in the report in hand in order to obtain a complete overview of the lessons learnt about the application of BUC to spent/irradiated UO₂ fuel assemblies of western PWR types.

1.2 Estimation of the isotopic composition of spent or irradiated fuel

1.2.1 Fuel characteristics

Fuel characteristics may affect the choice of the appropriate depletion code. For example, in the case of the presence of integral burnable absorbers in the fuel rods, for a fuel design application, a two-dimensional depletion code is certainly preferable to a point-depletion code.

Manufacturing tolerances in the fuel design parameters may affect the S/INF isotopic composition and hence the S/INF reactivity. Since the highest possible initial ²³⁵U concentration results, at given depletion conditions, given burn-up value and given cooling time, in the highest S/INF reactivity possible for a given S/INF configuration under given conditions, it is obvious that the tolerance in the pellet density is bounded by using the upper tolerance limit specified by the fuel vendor for the pellet density. The manufacturing tolerance in the pellet diameter is usually bounded by ignoring the dishing of the pellets, i.e. by modelling the fuel inside the fuel rods as cylindrical columns with a UO₂ density given by the upper tolerance limit of the pellet density.

The objective of a BUC CSA of the S/INF management system of interest usually is to determine the BUC loading criterion for this system. For BUC applications to S/INF from UO₂ fuel assemblies this criterion is usually given in form of a loading curve, which indicates the minimum burn-up necessary for the S/INF with a specific initial ²³⁵U enrichment to be loaded in the S/INF of interest. In other words, the loading curve presents the minimum required burn-up as a function of the initial ²³⁵U enrichment. Therefore, neither in the depletion analysis nor in the criticality calculations performed to estimate the loading curve it is necessary to take account of the tolerance in the initial enrichment of the PWR UO₂ fuel. This tolerance has to be considered in the application of the loading curve, i.e. in the third key step of BUC application when it is checked whether the loading curve is met or not (see Section 1.1).

Of course, the loading curve has to cover the whole range of initial ²³⁵U enrichments possible for the S/INF to be loaded in the S/INF system of interest. So the initial ²³⁵U enrichment defining the upper end point of the loading curve must not be less than \( e_{\text{max}} + \Delta e \), where \( e_{\text{max}} \) denotes the maximum possible nominal initial ²³⁵U enrichment and \( \Delta e \) is the upper tolerance (plus-tolerance) of the initial ²³⁵U enrichment.

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6. It is however recommended to confirm the validity of this statement in each and every application case.
7. Or a related parameter, see footnote 1.
As illustrated in Figure 1.1, when applying the loading curve to S/INF with a nominal enrichment value of $e_{\text{nom}}$ then that burn-up value of $B_{\text{min}}$ applies to the S/INF which is given by the loading curve for the initial enrichment value of $e_{\text{nom}} + \Delta e$. It is necessary to proceed in this way since the tolerance of the enrichment of a UF$_6$ charge and hence of the UO$_2$ pellets resulting from this UF$_6$ charge is significantly smaller (usually by one order of magnitude) than the tolerance specified for the un-irradiated fuel assemblies.

In the fuel to be loaded into the S/INF management system of interest there are usually pellets from a lot of different UF$_6$ charges. The frequency of occurrence distribution of initial enrichment in the fuel to be loaded in the S/INF system therefore consists of a lot of narrow peaks of different heights distributed within the initial enrichment tolerance interval specified for the fuel assemblies by the fuel vendor. The positions of these peaks within this tolerance interval and the respective heights of these peaks vary from fuel assembly to fuel assembly. Therefore, the frequency of occurrence distribution of initial enrichments within a fuel assembly usually remains unknown to the criticality safety analyst as well as to an applicant who checks the S/INF from the fuel vendor. The upper limit of the relevant initial enrichment tolerance interval has to be taken as the initial enrichment of the S/INF to be checked.

In order to help to prevent misloading events it is recommended to deliver a loading curve to an applicant, which is already shifted by the upper tolerance value $\Delta e$ of the initial $^{235}\text{U}$ enrichment to the left-hand side, as indicated in Figure 1.1. This is recommended since applicants are used to dealing with nominal initial enrichments.

8. The upper enrichment tolerance specified for today’s PWR fuel assembly designs is in the range of 0.01 wt.-% $^{235}\text{U}$ to 0.05 wt.-% $^{235}\text{U}$, whereas the enrichment tolerance of UF$_6$ charges is usually not greater than 0.0025 wt.-% $^{235}\text{U}$.
With respect to the tolerances in the fuel rod outer diameter, fuel rod pitch and guide tube inner and outer diameter, the following has to be observed:

- A smaller moderator volume within a fuel assembly lattice results in counteracting effects: While less moderation causes hardening of the neutron spectrum, a lower amount of soluble boron within the fuel assembly’s lattice results in a decrease of the neutron spectrum hardness.

- A higher moderator volume reverses these two effects, so that they remain counteracting: More moderation results in a decrease of the neutron spectrum hardness, but a higher amount of soluble boron in the fuel assembly’s lattice leads to spectrum hardening.

Because the spectrum hardness increases with increasing burn-up (see Section 1.3.4), it cannot be excluded that the effects of the tolerances in fuel rod outer diameter, fuel rod pitch and guide thimble diameters on the reactivity of the S/INF at the end of irradiation and after that depend on the burn-up of the fuel. It is therefore recommended to perform depletion calculations for the minimum possible moderator volume, nominal moderator volume as well as maximum possible moderator volume in the lattice of the fuel assembly of interest. Even though the differences of the S/INF’s reactivity values corresponding to these three cases are usually small, it is important to notice that the gradient of the decrease of the fuel’s reactivity with increasing burn-up is impacted by the moderator volume and depends on the burn-up.

1.2.2 Parameters for the depletion analysis

The parameters for depletion analysis are discussed in the following sections with particular attention being given to the sensitivity of the neutron multiplication factor of the S/INF management system of interest to variations in the depletion parameters. These variations are usually related to neutron spectrum hardening. Spectrum hardening results in an increased build-up rate of plutonium due to the increased neutron capture in $^{238}$U. The increased plutonium production concurrently leads to a decrease in the $^{235}$U fission rate due to an increase in the plutonium fission rate and has therefore the effect of increasing the reactivity of the fuel at shut-down and after that.

1.2.2.1 Specific power and operating history

The production rate of each fission product is related to the specific power via the fission rate. The higher the specific power, the higher the production rate, and therefore the higher the equilibrium level of unstable nuclides where the decay rate approaches the production rate [30]. It was in fact observed [33] that reactivity calculations with actinides plus fission products show a slight downward trend in the neutron multiplication factor with increasing specific power level, whereas calculations on the actinide-only level show the opposite trend. And both trends increase with increasing burn-up due to spectrum hardening.

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9. This approach makes it possible to use an isotopic composition which results, at given initial enrichment and given burn-up, in the highest reactivity of the S/INF. This approach therefore covers the reactivity effects due to the varying of the outer diameter of the fuel rod during depletion.

10. In full Monte Carlo uncertainty analysis approaches like CONCERT [48] the variations in fuel rod outer diameter, fuel rod pitch and guide thimble diameters due to the tolerances in these parameters can be taken into account by Monte Carlo sampling on these parameters.

11. The differences in the neutron multiplication factors are usually not greater than $\Delta k \leq 0.005$. However, depending on the S/INF management system of interest, a difference of $\Delta k = 0.005$ can result in a burn-up difference of about 1 MWd/kg U in the loading curve.
An operating history is simply a time varying specific power profile. To understand the effect of different operating histories on the reactivity of spent fuel, model histories in the form of specific power histograms were developed to represent the key aspects of operating histories (e.g. high power operation early or late in the fuel’s life, extended downtimes early or late in the fuel’s life, short or long inter-cycle downtimes etc.), [33]. In general, low power operation near the end of cycle results in a higher reactivity worth of the fuel due to the decreased production rate of the fission products. And the opposite is true again when only actinides are considered for burn-up credit.

However, all the reactivity effects studied in [33], those which are related to the downtimes as well as those which are related to low power operations or higher power operations at the end of cycle, were found to be really very small: On the actinide plus fission product scale the relative change in the neutron multiplication factor $k$ observed in [33] is not greater than 0.2%. Therefore, the conclusions are:

- Downtimes can be ignored in depletion calculations. This is conservative in case of the actinides – only BUC approaches. In case of actinides-plus-fission-products BUC approaches the impact on $k$ is insignificant (i.e. negligible) for typical downtimes; and for extended downtimes in the late life ignoring of the downtimes is conservative.
- Usually full power can be assumed in the depletion analysis. Whether or not extended low/high power operation should be included, that should be decided on the basis of the specific case of interest and the burn-up credit level that will be chosen.

It should, however, be noted that in cases of extended low power operations, at the end of a cycle for instance, control rods of at least one control rod bank are inserted into the fuel assemblies with a significant insertion depth. Insertion of control rods results in a significant increase of the S/INF’s reactivity, as will be told in Section 1.2.2.5.

1.2.2.2 Fuel temperature

Resonance neutron absorption in $^{238}$U is increased at higher fuel temperatures due to Doppler broadening. This leads to spectral hardening and hence to a higher reactivity worth of the S/INF. This effect increases with increasing burn-up due to the fact that increasing burn-up results in spectral hardening too. Therefore, bounding of the fuel temperature reactivity effect in the depletion analysis is recommended. An example for working out a bounding fuel temperature is given in [49].

1.2.2.3 Moderator temperature and related density

In an operating PWR, as the moderator temperature increases, the moderator density decreases. This leads to reduced moderation and hence spectral hardening. The effect on the neutron multiplication factor of a S/INF management system of interest is significant [33,50], a bounding moderator temperature value must be used, therefore.

An example for determining a bounding moderator temperature is given in [49]. The following conclusions can be drawn from this example [50]:

- Since the moderator temperature is increasing from the bottom end of the fuel zone to the top end of the fuel zone a bounding value for the moderator temperature is given by the moderator temperature in the top end zone of the fuel.
- The moderator temperature in the top end zone has to be analysed for each fuel assembly of interest. In other words, a hot-channel analysis has to be performed,
because the hot-channel temperature in the top end zone of the fuel may be higher than the mean outlet temperature which is often assumed to be bounding.

1.2.2.4 Presence of soluble boron

Neutron absorption by boron diluted in the PWR reactor coolant results in spectral hardening. Studies performed to assess the effect of soluble boron concentration used during depletion show a clear increase in reactivity with increased boron concentration [33,50,51]. Due to the fact that in a real operating PWR the boron concentration decreases during the cycle due to the increasing core burn-up, it has been found that use of the cycle-averaged boron concentration in the depletion analysis results in a reactivity worth of the S/INF at the end of irradiation and after that, which is bounding, if not conservative [50,51].

As shown in [49], it can be checked by analysing the reactivity change of the PWR core as a function of the fuel’s burn-up for different cycle-averaged boron concentrations whether the boron concentration value assumed to be the bounding value is really bounding with respect to the S/INF’s reactivity.

1.2.2.5 Use of fixed neutron absorbers

Fixed poison rods are commonly used for reactivity control as well as enhanced fuel utilisation. The effect of such poison rods is similar to that of soluble boron, but is more localised and impacts, therefore, the axial and horizontal distribution of the burn-up within the fuel assemblies. The effect on reactivity is significant [30], in particular when the rods are inserted for a long time.

Burnable poison rods and axial power shaping rods are depleted usually in one cycle, mostly in the first irradiation cycle of the lifetime of the fuel assemblies in which these rods are inserted. Therefore, the effect of these rods on the S/INF reactivity is dependent on the fuel exposure prior to depletion of these rods, the subsequent burn-up, and the possibly remaining poison loading within the rods. In any case, the effect on reactivity is significant, even after removal of these rods [30].

Whereas burnable poison rods and axial shaping rods are mostly depleted in the first irradiation cycle of the life of the fuel assemblies being involved, Control Rods (CR) may be used in all life cycles of the assemblies. The NEA EGBUC therefore decided to conduct a theoretical benchmark on the effect of CR insertion during irradiation of fuel assemblies on the S/INF composition and on the resultant reactivity of the S/INF [13]. In this benchmark the total irradiation time has been divided into three cycles each of which have a length equivalent to a burn-up of 15 MWd/kg U. It has been assumed that there are no downtimes between the cycles (see Section 1.2.2.1). Different periods of CR insertion have been studied: CR insertion in the first cycle only, in the first two cycles, in all cycles, as well as CR insertion in the second cycle only and in the third cycle only. To study the plain effects on the isotopic composition and the reactivity of the S/INF it has always been assumed that the entire fuel zones of the fuel assemblies are exposed to CR insertion (“full CR insertion”). Figure 1.2 shows an example for the results obtained for the benchmark. This example confirms that, due to spectrum hardening, CR insertion during depletion results in a significant increase of the S/INF reactivity. In addition, as appears from Figure 1.2, the reactivity increase due to CR insertion increases with increasing burn-up. This is due to the fact that an increase in burn-up results in an increase of the spectrum hardening, so that the relative increase in the number densities of $^{235}$U and $^{239}$Pu increases exponentially with increasing burn-up, (see Figure 1.3).

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12. Slightly higher, as it was the case in [49].
Figure 1.2. Example for the increase $\Delta k$ in the neutron multiplication factor due to the use of fixed neutron absorbers: Pin-cell calculation results for the impact of CR insertion on the S/INF reactivity

Calculations were performed by means of CASMO-4 [52] with 70-group cross-section library based on JEF 2.2 (depletion) [53] and SCALE/KEO V.a with 44GROUPNDF5 cross-section library (reactivity) [54]. The irradiation time is divided into three periods (cycles) each of which have a length equivalent to a burn-up of 15 MWd/kg U.

Usually, control rods cannot be fully inserted into the active zones of the fuel assemblies during a whole cycle. In most of the countries it is common practice in core operation that at least one CR bank is in a “target bite position”, i.e. at the beginning of cycle the control rods of this CR bank are inserted into the fuel zone of the fuel assemblies at the respective core positions with an insertion depth of usually not more than about 30 cm; and the insertion depth is then gradually reduced during the cycle and tends towards zero at the end of cycle. However, the situation is different for extended low power operation at the end of cycle. Then the control rods of at least one CR bank are inserted with a considerable insertion depth.

In BUC CSA practice it is very often conservatively supposed that, due to the lack of information about CR insertion histories, control rods are inserted during the entire irradiation time and that the insertion depth amounts to 80 cm at least. As follows from Figure 1.2, this assumption leads to an overly conservative estimate of the S/INF’s reactivity. Taking into consideration that, as a rule of thumb, a change of $\Delta k = 0.01$ in the neutron multiplication factor of a S/INF management system of interest may result in a change of about 2 MWd/kg U of the minimum burn-up required for S/INF to be loaded in this system, it is worthwhile to study CR insertion histories used in the plant for which the depletion analysis has been made. An example for determining a bounding CR insertion history is given in [49].

Furthermore, it has to be taken into account that different control rod insertion depths result in different effects on axial burn-up profiles and different effects due to axial burn-up profiles. Therefore, CR insertion during depletion also has to be treated together with the evaluation of reactivity effects due to axial burn-up profiles. It is discussed in Section 1.3.6.3.2.
Figure 1.3. Example for the relative change $\Delta N/N$ of isotopic number densities $N$ due to CR insertion during all three cycles specified in [13] (see Figure 1.2)

Relative change of isotopic number densities due to CR insertion (Zero cooling time)

Note that the relative increase in the number densities of $^{235}$U and $^{239}$Pu increases exponentially with increasing burn-up. Number densities were calculated by means of CASMO-4 [52] with 70-group cross-section library based on JEF 2.2 [53].

1.2.2.6 Initial presence of integral burnable absorber in the fuel

Integral burnable absorbers initially present in the fuel are also used for reactivity control and improved fuel utilisation. These absorbers are depleted in the first irradiation cycle of the life of the fuel assemblies. The reactivity of the fuel assemblies may therefore increase with increasing burn-up to a maximum and decrease after that. The effect of burnable absorber fuel rods on the spent fuel reactivity depends on their initial poison loading, their positions in the fuel assembly, on the distribution of the poison within the pellets (pellets coated with poison or poison homogeneously mixed with the fuel), the burn-up, and the possibly remaining poison loading within the rods [30].

The presence of integral burnable poisons results in spectrum hardening. However, spectral hardening not only leads to an increase of plutonium build-up and a delay to $^{235}$U depletion but also results in a delay to the burn-out of the integral burnable absorber, and this delay tends towards a decrease in the reactivity.

Due to remaining poison loadings after burn-out of the neutron absorbers [30] the use of gadolinium (Gd) or erbium (Er) usually does not result in any reactivity increase of the S/INF reactivity; on the contrary, usually a slight decrease of the S/INF reactivity is observed [30]. The use of IFBA rods may, however, result in a slight increase of the S/INF reactivity after burn-out of the absorber [30,37].

Integral burnable absorbers are usually used in the centre region of the active zone of the fuel assemblies only, i.e. the bottom and top end of the fuel zone do not contain any integral burnable absorbers. The axial length of these un-poisoned zones depends on the fuel assembly type: lengths ranging from about 15 cm up to about 40 cm are in use. If Gd or Er is used in the
poisoned zone then the initial $^{235}\text{U}$ enrichment is often (in older fuel designs in particular), due to technical reasons, lower than in the un-poisoned zones. But there are also fuel designs containing axial blanket $\text{UO}_2$ pellets with low-enriched or natural uranium at the top and bottom end of the un-poisoned end zones. This is often the case when IFBA rods are used.

All these different combinations of integral burnable absorbers and higher or lower enrichments in the un-poisoned end zones result in different effects on axial burn-up profiles and different reactivity effects due to axial burn-up profiles. Therefore, all these different fuel design characteristics have to be discussed together with the evaluation of reactivity effects due to axial burn-up profiles and discussed in Section 1.3.3.1.

1.2.2.7 Presence of MOX fuel in the core

Presence of MOX fuel assemblies in the core results in spectral hardening. The presence of these assemblies therefore needs to be considered in the depletion analysis. The degree of spectral hardening depends on the plutonium content and quality of the MOX fuel. MOX fuel assemblies have heterogeneous Pu content distributions, which may be taken into account in the depletion analysis.

1.2.2.8 Remarks about the selection of bounding depletion parameters

Apart from the case of using integral burnable absorbers, which results in a more complex reactivity behaviour, it seems to be clear that a bounding or rather conservative irradiation history can be generated by choosing the depletion parameters in such a way that neutron spectrum hardening is maximised. And, in fact, tendencies to proceed in this way are observed in practice: It has been already observed that the highest fuel temperature and the highest moderator temperature and hence the lowest moderator density are combined with the highest (or at least a very conservatively estimated) soluble boron concentration of the moderator and the assumption that control rods are completely inserted in the fuel assemblies during all the operation cycles. Furthermore, it is assumed that each of the $\text{UO}_2$ fuel assemblies, for which burn-up credit is intended to be taken, is completely surrounded by MOX fuel assemblies inside the core during all the operation cycles. Maximising spectrum hardening in such a way is however not credible. First of all, the combination of the highest fuel and moderator temperature with the highest (or a very high) soluble boron concentration and the case of fully inserted control rods is contradictory to physics. To obtain a bounding irradiation history it is not necessary to choose depletion parameter combinations which are contradictory to physics. It makes sense:

- first, to spend an adequate amount of effort on the study of the specific reactor operation strategies used in the nuclear power plant of interest and
- then, to resolve by means of sensitivity studies a depletion parameter combination suitable for the plant of interest [49].

It should be kept in mind that the chosen depletion parameter combination has a significant impact on the economic benefit of burn-up credit. For instance, as follows from Figure 1.2, the assumption that control rods are fully inserted during all the operation cycles leads to a significant decrease in the economic benefit of burn-up credit, since the significant reactivity increase due to CR usage makes it necessary to use more neutron absorbing material and/or greater distances between the fuel positions inside the S/INF system of interest. Both increase in the required amount of neutron absorbing material and decrease in the number of

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13. For the distinction of the terms “bounding” and “conservative” [26,30,55].
fuel cells per unit volume of the S/INF system result in a significant increase in the costs of manufacturing and operating the S/INF system.

1.2.3 Cooling time

Immediately after reactor shut-down, $^{135}$Xe builds up thereby reducing the reactivity of the spent fuel, but due to the rapid decay of $^{135}$I and $^{135}$Xe the reactivity of spent fuel will increase within the first four days after shut-down. At the same time, there is an accumulation of $^{239}$Pu due to the decay of $^{239}$Np. The maximum $^{239}$Pu inventory is at about 20 days after shut-down (half-life of $^{239}$Np is about 2.5 days). Four days after shut-down, the production of strongly absorbing nuclei like $^{149}$Sm through $\beta$-decay of $^{149}$Pm leads to a slight decrease in reactivity. After about 100 days, the production of $^{155}$Gd through $\beta$-decay of $^{155}$Eu and that of $^{241}$Am through $\beta$-decay of $^{241}$Pu become predominant and cause a stronger reactivity decrease for time periods covering all spent fuel management systems with the exception of disposal and, possibly, interim storage facilities for which lifetimes of some hundred years are recently discussed.

For periods of times greater than approximately 100 years, it has to be taken into account that the half-life of $^{238}$Pu and $^{240}$Pu as well as of $^{241}$Am are significantly shorter than the half-life of $^{239}$Pu, and that $^{239}$Pu decays via $\alpha$-decay to $^{235}$U. Thus the reactivity increases after a time of about 100 years until a peak is reached around 30 000 years. The minimum reactivity at about 100 years after shut-down depends on the burn-up and the initial enrichment of the fuel because the $^{238}$U capture rate decreases with increasing enrichment.

Due to the production and decay processes after irradiation, not only the neutron multiplication factor of a spent fuel management system changes with cooling time, but also its bias arising from the uncertainties in the depletion calculations [56]. This must be considered when credit for cooling time is taken.

1.2.4 Depletion calculation benchmarks

Comparisons of the ability of various depletion calculation code systems and nuclear data libraries to predict S/INF isotopic concentrations have been provided by the NEA EGBUC Benchmarks Phase I-B [9] and Phase II-D [13].

1.2.4.1 The Phase I-B benchmark for depletion in a simple pin-cell model

The purpose of the Phase I-B benchmark was to study the compatibility of S/INF isotopic concentrations calculated by means of different depletion calculation codes and nuclear data libraries used by various organisations, institutes and companies which participated in the benchmark [9]. For this purpose, a simple pin-cell model was derived from a Combustion Engineering 14x14 fuel assembly design by using the fuel actual pin dimensions but increasing the pin pitch to maintain the fuel-to-moderator ratio of the actual fuel assembly design. The depletion calculations were performed for given operating history data with three different specific power histories resulting in final burn-ups of 27.35 MWd/kg U ("case A"), 37.12 MWd/kg U ("case B"), and 44.34 MWd/kg U ("case C"). A cooling time of 1870 days was present. Figures 1.4 through 1.6 show the standard deviation of the calculated isotopic concentrations delivered by the participants of the benchmark relative to the respective
averages of these concentrations\textsuperscript{14}. As appears from these figures sizeable deviations from the average values were observed.

**Figure 1.4. Standard deviations of the isotopic concentrations calculated by the Phase I-B participants relative to the averages of these concentrations** [9]

In BUC CSA application cases the uncertainty in reactivity related to the uncertainties in the calculated S/INF isotopic concentrations becomes of interest. Therefore, comparisons of calculated reactivity values, obtained by using the average concentration values, with calculated reactivity values, resulting from using isotopic concentrations estimated by means of CASMO-3 [57], are given in Appendix A of [9]. The difference in the calculated reactivity values ranges from about 0.8\% in case A to about 3.2\% in case C [9], Table A.1). The significant contributions to these reactivity differences are resulting from the differences in the isotopic concentrations calculated for the isotopes $^{235}$U, $^{239}$Pu, $^{241}$Pu, $^{241}$Am, $^{103}$Rh, $^{149}$Sm, $^{151}$Sm and $^{155}$Gd (see Tables A.2 through A.4 of Ref. [9]).

A more general view than obtained by comparing the results of one depletion code and one nuclear data library with the average values of isotopic concentrations obtained by various codes and libraries is gained by estimating the reactivity uncertainties related to the standard deviations presented in Figures 1.4 through 1.6. Estimates of the changes in reactivity due to these standard deviations are in fact given in Appendix A of [9]. These changes amount to 2.8\% in case A (related to a $k_{\text{eff}}$ mean value of 1.017), 4.3\% in case B ($k_{\text{eff}}$ mean = 0.918), and 5.5\% in case C ($k_{\text{eff}}$ mean = 0.855). The significant contributions to these changes are related, as was to be expected, to the isotopes $^{235}$U, $^{239}$Pu, $^{240}$Pu, $^{241}$Pu, $^{149}$Sm, $^{151}$Sm, and $^{155}$Gd (see Table A.6 in [9]).

For the uranium and plutonium isotopes as well as for $^{237}$Np and some fission products measured isotopic concentrations were available for the Phase I-B benchmark. In Figures 1.7 through 2.9, comparisons of the measured concentration values to the average concentration values are presented.

\textsuperscript{14}. Note that not all of the participants were able to deliver results for all the BUC fission products specified in Figure 1.6 [9].
Figure 1.5. Standard deviations of the isotopic concentrations calculated by the Phase I-B participants relative to the averages of these concentrations [9].

Figure 1.6. Standard deviations of the isotopic concentrations calculated by the Phase I-B participants relative to the averages of these concentrations [9].

15. The grouping of the actinides in “major actinides” (see Figure 1.4) and “minor actinides” is based on the reactivity worth values of these isotopes in S/INF, [8].
Figure 1.7. Comparisons of measured isotopic concentration (M) to the average values of the calculated concentrations (C): $(M/C-1)$ [9]

![Figure 1.7](image)

Figure 1.8. Comparisons of measured isotopic concentration (M) to the average values of the calculated concentrations (C): $(M/C-1)$ [9]

![Figure 1.8](image)
However, these comparisons may be misleading for the following reasons:

- The measured concentrations are related to the actual configuration of the fuel sample pin during reactor operation. This actual configuration is, of course, different from the simple pin-cell model assumed for the Phase I-B depletion model.

- The uncertainties (variances and covariances) of the measured concentrations are not specified in [9]. It is impossible, therefore, to check whether the average concentrations are compatible with the measurement results or not.

In addition, the standard deviations of the calculated isotopic concentrations portend biases and uncertainties in the nuclear data and biases caused by algorithmic weaknesses in the calculation procedures. To estimate the biases of the calculated isotopic concentrations in a consistent way it is necessary to consider the uncertainties (variances and covariances) in the nuclear data, the uncertainties (variances and covariances) in the measured concentrations, and to estimate the resulting covariance matrix of the isotopic concentration biases [48].

1.2.4.2 The Phase II-D benchmark for depletion in a 17x17-24-1 fuel assembly geometry taking account of different control rod insertion histories

In contrast to the Phase I-B benchmark, the Phase II-D benchmark addressed depletion in a two-dimensional configuration given by a 17x17-24-1 fuel assembly geometry, which is representative of real 17x17-24-1 fuel assembly designs, (see [13] in Appendix A).

16. Due to the measurement methods applied in radiochemical analysis [58] the measurement results are correlated [48,59].

17. The notation “17x17-24-1” is usually used to identify a fuel assembly design with 264 fuel pins, 24 guide thimbles and one instrumentation tube, arranged in a 17x17 square lattice. (The instrumentation tube is placed in the centre of the fuel assembly.)
purpose of the Phase II-D benchmark was to study the effect of Control Rod (CR) insertion modelling on calculated isotopic concentrations and related reactivity values of S/INF configurations. The benchmark therefore included two main parts:

- The depletion calculations for the above-mentioned representative 17x17-24-1 fuel assembly geometry: All the data and information required to perform these calculations were present in the benchmark specification given in Appendix A of [13], which are the following:
  - the geometry data;
  - the material data (the initial fuel composition, cladding material, guide thimble and instrumentation tube materials, absorber material and cladding material of the CRs);
  - the depletion parameters (fuel temperature, cladding temperature, moderator temperature and density, boron concentration of the moderator, specific power);
  - the irradiation histories: as appears from Table 1.1, twelve cases were considered including irradiation histories without any CR insertion and histories with CR insertion during different irradiation times combined with two different total irradiation times, as well as;
  - the cooling time (see Table 1.1).
- Calculation of the neutron multiplication factor for an infinite array of the irradiated fuel assemblies of the above-mentioned type: As indicated in Table 1.2, the results of each depletion case (see Table 1.1) were two times applied to the reactivity calculations: For one thing the actinides are only used, and for another thing the actinide-plus-fission-product BUC methodology is applied. In addition, reactivity calculations were also performed for present isotopic composition sets (cases 13b and 14b) and for the un-irradiated fuel (case 15).

Table 1.1 Phase II-D irradiation histories

<table>
<thead>
<tr>
<th>Cooling time (End of irradiation)</th>
<th>CRs</th>
<th>Period of CR insertion</th>
<th>Fuel inventory burnup</th>
<th>Case number</th>
</tr>
</thead>
<tbody>
<tr>
<td>0 day</td>
<td>Yes</td>
<td>0-30 GD/1U</td>
<td>45 GD/1U</td>
<td>2</td>
</tr>
<tr>
<td>0 day</td>
<td>No</td>
<td>-</td>
<td>45 GD/1U</td>
<td>3</td>
</tr>
<tr>
<td>5 years</td>
<td>No</td>
<td>-</td>
<td>45 GD/1U</td>
<td>8</td>
</tr>
<tr>
<td>5 years</td>
<td>Yes</td>
<td>0-30 GD/1U</td>
<td>45 GD/1U</td>
<td>9</td>
</tr>
<tr>
<td>5 years</td>
<td>yes</td>
<td>0-45 GD/1U</td>
<td>45 GD/1U</td>
<td>10</td>
</tr>
<tr>
<td>5 years</td>
<td>no</td>
<td>-</td>
<td>45 GD/1U</td>
<td>11</td>
</tr>
<tr>
<td>5 years</td>
<td>yes</td>
<td>0-45 GD/1U</td>
<td>45 GD/1U</td>
<td>12</td>
</tr>
</tbody>
</table>

Note: table copied from [13] in Appendix A.

Figures 1.10 and 1.11 show the standard deviation of the calculated isotopic concentrations, delivered by the participants of the Phase II-D benchmark, relative to the averages of these concentrations. With a few exceptions ($^{163}$Rh and $^{155}$Gd in particular), the standard deviations are smaller than those observed in the Phase I-B benchmark (see Figures 1.4 through 1.6). The Phase I-B calculations were performed during 1993 and 1994, whereas
the Phase II-D calculations were performed about 10 years later. Thus, improvements in nuclear data evaluations and code algorithms introduced in the time period between Phase I-B and Phase II-D might have result in a higher degree of uniformity of the calculation routes and hence, with a few exceptions, in a lower degree of variation of the results from different calculation routes. This is also reflected in the variations of the reactivity calculation results: As shown in Figure 1.12, the relative deviations of the neutron multiplication factors $k_{\infty}$, calculated for the benchmark exercises 1a through 12b, from the respective averages of these $k_{\infty}$ values fall, with a few exceptions, in a band ranging from about -1 % to about +1 %. However, most of the results of the “participant” named 18P_18 lead to deviation values outside this band, but this can be attributed to the fact that this “participant” used a one-dimensional depletion calculation code whereas all the other participants applied two-dimensional depletion calculation procedures. Application of a two-dimensional depletion code to a two-dimensional geometry is preferable to the use of a one-dimensional or a point-depletion code.

Comparison of the deviations observed for the reactivity calculation cases 1a through 12b to the deviations obtained for the cases 13b and 14b using prescribed SNF isotopic number densities show that the deviation band of about (-0.5%, +5%), which seems to be characteristic of reactivity calculations with a single (unitary) SNF isotopic concentration set, is increased to about (-1%, +1%) by using SNF isotopic concentration sets resulting from different depletion calculation procedures appropriate for the depletion task.

Figure 1.10. Standard deviations of the isotopic concentrations, calculated by the Phase II-D participants, relative to the averages of these concentrations [13]

---

18. “Participant” does not stand for an organisation here, but for a calculation procedure [13].
Figure 1.11. Standard deviations of the isotopic concentrations, calculated by the Phase II-D participants, relative to the averages of these concentrations [13]

Figure 1.12. Relative deviations of the calculated neutron multiplication factors $k_{inf}$ delivered by the Phase II-D participants, from the respective averages of these $k_{inf}$ values [13]
Table 1.2. Phase II-D reactivity calculation cases (AO:= Actinide-only BUC, ApFP:= Actinide-plus-Fission-Product BUC) [13]

<table>
<thead>
<tr>
<th>Reactivity Calculation No.</th>
<th>Depletion Case No.</th>
<th>BUC methodology</th>
</tr>
</thead>
<tbody>
<tr>
<td>1a</td>
<td>1</td>
<td>AO</td>
</tr>
<tr>
<td>1b</td>
<td></td>
<td>ApFP</td>
</tr>
<tr>
<td>2a</td>
<td>2</td>
<td>AO</td>
</tr>
<tr>
<td>2b</td>
<td></td>
<td>ApFP</td>
</tr>
<tr>
<td>3a</td>
<td>3</td>
<td>AO</td>
</tr>
<tr>
<td>3b</td>
<td></td>
<td>ApFP</td>
</tr>
<tr>
<td>4a</td>
<td>4</td>
<td>AO</td>
</tr>
<tr>
<td>4b</td>
<td></td>
<td>ApFP</td>
</tr>
<tr>
<td>5b</td>
<td>5</td>
<td>ApFP</td>
</tr>
<tr>
<td>6b</td>
<td>6</td>
<td>ApFP</td>
</tr>
<tr>
<td>7b</td>
<td>7</td>
<td>ApFP</td>
</tr>
<tr>
<td>8b</td>
<td>8</td>
<td>ApFP</td>
</tr>
<tr>
<td>9a</td>
<td>9</td>
<td>AO</td>
</tr>
<tr>
<td>9b</td>
<td></td>
<td>ApFP</td>
</tr>
<tr>
<td>10a</td>
<td>10</td>
<td>AO</td>
</tr>
<tr>
<td>10b</td>
<td></td>
<td>ApFP</td>
</tr>
<tr>
<td>11a</td>
<td>11</td>
<td>AO</td>
</tr>
<tr>
<td>11b</td>
<td></td>
<td>ApFP</td>
</tr>
<tr>
<td>12a</td>
<td>12</td>
<td>AO</td>
</tr>
<tr>
<td>12b</td>
<td></td>
<td>ApFP</td>
</tr>
<tr>
<td>13b</td>
<td></td>
<td></td>
</tr>
<tr>
<td>given isotopic composition: fuel depleted without CR insertion (see [13], Appendix A, Table 1)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>14b</td>
<td></td>
<td></td>
</tr>
<tr>
<td>given isotopic composition: fuel depleted with CR insertion (see [13], Appendix A, Table 1)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>15</td>
<td></td>
<td></td>
</tr>
<tr>
<td>fresh (un-irradiated) fuel (see [13], Appendix A, Section 1.2.2)</td>
<td>----</td>
<td></td>
</tr>
</tbody>
</table>

As shown in Figure 1.12, comparison of case 15 to cases 13b and 14b indicates a slight increase in the variation of the $k_{inf}$ results when changing from un-irradiated to irradiated fuel.

For the benchmark exercises 13b, 14b and 15 it is observed that the relative deviations of the $k_{inf}$ results delivered by participant 10P are not greater than the relative deviations of the results from all the other participants (see Figure 1.12). This observation confirms that a two-dimensional (at least two-dimensional) depletion code should be applied to depletion analysis of real fuel designs and reactor operation conditions bounding, with respect to the S/INF’s reactivity, the real operation conditions of the nuclear power plant of interest. Real operation conditions always include partial CR insertion in several fuel assemblies during their lifetime (see Section 1.2.2.5 and Section 1.3.6.3.2).
The increase in reactivity of S/INF due to CR insertion during irradiation has been already discussed in Section 1.2.2.5. Even if different in diagram type, Figure 1.13 is similar to Figure 1.2, but the $\Delta k$ values presented in Figure 1.13 are now derived from the average $k_{inf}$ values presented in Table 4.1 of [13]; accordingly, the error bars shown in Figure 1.13 are given by the standard deviations of the $\Delta k$ values resulting from the standard deviations of the $k_{inf}$ values. As stated in Section 1.2.2.5, the increase in reactivity due to CR insertion increases with increasing burn-up. This is due to the fact that an increase in burn-up results in an increase in spectrum hardness because of the build-up of the Pu-isotopes $^{239}\text{Pu}$, $^{240}\text{Pu}$, and $^{241}\text{Pu}$. Therefore, the harder the spectrum, the higher the increase in the S/INF’s reactivity due to CR insertion; and CR insertion enhances the spectrum hardness and hence the $^{238}\text{U}$ conversion rate.

**Figure 1.13. Phase II-D: Increase $\Delta k$ in the S/INF’s neutron multiplication factor due to CR insertion ($\Delta k$ values and their standard deviations [13] reactivity calculation cases 3b, 4b, 5b, 6b, 7b, 8b)**

As shown in Figures 1.14 and 1.15, the virtually only significant changes of the isotopic number densities due to CR insertion during irradiation are observed for the non-fissile isotope $^{238}\text{U}$ and the fissile isotopes $^{239}\text{Pu}$ and $^{235}\text{U}$ (decrease of the $^{238}\text{U}$ number density and net increase of the $^{239}\text{Pu}$ number density due to the enhanced conversion of $^{238}\text{U}$ to $^{239}\text{Pu}$, and increase of the $^{235}\text{U}$ number density due to the increase of the $^{239}\text{Pu}$ fission rate at fixed power level).
It follows, therefore, that a change in the BUC methodology from the actinide-plus-fission-product BUC procedure to the actinide-only method does not result in a really significant change of the S/INF’s reactivity increase caused by CR insertion. And, likewise, because of the half-lives of $^{235}\text{U}$, $^{238}\text{U}$ and $^{239}\text{Pu}$, a change of the cooling time from zero to five years$^{19}$ cannot result in a really significant change of the S/INF’s reactivity increase resulting from CR insertion during depletion. As appears from Figure 1.16, both conclusions are confirmed by the Phase II-D reactivity calculation results$^{20}$.

Since CR insertion impacts axial burn-up profiles of irradiated fuel assemblies the impact of CR insertion on the S/INF’s reactivity will be continued in Section 1.3.6.3.2.

Figure 1.14. Phase II-D: Absolute change $\Delta N$ of isotopic number densities $N$ due to CR insertion during irradiation

The related relative changes $\Delta N/N$ have been presented in Figure 1.3. Number densities were calculated by means of CASMO-4 [52] with 70-group cross-section library based on JEF 2.2 [53].

---

19. Zero cooling time (but assuming complete decay of $^{239}\text{U}$ and $^{239}\text{Np}$ to $^{239}\text{Pu}$) is usually used in BUC CSA of SNF wet storage pools, 5 years cooling time is often used in BUC CSA of storage or transport casks.
20. Of course, the $k_{eff}$ values are changing significantly (see Table 4.1 in [13]), but the related differences $\Delta k$, presented in Figure 1.13, remain virtually unchanged.
Figure 1.15. Phase II-D: Change of isotopic number densities $N$ due to CR insertion: Comparison of the number densities calculated for the case of no CR insertion to the number densities obtained for CR insertion during the whole irradiation time. Number densities were calculated by means of CASMO-4 [52] with 70-group cross-section library based on JEF 2.2 [53].

Figure 1.16. Phase II-D: Increase $\Delta k$ in the S/INF’s neutron multiplication factor due to CR insertion: Comparison of $\Delta k$ values obtained by using different BUC procedures and different cooling times ($\Delta k$ values and related standard [13] reactivity calculation cases 1a, 2a, 3a, 4a, 9a, 10a, 11a, 12a, and 1b, 2b, 3b, 4b, 9b, 10b, 11b, 12b)
1.3 Burn-up credit criticality safety analysis

The main steps of a CSA of a S/INF management system designed for BUC, which have been already listed in Section 1.1, will be discussed in the following sections with particular attention focused on:

- some aspects that have to be considered in the evaluation of uncertainties which are inherent in BUC CSA;
- effects which may impact the reactivity worth of the S/INF under the conditions of the S/INF management system of interest.

The objective here is to recommend how bounding BUC CSA approaches can be achieved and how overly conservative approaches can be avoided. A bounding approach is a calculation model which is justified by physics arguments demonstrating that the use of this model does not result in an underestimation of the neutron multiplication factor of the fuel management system of interest [26,30,55].

1.3.1 Isotopic selection and validation

1.3.1.1 Isotopic selection

A bounding use of BUC:

- requires consideration of all fissile isotopes;
- allows consideration of any neutron absorbing isotope the use of which can be validated.

The neutron absorbing isotopes to be used in a criticality calculation should be selected on the basis of:

- their reactivity worth;
- their nuclear stability;
- their chemical stability.

As was shown in several studies [30,33,60], the change in reactivity due to burn-up and cooling time can be adequately represented by a relatively small set of isotopes meeting the requirements of nuclear and chemical stability.

The requirement of nuclear stability means that the half-life of a radioactive isotope has to be sufficiently large so that the calculated concentration of this isotope can be validated. Any increase in the reactivity of the S/INF of interest due to the decay of radioactive isotopes has to be taken into account in the CSA.

The requirement of chemical stability means that neutron absorbing isotopes of elements or compounds of these elements as they are present in the S/INF will not be considered in the CSA if these elements or compounds are volatile under any condition (normal, abnormal or accidental condition) to be analysed.

Note that the selection of neutron absorbing isotopes approved of being used in CSA can be considerably restricted by national regulations and criticality safety standards [24,26].
1.3.3.2 Isotopic validation

Isotopic validation can be achieved:

- by correcting the isotopic concentrations, calculated for the S/INF of interest (application case), by means of Isotopic Correction Factors (ICFs) derived from comparisons with chemical assay data (see Figure 1.17), or;
- by estimating the bias in the neutron multiplication factor of the S/INF facility of interest (application case) due to the bias of the concentration of the individual isotopes used (see Figure 1.18).

It has to be considered in an isotopic validation procedure that, as indicated in Figure 1.19, due to the variances and covariances of the nuclear data and due to the variances and covariances of the measured isotopic concentrations, the bias corrected isotopic concentrations (see Figure 1.17) or the isotopic biases ($\Delta k_{AC}$) (see Figure 1.18) are mutually correlated. These correlations have to be taken into account in the uncertainty analysis which is, as stipulated by any criticality safety regulation permitting BUC, part of the BUC CSA of the S/INF management system of interest (see Section 1.4).

The reactivity worth of the isotopes is affected by the depletion conditions as well as by the characteristics of the S/INF management system analysed. Depletion conditions resulting in spectrum hardening cause not only an increased build-up rate of plutonium and a decrease in the $^{235}$U fission rate due to an increase in the plutonium fission rate, but also a decrease in neutron absorption in some fission products. Therefore, bounding depletion conditions usually results in higher concentrations of some fission products (e.g. $^{149}$Sm, see Figure 1.17) than more realistic conditions. Nevertheless, the isotopic inventory obtained under the bounding depletion conditions – and this makes these conditions bounding - results in a higher spent fuel reactivity due to the increased build-up of plutonium and the decrease in the $^{235}$U fission rate due to an increase in the plutonium fission rate.

The use of neutron absorbers in a S/INF management system usually results in spectral hardening. This may lead to less neutron absorption in the neutron absorbing isotopes of the S/INF. In other words, the relative reactivity worth of the neutron absorbing fission products and (non-fissile) actinides in the S/INF may be impacted by the S/INF management system’s characteristics.
Figure 1.17. Definition and application of Isotopic Correction Factors (ICFs)

\[
\text{ICF} = \frac{M - c_0}{C - c_0}
\]

Bias-corrected isotopic concentrations of the Application Case (AC)

\[
c_{AC}^{\text{bias-corrected}} = (c_{AC}^{AC})_0 + \text{ICF} \cdot ((c_{AC}^{AC})_{\text{calculated}} - (c_{AC}^{AC})_0)
\]

(M := Measured concentration, C := Calculated concentration, B := Burn-up, c_0, (c_{AC})_0 := concentration at begin of irradiation), [26,48].

Figure 1.18. Isotopic validation by calculating isotopic $\Delta k$ values for the application case which are due to the difference between measured and calculated isotopic concentrations

\[
\Delta k_{AC} = k_{AC}(M_i, (c_{AC})_{i,\text{meas}}) - k_{AC}(C_i, (c_{AC})_{i,\text{calculated}})
\]

Correction of the neutron multiplication factor $k_{AC}$ of the application case

\[
k_{AC}^{\text{DC-bias-corrected}} = k_{AC}((c_{AC})_{i=1,...,n}) + \sum_{i=1}^{n} (\Delta k_{AC})_i
\]

(DC: = Depletion Calculation; “DC-bias-corrected” indicates that this figure shows the correction of the neutron multiplication factor $k$ for the isotopic concentration biases only), [26].
1.3.2 Criticality calculation validation

Criticality calculation validation is performed by evaluating experimental benchmarks, including:

- critical experiments [61];
- reactivity worth measurements [24] and [61-64];
- reactor critical configurations [65].

which are representative of the S/INF management system of interest (application case).

The decision whether a benchmark is representative or not is based on applying some methods of evaluating similarities between benchmark system and application case. Traditional methods are mainly based on expert judgement and consist in:

- comparison of materials (fuel compositions, neutron absorbing materials, etc.);
- comparison of dimensions and geometries (e.g. fuel storage arrangements);
- comparison of gross integral parameters (e.g. fuel-to-moderator ratio, lethargy of average neutron energy causing fission);
- comparison of neutron spectra.

Today’s methods consist in evaluating neutron-physics properties of benchmark and application case:

- estimation of the correlation of the neutron multiplication factors of the benchmark system and the application case, [65-67];
- comparison of the neutron energy dependence of isotope-specific and nuclear-reaction-specific sensitivity coefficients \( \frac{\partial k}{\partial \Sigma_i} \) of the neutron multiplication factors of the
benchmark system and the application case ($\Sigma_i$ some macroscopic cross-section of some isotope $i$), [64-65].

Today’s methods are based on the fact that the nuclear data compiled in the nuclear data evaluations used to generate libraries for CSA have variances and covariances resulting:

• not only in correlations between the neutron multiplication factors of the application case and the neutron multiplication factors of the benchmarks just indicating the representativeness of these benchmarks with respect to the application case [66,67];

• but also in mutual correlations of the neutron multiplication factors of all the benchmark systems selected for validation of the CSA of the application case [67].

In addition to the correlations due to the nuclear data uncertainties and correlations, another source of mutual correlations between benchmark neutron multiplication factors is the use of same materials (e.g. same fuel pins, same absorber plates etc. [61]) in different benchmark configurations 21. These correlations are due to the manufacturing tolerances of these materials resulting in uncertainties in the parameters that describe the isotopic compositions and the geometric dimensions of these materials [67,68].

All these correlations have to be taken into account in the uncertainty analysis, which is part, as already mentioned, of the BUC CSA of the application case (see Section 1.4).

1.3.3 Reactivity effects of axial and horizontal burn-up distributions

1.3.3.1 Axial burn-up distributions of PWR UO$_2$ fuel assemblies

The axial power distribution in a fresh fuel assembly in a PWR core is more cosine-shaped at the beginning of cycle. The fuel near the axial centre of the assembly is therefore depleted at a faster rate than at the ends. With increasing burn-up the power shape flattens out due to the higher fuel depletion and fission product poisoning near the centre. However, due to the neutron leakage at the ends of the fuel zone the burn-up drops off rapidly near the ends (see Figure 1.20).

The axial burn-up shapes and the related axial isotopic composition distributions are usually asymmetric because of the higher moderator temperature and hence lower moderator density in the upper region of the core. The asymmetry at end of cycle is:

• dependent on the average burn-up of the fuel assemblies and;

• significantly impacted by:

  – control rod insertion during the cycle;
  – use of burnable poison rods or axial power shaping rods in the cycle;
  – presence of integral burnable poisons in the fresh fuel assemblies;
  – presence of axial blankets in the fuel assemblies, as well as;
  – reload patterns determining the interactions between fresh fuel assemblies and fuel assemblies with different burn-up shapes at begin of cycle.

21. This is not only the case for benchmark series described in [61] under a specific identification number, but also for benchmark series compiled under different identification numbers. For example, the fuel pins used in the benchmark series LEU-COMP-THERM-34 were also used in the benchmark series LEU-COMP-THERM-37 and other series; and it seems that they were also used in LEU-COMP-THERM-007.
The reactivity of a Spent or Irradiated Fuel Assembly (S/IFA) is affected by the non-uniformity and the asymmetry of the axial burn-up shape and the related axial isotopic distribution of the S/IFA. The reactivity effect due to non-uniformity and asymmetry is commonly named as “axial end effect” or, briefer, “end effect” and is usually defined as the difference $\Delta k$ end effect of the neutron multiplication factor $k_{\text{eff (shape)}}$ of the S/IFA obtained with the axial burn-up shape and the neutron multiplication factor $k_{\text{eff (unif.dist.)}}$ obtained by assuming a uniform distribution of the average burn-up of the actual shape:

$$\Delta k_{\text{end effect}} = k_{\text{eff (shape)}} - k_{\text{eff (unif.dist.)}}$$

For low average burn-up values, the end effect of S/IFAs in a S/INF management system may be negative. This is due to the fact that the calculational fission density distribution (i.e. fission probability density distribution) is centred around the axial centre of the fuel zone of the S/IFA where the actual burn-up is higher than the respective average burn-up value, so that $k_{\text{eff (unif.dist.)}}$ is greater than $k_{\text{eff (shape)}}$. With increasing burn-up, however, the calculational fission density distribution is shifted, due to the increasing degree of non-uniformity (see Figure 1.20) and due to the asymmetry of the axial isotopic composition distribution, more and more towards the top region of the fuel zones of the S/IFA. The actual burn-up in that region is lower than the average burn-up (see Figure 1.20), so that the end effect $\Delta k_{\text{end effect}}$ may become positive since $k_{\text{eff (shape)}}$ may become greater than $k_{\text{eff (unif.dist.)}}$. However, whether the end effect is ever negative and, if it is, whether it actually becomes positive and, if it does, at which average burn-up value becomes positive depends on:

- the design and the active length of the fuel assemblies;
- the depletion conditions impacting the axial burn-up shapes and the asymmetry of the axial isotopic composition distributions;
- the cooling time considered in the BUC CSA of the S/IFAs of interest because the isotopic composition distribution changes with the cooling time due to the decay of the radioactive isotopes in the S/INF;
- the materials between and/or surrounding the S/IFAs in the S/INF management system of interest.

as shown in several studies on the axial end effect [10-12], [14], [16-19], [21-32], [42] and [50]. It is therefore obvious that the axial end effect has to be explicitly evaluated for the specific S/IFAs of interest under consideration of the specific irradiation histories of these S/IFAs and under consideration of the specific conditions of the S/INF system of interest.
1.3.3.2 Horizontal burn-up distributions of PWR UO₂ fuel assemblies

Radial variations in the neutron flux in an operating reactor, which are mainly due to leakage at the core periphery and to burn-up differences between neighbouring assemblies, result in a non-uniform horizontal burn-up distribution over the radial extent of the core. It has been shown [27,50] that non-uniform horizontal burn-up profiles might result in a slight increase of the neutron multiplication factor of the spent fuel management system of interest. The magnitude of this increase is affected, due to spectral effects, by the characteristics of this system and depends on the fuel assembly type (see Lecture 4.3.2 in [30]). The reactivity effect due to horizontal burn-up distribution has therefore to be evaluated for the specific S/FAs of interest under consideration of the specific irradiation histories of these S/IFAs and under consideration of the S/INF system of interest.

1.3.4 Estimation of the loading criterion

As stated in Section 1.2.1, the objective of a BUC CSA of a S/INF management system of interest is to determine the BUC loading criterion for this system. This criterion is usually presented in form of a loading curve indicating the minimum required average burn-up of the S/INF as a function of the initial ²³⁵U enrichment of the S/INF.

A loading curve of a S/INF system is usually generated by applying a reactivity equivalence condition, i.e. each point of the loading curve is defined by a fixed numerical value of the neutron multiplication factor $k_{\text{eff}}$ of the S/INF system [27]. Usually that $k_{\text{eff}}$ value is chosen which is, according to the relevant criticality safety regulations or standard, the maximum permissible one. Thus, at each point the numerical values of the initial enrichment $e$ and the average burn-up $B$ are determined such that $k_{\text{eff}}$ is constant along the whole loading curve. This does not mean that the neutron-physical properties of the S/INF system are constant. This is obvious, since a change in initial enrichment requires a change in average burn-up to keep the system’s $k_{\text{eff}}$ value constant. Any change in initial enrichment and average
burn-up results in a change of the isotopic composition of the S/INF and hence in a change of the neutron-physical properties of the S/INF system. In particular, increase in burn-up results in neutron spectrum hardening because of the build-up of plutonium isotopes. This increase in spectrum hardening with increasing burn-up is conspicuous when in a CSA of PWR S/INF wet storage pool BUC is combined with Partial Boron Credit (PBC). In this case, the loading curve is based on a $k_{\text{eff}}$ value higher than the maximum allowable. To comply with the maximum permissible $k_{\text{eff}}$ value credit is taken for some portion of the boron solved in the pool coolant. As shown in Figure 1.21, even though the loading curve is based on a constant $k_{\text{eff}}$ value, the minimum PBC required to keep $k_{\text{eff}}$ at its maximum permissible value increases along the loading curve. This is obviously due to spectrum hardening with increasing burn-up. The increase in the required PBC is the reactivity equivalent of the increase of the spectrum hardness with increasing burn-up\textsuperscript{22}. Therefore, it is obvious due to physics that the validity of a reactivity equivalence relation used for instance to determine a loading curve is bounded to the design basis to which this relation is applied\textsuperscript{23}. This relation is not retained when the design basis is changed. It has been observed that a lot of erroneous assumptions have been made about the validity of reactivity relations \[70\] and, for PWR spent fuel pool storage \[34\].

A loading curve usually applies to any fuel position inside a S/INF management system configuration of interest and does not include any credit for any real loading scheme for the system. A loading curve must therefore cover the variety of irradiation histories possible in the PWR core of interest. In addition, since indicating minimum required average burn-up values, a loading curve must cover the variety of axial and horizontal burn-up profiles and related isotopic compositions which result in possibly positive axial end effects and positive horizontal reactivity effects, respectively. So therefore, the task of estimating a loading curve implies the need for:

- looking for a bounding irradiation history given by those reactor operation conditions leading, at given initial enrichment and given burn-up, to the highest reactivity of the S/INF under the conditions of the S/INF system of interest;
- generating a bounding axial burn-up profile, i.e. a model profile which covers, under the conditions of the S/INF system of interest, the end effects of all the real axial burn-up profiles to be taken into account;
- generating a bounding horizontal burn-up profile, i.e. a model profile which covers the reactivity effects of all the horizontal burn-up profiles to be considered.

It is preferable to estimate a loading curve as a continuous function of the initial enrichment\textsuperscript{24}. Therefore, both the shape of the bounding axial burn-up profile and the shape of the bounding horizontal profile have to be described as continuous functions of the average burn-up \[27,50,71\].

\textsuperscript{22}. If that minimum PBC required for the starting point of the loading curve where no BUC is needed (in Figure 1.21; about 250 pcm boron at about 1.7 wt.-% initial enrichment) were taken, then the neutron multiplication factor would increase with increasing burn-up along the loading curve.

\textsuperscript{23}. The design basis is characterised by all the parameters describing the S/INF system of interest which are kept constant when a reactivity equivalence relation is applied to determine values for the remaining parameters of the system. For example, in Figure 1.21, the remaining parameters are the initial enrichment and the average burn-up, all the other parameters characterising the S/INF system (wet storage pool for PWR fuel assemblies) are kept constant.

\textsuperscript{24}. It is observed that discontinuous loading curves are presented very often. Such loading curves are in fact not only ambiguous, but also bizarre since contradicting physics. There is no problem to estimate continuous loading curves \[71\].
As mentioned in Section 1.3.3.1, the calculational fission density distribution is shifted more and more towards the top region of the fuel zones of the S/IFAs of interest. The $k_{\text{eff}}$ value of the S/IFAs is therefore more and more determined by the isotopic composition distribution in the top region of the SFAs' fuel zones. Thus, the determination of a bounding irradiation history, i.e. the determination of bounding depletion parameters have to be discussed together with the physical effects due to the non-uniformity of burn-up distributions in S/IFAs, as discussed in Section 1.3.8.

1.3.5 Analysis of abnormal and accident conditions

In BUC CSA of PWR S/INF wet storage pools, the bounding normal operation geometric configuration of fuel assemblies, storage cells and storage racks as well as the bounding normal operation pool coolant temperature usually make up the design basis for the loading curve. Because of the increase in spectrum hardness with increasing burn-up along the loading curve it is obvious that the analysis of abnormal or accidental conditions has usually to be based on the initial enrichment and the burn-up defining the upper end point of the loading curve since the efficiency of neutron absorbers used in the system decreases with increasing spectrum hardness. What is true for the PBC (Partial Boron Credit) discussed in the preceding section is also true for the boron credit required for abnormal or accidental events. Since the abnormal or accidental configuration is different from the design basis of the loading curve, use of the fuel's isotopic composition defining the lower end point of the loading curve\(^{25}\) in the analysis of the abnormal or accidental configuration results in a significant underestimation of the minimum boron content of the pool water required for maintaining sufficient subcriticality [34].

In fact, use of any point of the loading curve different from the upper end point of the loading curve results in an underestimation of the minimum required boron content. Figures 1.22 and 1.23 give an example for this fact:

- Figure 1.22 shows a PWR fuel assembly wet storage pool loading curve obtained by assuming zero boron content in the pool water, the bounding normal operation pool coolant temperature as well as the bounding normal operation geometric configuration of the fuel assemblies, storage cells and storage racks. The actual upper end point of this loading curve is the burn-up value (40.08 MWd/kg U) at 5.0 wt.-\(^{235}\text{U}\) initial enrichment since higher enrichments are not allowed in the storage pool analysed.

- Figure 1.23 summarises the results of the analysis of the accidental event of an inadvertent placement of a fresh fuel assembly outside and adjacent to a storage rack designed for burn-up credit according to the loading curve Figure 1.22. The misplaced fresh fuel assembly is assumed to have the maximum possible enrichment of 5 wt.-\(^{235}\text{U}\).

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\(^{25}\) The lower end point of the loading curve is given by the highest enrichment value allowable without taking credit for burn-up (see Figure 1.22: Lower end point at 2.20 wt.-\(^{235}\text{U}\) enrichment).
First the loading curve is determined using a fixed $k_{eff}$ value (here $k_{eff} = 0.999$) higher than the maximum allowable value. Then the initial enrichment values and the related burn-up values of the loading curve are taken to determine the minimum PBC required to comply with the maximum allowable $k_{eff}$ value (here $k_{eff} = 0.95$), [69].

As shown in Figure 1.23, use of any point of the loading curve different from the upper end point of the loading curve results in an underestimation of the maximum $k_{eff}$ value possible in the accidental event analysed; so therefore, use of any point of the loading curve different from the upper end point of the loading curve results in an underestimation of the minimum boron content required for meeting the subcriticality acceptance criterion (which is $k_{eff} \leq 0.92$ in Figure 1.23).

The fact that the validity of a reactivity equivalence relation used for instance to determine a loading curve is strictly bounded to the design basis to which this relation is applied has been demonstrated here for PWR wet storage pools, namely for the usual case that the design basis of a loading curve does not include any credit for the boron content of the pool coolant. However, the statement, that any reactivity equivalence relation becomes invalid when the design basis of this relation is changed or left, goes of course, due to physics, for any case. Different examples demonstrating this fact can be found in [70] and in the proceedings of the BUC training course [26] (see Session 3 of that course, presentation “Reactivity equivalence and BUC loading curve”). It is demonstrated in these references that, whatever the fuel type is and whatever the spent fuel management system is, application of a reactivity equivalence relation to a configuration or case different from the design basis of the reactivity equivalence relation does result in an incorrect estimate of the reactivity of this configuration or case. It is shown that the reactivity is dramatically underestimated in many cases. And it is stated in addition that equating the reactivity of spent fuel to fresh fuel really makes no sense since one has to calculate the isotopic content of the spent fuel in any case so that this calculated isotopic content can be directly applied to the application case of interest. The objective of generating a loading curve is not to equate the reactivity of spent fuel to fresh fuel but to estimate the minimum required burn-up as a function of the initial enrichment of the fuel.
Figure 1.22. Example for a PWR fuel assembly wet storage pool loading curve obtained by assuming zero boron content in the pool water.

The actual upper end point of the loading curve is the burn-up value at 5.0 wt.-% \(^{235}\text{U}\) initial enrichment since higher enrichments are not allowed.

Figure 1.23. Analysis of the accidental event of an inadvertent placement of a fresh, 5 wt.-% \(^{235}\text{U}\)-enriched fuel assembly outside and adjacent to a storage rack designed for burn-up credit according to the Loading Curve (LC).

Figure 1.22: Use of three different LC points: LC (e = 3.0 wt.-%): Point at 3.0 wt.-% \(^{235}\text{U}\) initial enrichment, Burn-up = 13.82 MWd/kg ULC (e = 4.5 wt.-%): Point at 4.5 wt.-% \(^{235}\text{U}\) initial enrichment, Burn-up = 34.20 MWd/kg ULC (e = 5.0 wt.-%): Point at 5.0 wt.-% \(^{235}\text{U}\) initial enrichment, Burn-up = 40.08 MWd/kg U.
1.3.6 Criticality calculation benchmarks

Comparisons of the ability of various criticality calculation code systems and nuclear data libraries to predict the neutron multiplication factor of given S/INF systems with given isotopic compositions have been provided by the NEA EGBUC Benchmarks Phase I-A (Ref. [8]) as well as Phases II-A, II-B, II-C, and II-E [10-12] and [14]. Phase I-A was a basic benchmark addressed to eigenvalue calculations for a simple pin-cell configuration. The benchmarks of Phase II were addressed to investigations of the reactivity effects due to axial burn-up profiles, first using idealised burn-up profiles symmetric in shape and isotopic composition (Phases II-A and II-B), then using burn-up profiles bounding realistic axial burn-up distributions (Phases II-C and II-E).

1.3.6.1 The Phase I-A benchmark for eigenvalue calculations for a simple pin-cell model

The eigenvalue calculations were performed to analyse the impact of the parameters:

- burn-up: burn-up values of 0 MWd/kg U (fresh fuel), 30 MWd/kg U and 40 MWd/kg U were chosen;
- cooling time: cooling times of 1 year and 5 years were used in different combinations with the specified burn-up values of 30 MWd/kg U and 40 MWd/kg U, as well as the impact of selecting different groups of isotopes;
- major actinides only (see Figure 1.4);
- all actinides (i.e. major plus minor actinides in Figures 1.4 and 1.5);
- actinides plus major fission products (all fission products specified in Figure 1.6 but $^{135}$Cs).

The geometrical data of the pin cell and the isotopic number densities were given in the benchmark specification [8] for all the specified burn-up values and cooling times.

The Phase I-A benchmark report is mainly addressed to comparisons of the results delivered by the participants of the benchmark for the multiplication factors, the neutron spectra, the isotopic reaction rates (absorption, production, neutrons per fission). Trends due to burn-up and cooling time were only extracted from the results delivered for the neutron multiplication factors. Accordingly, the main result of the Phase I-A benchmark exercise was obtained from the analysis of the contributions of the selected isotope groups to the decrease in reactivity due to burn-up and cooling time:

- the major actinides contribute more than 50% to the reactivity loss;
- the contribution of the minor actinides is less than 10%;
- the contribution of the major fission groups amounts to approximately 30%.

So, the contribution of all the remaining fission products is not greater than about 10%.

Note that these contributions refer to the pin-cell model. In systems with harder neutron spectra, the reactivity worth of several neutron absorbing nuclides may be lower, so that the relative contribution of the major actinides to the reactivity loss may be greater. Anyway, the contributions observed in the Phase I-A Benchmark confirm that the relatively small set of the specified isotopes (major actinides, minor actinides, and major fission products) can represent about 90% of the reactivity decrease due to burn-up and cooling time.

As for the impact of the cooling time, it was found – as was to be expected according to Section 1.2.3 of the report in hand – that the increase in cooling time from 1 year to 5 years at
given burn-up results in a reactivity decrease and that the amount of this decrease becomes more pronounced when the fission products are included\textsuperscript{26}.

1.3.6.2 Benchmark studies Phase II-A and Phase II-B on reactivity effects due to axial burn-up profiles assumed to be symmetric in shape and isotopic composition

In Phase II-A, an array of PWR fuel assemblies, which was assumed to be of infinite lateral extent, was examined for the reactivity effect of axial burn-up profiles [10]. In Phase II-B, a configuration of 21 PWR spent fuel assemblies in a stainless steel transport cask was taken as a basis for evaluating the reactivity effect of axial profiles [11]. The 21 fuel assemblies were assumed to be positioned in a borated stainless steel basket centred in the transport cask.

In Phase II-A and Phase II-B, idealised burn-up profiles were applied, each characterised by an axially symmetric burn-up distribution represented by nine uniform zones. Even though real PWR axial burn-up profiles are axially asymmetric due to the lower moderator density in the upper half of an operating core, some important observations have been made in the benchmark studies Phase II-A and Phase II-B:

- The calculational fission density distribution of an isotopic composition, which is uniformly distributed over the full active length of a fuel assembly is cosine-shaped irrespective of whether the fuel is fresh or irradiated.

- The axial end effect may be negative at lower average burn-up values. If so, the end effect reaches a minimum at some average burn-up value and increases then with increasing average burn-up due to the increasing non-uniformity of the burn-up profile\textsuperscript{27}.

- The increasing non-uniformity of burn-up profiles with increasing average burn-up results in a progressive reshaping of the related calculational fission density distributions: For the idealised burn-up profiles used in Phase II-A and Phase II-B, it is observed that, first, the fission density distribution flattens out more and more, increases more and more near the ends of the fuel assembly’s fuel zone and hence drops more and more around the centre of the fuel zone, so that it becomes a double-peak distribution. The peaks increase and shift more and more towards the ends of the fuel zone with increasing burn-up, and the fission density in the centre region of the fuel zone decreases to meagre values.

Due to the idealised burn-up profiles assumed to be axially symmetrically in shape and isotopic composition, the calculational fission density distributions observed in Phase II-A and Phase II-B are axially symmetrically. Because real axial burn-up profiles are usually asymmetric in shape and isotopic composition, which is due to the mere fact that the moderator density in the upper region of the core is lower than in the bottom region, it can be concluded that the peak at the top end of the fuel assembly’s fuel zone will be significantly higher than the peak at the bottom end of the fuel zone, provided that all the other conditions assumed in the Phase II-A and Phase II-B studies remain unchanged.

- Application of the actinide-only BUC approach to a given axial burn-up profile yields a lower value for the axial end effect than application of the actinide-plus-fission-product BUC approach. This is due to the fact that the fission product concentration is

\textsuperscript{26} As stated in Section 1.2.3, there is a minimum in reactivity at around 100 years cooling time.

\textsuperscript{27} The wording “increasing non-uniformity” is used to describe the fact that the ratio between the burn-up in the plateau region of a burn-up profile and the burn-up at the ends of a fuel assembly’s fuel zone increases with increasing average burn-up (see Figure 1.20).
considerably higher in the centre region than in the end regions of the fuel assembly’s fuel zone. The reactivity worth of the centre region is therefore more overestimated in the actinide-only approach than the reactivity worth of the end regions.

- For the cooling times of 1 year and 5 years assumed in the Phase II-A and Phase II-B studies, it is observed that the axial end effect increases, at given average burn-up and given axial burn-up shape, with increasing cooling time. This is due to the fact that the reactivity worth of the centre region decreases faster with increasing cooling time than the reactivity worth of the end zones because the plutonium and fission product concentration is higher in the centre region [39]. It is shown that the end effect increases with cooling time for cooling times up to about 100 years.)

1.3.6.3 The benchmark studies Phase II-C and Phase II-E on reactivity effects due to axial burn-up profiles bounding realistic axial burn-up distributions

Whereas idealised axial burn-up profiles were used in Phases II-A and II-B, and whereas a uniform burn-up distribution was used in Phase II-D (see Section 1.2.4.2), realistic axial burn-up profiles extracted from databases of real axial burn-up profiles were used in the benchmarks Phase II-C and Phase II-E, [12], [14], and [72]. As in Phase II-B, a configuration of 21 PWR spent fuel assemblies in a stainless steel transport cask was taken as a basis for evaluating the reactivity effect of the axial burn-up profiles; and as in Phase II-B, the fuel assemblies were assumed to be positioned in a borated stainless steel basket centred in the transport cask.

- 1.3.6.3.1 The Phase II-C benchmark

The objective of the Phase II-C benchmark was to study the impact of the asymmetry of axial burn-up shapes on the end effect. To describe the asymmetry of an axial burn-up shape, a parameter named as “top end parameter $S_{kn}$” defined by Equation (2) was introduced:

$$S_{kn} = \sum_{\nu=1}^{n} \alpha_{\nu\mu}$$ with $k = 6$ and $n = 32$. (see Figure 1.20)  \hspace{1cm} (2)

where $\alpha_{\nu\mu}$ is the ratio of the burn-up $B_{\nu\mu}$ of the $\mu$-th profile at node $\nu$ to the averaged burn-up $\overline{B}_{\mu}$ of this profile:

$$\alpha_{\nu\mu} = B_{\nu\mu} / \overline{B}_{\mu}.$$ \hspace{1cm} (3)

Since the nodes of the axial shapes used in Phase II-C are equidistant and since the distance of the bottom node to the bottom end of the active zone as well as the distance of the top node to the top end of the active zone are just given by the half of the distance between two neighbouring nodes the averaged burn-up $\overline{B}_{\mu}$ is given by Equation (4):

$$\overline{B}_{\mu} = \frac{1}{n} \sum_{\nu=1}^{n} B_{\nu\mu}, \quad n = 32.$$ \hspace{1cm} (4)

It follows, therefore,

$$\sum_{\nu=1}^{n=32} \alpha_{\nu\mu} = n = 32.$$ \hspace{1cm} (5)

The Phase II-C benchmark is based on the evaluation of a database of 850 axial burn-up profiles, which has been provided by the German Convoy Series nuclear power plant Neckarwestheim II [12]. All the fuel assemblies from which these axial burn-up profiles, based
on evaluation of in core flux map measurements, have been obtained are of one and the same type.

The 850 axial burn-up profiles were normalised according to Equation (3) and grouped into seven groups according to their average burn-up as specified in Figure 1.24. In this figure the average $\alpha_{\nu\mu}$ values of the normalised burn-up profiles of each of the groups are presented. It appears from these group-averages $\alpha_{\nu\mu}$ that

- the asymmetry of axial burn-up profiles tends to decrease with increasing average burn-up of the profiles.

For the Phase II-C benchmark, the burn-up groups 3 and 6 were used, (see Figure 1.24). Two profiles named as “B32A222222” and “B50A222222” were formed as references cases by using the upper bounds 32 MWd/kg U and 50 MWd/kg U, respectively, of the two burn-up groups as average burn-up values and the average $\alpha_{\nu\mu}$ values of all the 850 axial burn-up profiles (these values are given by the normalised profile specified as “total” in Figure 1.24). From each reference case, a set of profiles was derived by replacing successively the $\alpha_{\nu\mu}$ values of nodes 1 through 6 of the reference case by the group-specific minimum or maximum $\alpha_{\nu\mu}$ values observed in the database and by taking into account the normalisation condition Equation (5). Figure 1.25 shows the reference cases and the profiles with the highest asymmetry (BbbA111111 with bb = 32 and 50, respectively) and the lowest asymmetry thus obtained (BbbA333333 with bb = 32 and 50, respectively). (The digit “$\nu$” in the profile’s identification name “BbbAn_1n_2n_3n_4n_5n_6” is taken to be 2, when the total average $\alpha_{\nu\mu}$ value is used for the $\nu$-th node, is set to 1, when the group-specific minimum $\alpha_{\nu\mu}$ value is applied to the $\nu$-th node, and is chosen to be 3, when the group-specific maximum $\alpha_{\nu\mu}$ value is used for the $\nu$-th node.)

**Figure 1.24. Evaluation of the axial burn-up profiles from the database of the 850 axial burn-up profiles from Neckarwestheim II: Averages $\alpha_{\nu\mu}$ for the burn-up groups into which the normalised burn-up profiles were grouped according to their average burn-up values**
The decision to vary only the $\alpha$ values for the six top nodes and to choose $\kappa = 6$ for the top end parameter $S_\kappa$, Equation (2), is justified by the Phase II-C benchmark results:

- Figure 1.26 shows for the 50 MWd/kg U average burn-up cases the normalised least-squares fit curves $f(z)$ obtained from the fission densities calculated in the Phase II-C benchmark [12]. As expected (see Section 1.3.6.2), the fission density distributions are strongly peaked in the top end region of the fuel zone only; and the more the peaks are shifted towards the top end of the active length the higher, at given burn-up, the asymmetry of the profiles and the higher, at given asymmetry the average burn-up. This can be demonstrated by plotting the “top end content” of the fission density distributions $f(z)$ against the top end parameter $S_6$, (see Figure 1.27).

$$C_6 = \int z f(z) \text{ with } \zeta_6 = \frac{Z_6 + Z_7}{2}$$

(L in Equation (6) denotes the active length of the fuel assemblies, and $Z_j$ is the distance of the locus of the $j$-th node from the bottom end of the active zone.)

- Therefore, the neutron multiplication factor of a given spent fuel management system the design of which is comparable with the Phase II-C configuration is virtually solely determined by the top end region of the active zone of the spent fuel assemblies.

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28. This means that, in particular, neutron moderation and reflection conditions inside and outside the configuration will not change with the height $z$ of the fuel zone, and that the neutron absorbing materials along the height $z$ will not change in material composition and geometry, (see [12], Sections 1.3.5 and 1.7.3).
Figure 1.26. Phase II-C: Normalised fission density distributions obtained for the profiles with 50 MWd/kg U average burn-up

Figure 1.27. Regression analysis of the C6 values obtained for the Phase II-C axial burn-up profiles

Top End Content C6 as a Function of the Top End Parameter S6

Equation 2 shows that the higher the S6 value, the lower the asymmetry of the axial profile.
Figure 1.28. Phase II-C: Regression analysis of the observed end effect values $\Delta k_{ee}(B32)$ and $\Delta k_{ee}(B50)$ as a function of the top end parameter $S6$

Figure 1.28 shows the results obtained for the end effect. As appears from this figure, the end effect increases:

- at given burn-up, with increasing asymmetry;
- at given asymmetry, with increasing average burn-up.

The values of the sample correlation coefficient $R^2$ of the regression functions obtained for the end effect are indicated in Figure 1.28. As can be seen, the $R^2$ value achieved for the 50 MWd/kg U average burn-up cases is significantly lower than the $R^2$ value obtained for the 32 MWd/kg U cases. As shown in Figure 1.20, the more the presence of a spacer grid in the top end region of the fuel zone impacts the shape of an axial burn-up profile, the higher the average burn-up of the profile is. To take account of the impact of this “local asymmetry” of the profile on the neutron multiplication factor $k_{eff}(\text{shape})$ and hence the end effect Equation (1), the “local asymmetry parameter” has been introduced in the evaluation of the Phase II-C benchmark results [12]:

$$LA(\mu) = \frac{SI3(\mu)}{S6(\mu)} \quad \text{with} \quad SI3(\mu) = \frac{1}{n} \sum_{\nu=1}^{3} \alpha_{\nu\mu}, \quad n = 32$$

(7)

In Figure 1.29, the observed end effects are plotted against the parameter:

$$A = S6 + g \cdot LA = S6 + g \cdot \frac{SI3}{S6}.$$  

(8)
Figure 1.29. Phase II-C: Regression analysis of the observed end effect values $\Delta k_{eef}(B32)$ and $\Delta k_{eef}(B50)$ as a function of the parameter $S6+g\cdot LA$ as shown in Equation (8).

The factor $g$ in Equation (8) couples the profile’s asymmetry with the “local asymmetry” of the profile’s top end shape. In the “uncoupled” case, i.e. with $g = 0$ one gets the regression curves presented in Figure 1.28. In Figure 1.29, these curves serve as starting curves, and the coupling factor $g$ is then increased such that the sample correlation coefficient $R^2$ of the resultant regression functions is maximised. As shows in Figure 1.29, the increase in $R^2$ obtained for the 32 MWd/kg U axial profiles is negligible, whereas the increase in $R^2$ found for the 50 MWd/kg U axial profiles is significant. This confirms that:

- the impact of the “local asymmetry” on the end effect increases with increasing average burn-up.

So, in summary, the following observations were made in Phase II-C:

- The asymmetry of axial burn-up profiles tends to decrease with increasing average burn-up of the profiles.
- At given burn-up the end effect increases with increasing asymmetry.
- At given asymmetry the end effect increases with increasing average burn-up.
- The end effect is significantly impacted by the “local asymmetry” of the profile in the region of the top end of the fuel zone of the fuel assemblies. This impact increases with increasing burn-up.

1.3.6.3.2 The Phase II-E benchmark

As already stated above, in Phase II-D the burn-up was always assumed to be uniformly distributed over the active length of the fuel assemblies. Consequently, either zero Control Rod (CR) insertion or full CR insertion (insertion over the full active length) were only assumed in Phase II-D (see Section 1.2.4.2 and [13]). Therefore, it was the objective of the Phase II-E benchmark to combine the asymmetry effect on the end effect observed in Phase II-C with the CR insertion effect on the isotopic inventory as set forth below:
Since the asymmetry of the axial profiles and the end effect are dependent on the average burn-up of the profiles two profiles related to different average burn-up values were chosen, (see Figure 1.30).

To be representative and bounding, the two axial burn-up profiles chosen were generated from a database of real axial burn-up profiles by means of the methods described in [71].

For each of these profiles the end effect was studied for different CR insertion depths ranging from 0 cm (no insertion) to full insertion.

For Phase II-E virtually the same transport cask configuration has been assumed as the one used in Phase II-C [14]. The neutron multiplication factor of this cask configuration and the related end effect were analysed as a function of the control rod (CR) insertion depth $d_{CR}$ in the assemblies’ fuel zone during depletion. So, for CR insertion depths $0 < d_{CR} < L$ the fuel zone of the fuel assemblies was divided into two zones, the zone at the top end of the fuel zone which was exposed to CR insertion during depletion, and the remainder of the fuel zone which was not exposed to CR insertion. Accordingly, the axial burn-up profiles shown in Figure 1.30 as well as the uniform burn-up distribution of the average burn-up values of the profiles were divided into these two zones.

As known from the Phase II-D benchmark exercise, CR insertion leads, due to spectrum hardening, to a significant increase in the number densities of $^{235}$U and $^{239}$Pu and hence to a significant increase in the fuel’s reactivity compared to the case of no CR insertion. The increase in the number densities of $^{235}$U and $^{239}$Pu and hence the increase in reactivity increases with increasing burn-up since increasing burn-up results in increasing spectrum hardening. Thus, the increase in the reactivity importance due to CR insertion increases faster in axial fuel zones with higher depletion rates and hence higher burn-ups. From that it follows that the impact of CR insertion on the neutron multiplication factor of a PWR UO$_2$ configuration of interest and hence on the end effect related to a given axial burn-up profile is strongly...
dependent on the CR insertion depth during depletion. In particular, it can be expected that full CR insertion into the entire fuel zone of a fuel assembly during depletion results, compared to the case of no CR insertion, in a significant increase of the configuration’s neutron multiplication factor but, at the same time, in a significant decrease of the end effect since the reactivity importance of the centre zone of the fuel zone increases faster with increasing spectrum hardening than the reactivity importance of the end zones of the fuel zone.

Conclusions on the changes of the configuration’s neutron multiplication factors $k_{\text{eff}}$ (shape) and $k_{\text{eff}}$ (unif. dist.) and hence, according to Equation (1), on the change of the end effect with changing CR insertion depth can be drawn from the outcomes of the Phase II-C benchmark by following simply, from the top end to the bottom end of the fuel zone, the fission density distribution $f(z)$ associated with the given axial burn-up profile at zero CR insertion depth (see Figure 1.31) and by starting, at zero CR insertion depth, with the fission density distribution of the uniform distribution of the profile’s average burn-up (see Figure 1.32).

**Figure 1.31. Phase II-C: Comparison of the non-normalised fission density distributions obtained for the reference profiles B32A222222 and B50A222222**
In fact, to predict the behaviour of $k_{\text{eff}}$ (shape) qualitatively, one needs only to follow the increase of the probability content:

$$C(\zeta) = \int_{L-\zeta}^{L} dz \ f(z)$$ \hspace{1cm} (9)

as given by the fission density distribution $f(z)$ with increasing distance $\zeta$ from the top end of the fuel zone:

- As shown in Figure 1.31 for example, at the beginning, i.e. at small CR insertion depths $\zeta = d_{\text{CR}}$, the fission probability $C(\zeta)$ increases very rapidly with increasing $\zeta$, and it is therefore to be expected that the neutron multiplication factor $k_{\text{eff}}$ (shape) rapidly increases since the number densities of $^{235}\text{U}$ and $^{239}\text{Pu}$ in the region $[L-\zeta, L]$ are increased due to CR insertion, in fact, the more they are increased the higher the burn-up becomes with increasing $\zeta = d_{\text{CR}}$.

- Then, with further increasing CR insertion depth $\zeta = d_{\text{CR}}$, the increase of the fission probability $C(\zeta)$ slows down due to the shape of the fission density distribution; and when $\zeta$ exceeds the value $\zeta_{M}$ where the maximum of the fission density distribution is located, then the increase in $C(\zeta)$ goes down more and more. It is therefore to be expected that the neutron multiplication factor $k_{\text{eff}}$ (shape) still increases, but that the amount of its increase slows down more and more with increasing insertion depth $\zeta = d_{\text{CR}}$.

- Finally, when $\zeta = d_{\text{CR}}$ reaches a certain value $\zeta_{p}$ such that the region $[L-\zeta_{p}, L]$ virtually contains the entire fission density peak then any increase in $\zeta$ results in a negligible increase of $C(\zeta)$ only, and it is then to be expected that $k_{\text{eff}}$ (shape) virtually remains constant for any value $\zeta > \zeta_{p}$.
The values $\zeta_M$ and $\zeta_P$ tend to decrease with increasing average burn-up (see Figure 1.31). It is therefore to be expected that both, the rapidity with which the neutron multiplication factor $k_{\text{eff}}(\text{shape})$ increases with increasing insertion depth $\zeta = d_{\text{CR}}$ at the beginning of the CR insertion, and the rapidity with which $k_{\text{eff}}(\text{shape})$ converges towards a certain case-specific limit, increase with increasing average burn-up.

Of course, CR insertion affects the shape of a fission density distribution for a given axial burn-up profile. In addition, CR insertion may impact the shape of the axial burn-up profile and increase the asymmetry of the profile in particular. Nevertheless, for a given axial burn-up profile (given, for instance, by a bounding profile as needed for the determination of a burn-up credit loading curve, see Section 1.2.4) the associated fission density distribution at zero CR insertion is, so to speak, the “starting condition” which significantly affects the rapidity with which $k_{\text{eff}}(\text{shape})$ can change due to the changes in the axial isotopic composition distribution caused by CR insertion.

In fact, the cosine-shaped fission density distribution associated with the uniform distribution of the average burn-up (see Figure 3.16) provides a completely different “starting condition”. Before a significant response of the neutron multiplication factor $k_{\text{eff}}(\text{unif. dist.})$ to a change in the isotopic composition due to CR insertion can be expected, a significant increase in the fission density must occur at the top end of the fuel zone. This requires a sizeable insertion depth $\zeta = d_{\text{CR}}$ since a potential increase in the reactivity due to the change in the isotopic composition at the top end region of the fuel zone competes with increased leakage due to the close proximity to the end of the fuel zone. In other words, a significant “reorientation” of the fission density distribution such that a proper peak of the fission density in the top end region of the fuel zone can be obtained requires a proper CR insertion depth $\zeta = d_{\text{CR}}$. Therefore, it is to be expected that the neutron multiplication factor $k_{\text{eff}}(\text{unif. dist.})$ starts to increase at a significantly higher $\zeta = d_{\text{CR}}$ value than the neutron multiplication factor $k_{\text{eff}}(\text{shape})$.

After the neutron multiplication factor $k_{\text{eff}}(\text{unif. dist.})$ has started to increase, it continues to increase with any further increase of the CR insertion depth $\zeta$ till $\zeta = L$ is reached. This is due to the fact that any increment $\Delta \zeta$ in the insertion depth $\zeta$ means that in the range $[\zeta, \zeta + \Delta \zeta]$ one uniform isotopic composition is exchanged for another isotopic composition which has a higher reactivity due to spectrum hardening. This exchange is always the same for any interval $[\zeta, \zeta + \Delta \zeta]$ since a uniform burn-up distribution is examined. After a certain insertion depth is reached the increase in the neutron multiplication factor will slow down more and more since the relative increase of the axial length of the fuel zone containing already the more reactive isotopic composition decreases with increasing $\zeta$ according to $1/(1 + \zeta/\Delta \zeta)$. And finally, the maximum of the fission density distribution will return, step by step, with increasing $\zeta$ to the centre of the fuel zone, till at $\zeta = L$ the fission density distribution is again cosine-shaped.

Therefore, because the neutron multiplication factor $k_{\text{eff}}(\text{unif. dist.})$ starts to increase at a higher insertion depth $\zeta$ than the neutron multiplication factor $k_{\text{eff}}(\text{shape})$ and because $k_{\text{eff}}(\text{unif. dist.})$ does not cease to increase – even if the amount of the increase slows down more and more for higher $\zeta$ values – till $\zeta = L$ is reached, whereas $k_{\text{eff}}(\text{shape})$ reaches its case-specific limit at a $\zeta$ value which is significantly lower than $L$, it can be inferred that the end effect, given according to Equation (1), has a maximum at a relatively low $\zeta$ value, which
decreases with increasing average burn-up. In addition, since the increase in the fuel’s reactivity due to the spectrum hardening caused by CR insertion increases with increasing burn-up it is to be expected, as already stated, that the end effect is lower for the case $\zeta = L$ than for the case $\zeta = 0$.

As appears from Figures 1.33 through 1.40, all these predictions are confirmed by the outcomes obtained in the Phase II-E benchmark calculations:

- Starting with the CR insertion, the neutron multiplication factor $k_{\text{eff}}(\text{shape})$ responds nearly promptly and increases very rapidly; and the response of $k_{\text{eff}}(\text{shape})$ is the more prompt, the higher the average burn-up (see Figures 1.33 and 1.35). Then, around a CR insertion depth $d_{\text{CR}}$ where the maximum of the axial fission density distribution is located (see Figure 1.34) the increase of $k_{\text{eff}}(\text{shape})$ begins to slow down; and for insertion depths $d_{\text{CR}}$ greater than approximately 100 cm, where most of the fission density distribution is already covered by the integral Equation (9), no further increase of $k_{\text{eff}}(\text{shape})$ is observed.

- In contrast to the behaviour of $k_{\text{eff}}(\text{shape})$, the response of the neutron multiplication factor $k_{\text{eff}}(\text{unif. dist.})$ of the uniform burn-up distribution is “delayed”, i.e. a sizeable insertion depth $d_{\text{CR}}$ has to be reached before a significant increase in $k_{\text{eff}}(\text{unif. dist.})$ can be observed (see Figures 1.36 and 1.38). Then, after a sufficient “reorientation” of the fission density distribution is reached (see Figure 1.37), $k_{\text{eff}}(\text{unif. dist.})$ starts to increase rapidly due to a more and more pronounced peaking of the fission density distribution in the top end region of the fuel. With increasing CR insertion depth more and more of the content below the fission density distribution is covered by the integral Equation (9) even though the peaking of the fission density distribution becomes less and less pronounced. The increase in $k_{\text{eff}}(\text{unif. dist.})$ slows down, therefore, the relative increase of the axial length of the fuel zone containing already the more reactive isotopic composition decreases with increasing CR insertion depth. However, as expected, the increase in $k_{\text{eff}}(\text{unif. dist.})$ continues till $d_{\text{CR}} = L$ is reached (see Figures 1.36 and 1.38).

- Consequently, as expected, starting the CR insertion the end effect first increases significantly, reaches then a maximum and slows down till it reaches at full CR insertion a value which is lower than the value of the end effect at zero CR insertion (see Figures 1.39 and 1.40).
Figure 1.33. $K_{eff}$ as a function of CR insertion depth bounding profile, average burn-up=30 MWd/kg U [14,72]

Figure 1.34. Fission densities axial burn-up profile average burn-up B=30 MWd/kg U (not normalised to unity) [14,72]
Figure 1.35. $K_{\text{eff}}$ as a function of CR insertion depth
bounding profile, average burn-up=50 MWd/kg U [14,72]

Figure 1.36. $K_{\text{eff}}$ as a function of CR insertion depth
uniform burn-up distribution, burn-up=30 MWd/kg U [14,72]
As shown in Figure 1.39, in cases of average burn-up of 30 MWd/kg U, the end effect becomes negative for full CR insertion. A negative end effect means that the so-called “bounding profile” is no longer bounding. The use of a so-called “bounding profile” at a negative end effect results in an underestimation of the neutron multiplication factor of a fuel system of interest. So, one should be cautious with the use of so-called bounding profiles when CR insertion has to be considered. The bounding profile at negative end effect is the uniform burn-up distribution. This goes irrespective of whether CR insertion has to be taken into account or not.
Thus, one of the lessons that can be learnt from the results of the Phase II-C through Phase II-E benchmarks is

- that it is of course necessary in burn-up credit applications to look for bounding axial burn-up profiles (see Section 1.3.4);
- but that it is also necessary to control whether the end effect obtained with a so-called “bounding profile”, is negative or not.

If the end effect is negative the uniform burn-up of the average burn-up of the profile is the bounding profile. A non-uniform burn-up distribution can only be bounding, if the end effect obtained with this distribution, is not negative.

Another lesson that can be learnt from Phase II-E in particular is that relatively small CR insertion depths have to be considered in burn-up credit applications. It is in fact common practice in core operation that at least one CR bank is in a “target bite position”, i.e. at the beginning of cycle the control rods of this CR bank are inserted into the fuel zone of the involved fuel assemblies with an insertion depth of usually not more than about 30 cm, and the insertion depth is then gradually reduced during the cycle and tends towards zero at the end of cycle [49].

It is also quite common practice in core operation to use extended low power operation at the end of cycles. Then the control rods of at least one CR bank are inserted with a significant insertion depth [49]. As learnt from Phase II-D, the increase in reactivity of spent fuel due to spectrum hardening due to CR insertion during irradiation increases with increasing burn-up of the fuel because increasing burn-up results in increasing spectrum hardening.

Further lessons that can be learnt from Phase II-C through Phase II-E benchmark results are given in the following sections.

Figure 1.39. End effect $\Delta k$ as a function of CR insertion depth, average burn-up=30 MWd/kg U
1.3.7 Observations on the case that a section of the top end of the fuel zone of the fuel assemblies juts out of the neutron absorber channels of a spent fuel storage or transport system

It has been observed that in some spent fuel storage racks of wet storage pools as well as in some spent fuel storage and transport casks the nominal length of the absorber material of the channels forming the fuel assembly storage positions is chosen equal to the nominal active length specified for the un-irradiated fuel assemblies of the type of interest. Therefore, it cannot be excluded already for the case of un-irradiated fuel assemblies that, due to the manufacturing tolerances in the un-irradiated fuel assemblies’ active length and in the absorber length, a section of the fuel zone of the fuel assemblies protrudes from the neutron absorber channels. Furthermore, it has to be considered that the active length of fuel under irradiation increases with increasing irradiation time, so that the active length of spent fuel can be enlarged by a factor up to about 1.008. Thus, assuming an active length of 365.76 cm (often used for 17x17 fuel assemblies, for instance) plus the usual tolerance of 0.7 cm (half a pellet length) for the un-irradiated fuel assembly, the active length can be increased up to 369.39 cm due to irradiation. Assuming the quite common tolerance of 0.5 cm for the absorber length, it follows that a section of up to 4.13 cm of the fuel zone of the fuel assemblies may jut out of the neutron absorber channels. The question is whether such an amount of jutting-out of the absorber channels affects the neutron multiplication factor \( k_{\text{eff}} \) (shape) of the spent fuel configuration of interest or not.

Due to the outcomes of the Phase II-C benchmarks the case that the top end region of the fuel zone juts out of the neutron absorbing channels is of particular interest. Accordingly, even though the amount of the impact on the end effect may be significantly different, qualitatively the same that has been told in the preceding section about the impact of CR insertion during depletion on the end effect applies to the case that the fuel zone of the fuel assemblies is only partially inserted in the absorber channels. One has only to identify now the parameter \( \zeta \) with the axial length of the fuel region which is not inserted into the neutron absorbing material zone. In fact, starting at full coverage of the entire fuel zone, i.e. starting with a “non-coverage” of \( \zeta = 0 \) the fission probability \( C(\zeta) \) due to the fission density distribution \( f(z) \) associated
with the applied axial burn-up profile increases very rapidly with increasing $\zeta$, and it is therefore to be expected that the neutron multiplication factor $k_{\text{eff}}(\text{shape})$ rapidly increases due to the significant change in the neutron absorption and reflection conditions caused by the “disappearance” of the neutron absorber in horizontal direction. Then, due to the shape of the fission density distribution $f(z)$, the increase in $C(\zeta)$ and hence the increase in $k_{\text{eff}}(\text{shape})$ slows down more and more, in particular when $\zeta$ has exceeded the value $\zeta_M$ where the maximum of $f(z)$ is located. Finally, when $\zeta$ has reached the value $\zeta_P$ such that the whole region $[L - \zeta_P, L]$ which virtually contains the entire fission density peak is uncovered then $k_{\text{eff}}(\text{shape})$ virtually remains constant for any value $\zeta > \zeta_P$.

In contrast to that the “reorientation” of the fission density distribution of the uniform burn-up distribution requires a sizeable non-coverage $\zeta$. Therefore, the neutron multiplication factor $k_{\text{eff}}(\text{unif. dist.})$ starts to increase at a significantly higher $\zeta$ value than the neutron multiplication factor $k_{\text{eff}}(\text{shape})$. The neutron multiplication factor $k_{\text{eff}}(\text{unif. dist.})$ continues to increase till $\zeta = L$ is reached, but the amount of its increase will slow down at higher $\zeta$ values since the relative increase in the length of the uncovered fuel region due to an increment $\Delta \zeta$ of this length goes down according to $1/(1 + \zeta/\Delta \zeta)$.

Thus, starting at $\zeta = 0$, it is to be expected that the end effect first increases rapidly with increasing $\zeta$, then reaches a maximum and, afterwards, decreases monotonously with further increasing $\zeta$. Of course, it cannot be expected now, in contrast to the CR insertion case, that the end effect at $\zeta = L$ is smaller than at $\zeta = 0$ because the increases in $k_{\text{eff}}(\text{shape})$ and $k_{\text{eff}}(\text{unif. dist.})$ are not caused by changes in the isotopic composition of the fuel.

These predictions have been checked by means of the configuration shown in Figure 1.41 using the axial burn-up profile with 30 MWd/kg U average burn-up presented in Figure 1.30 and assuming zero CR insertion.

Figure 1.41 shows only the top end region of the geometry model used. This model consists of one 17x17-25 fuel assembly surrounded by the same neutron absorbing material as was used in the Phase II-E benchmark. The fuel assembly has been modelled analogously to Phase II-E, but in $\pm Z$-direction reflected by water only since no cask material was assumed. In $\pm X$-direction and $\pm Y$-direction the geometry model was mirror reflected so that a configuration has been simulated which is infinite in lateral extent with respect to the axial direction ($\pm Z$-direction) of the fuel assemblies. The mirror reflection boundaries were defined by the outer surfaces of the absorber channel shown in Figure 1.41 so that neighbouring fuel assemblies in the simulated configuration were just separated by one absorber panel (as it is usually the case in those storage racks of spent fuel ponds which are designed for burn-up credit). The fuel assemblies in the simulated configuration were gradually pulled out of the absorber channels in $+ Z$-direction; and the neutron multiplication factors $k_{\text{eff}}(\text{shape})$ and $k_{\text{eff}}(\text{unif. dist.})$ were analysed as a function of the “non-coverage”-parameter $\zeta$.

As appears from Figure 1.41, first the fuel assemblies have been assumed to be completely inserted in the absorber channels so that the non-coverage parameter $\zeta$ is taken to be negative at the beginning, i.e. before the pulling-out of the assemblies has been started. $\zeta$ is taken to be
zero when the top end of the fuel zone reaches the Z-height of the top end of the absorber channels.

The results obtained for $k_{\text{eff}}$ (shape), $k_{\text{eff}}$ (unif. dist.) and the end effect as a function of the non-coverage parameter $\varsigma$ are presented in Figure 1.42. As appears from this figure, the predictions made above about $k_{\text{eff}}$ (shape), $k_{\text{eff}}$ (unif. dist.) and the end effect as a function of $\varsigma$ are fully confirmed.

It is worthwhile to note that $k_{\text{eff}}$ (shape) already responds slightly at negative $\varsigma$ values to the increase of $\varsigma$. Then, for $\varsigma > 0$ $k_{\text{eff}}$ (shape) increases promptly and rapidly. Already for a non-coverage of $\varsigma = 5$ cm a significant increase of $k_{\text{eff}}$ (shape), compared to the values obtained for $k_{\text{eff}}$ (shape) at $\varsigma \leq 0$, is found. So therefore, it has to be considered that cases as those described in the first paragraph of this section result in significant impacts on $k_{\text{eff}}$ (shape). In other words, caution should be used when choosing the nominal length of absorber channels to be equal to the nominal active length specified for the un-irradiated fuel assemblies.

**Figure 1.41. 17x17 Assembly geometry [72]**

If this choice is made for a burn-up credit transport cask it has to be taken into account that the non-coverage of the fuel zone of the fuel assemblies may be increased due to slipping of the fuel assemblies under accident conditions which results, if flooding of the cask is assumed to be caused by these accident conditions, in a significant increase of $k_{\text{eff}}$ (shape), as shown in Figure 1.42. Also, it should be kept in mind that the increase of $k_{\text{eff}}$ (shape):

- takes place the more promptly, the higher the average burn-up of the axial burn-up profiles is;
- is significantly enhanced if CR insertion during depletion of the fuel assemblies has to be considered.
In conclusion, it is strongly recommended to ensure full coverage of the fuel zones under all conditions to be analysed in a burn-up credit application case.

It has been shown that it is possible to predict qualitatively, on the basis of the results obtained in the Phase II-C benchmark, the behaviour of $k_{\text{eff}}$ (shape), $k_{\text{eff}}$ (unif. dist.) and hence the end effect for the Phase II-E configurations as well as for the case that the fuel zone of spent fuel assemblies is not fully shielded by neutron absorbing channels. The lessons learnt from elaborating these predictions and from the results obtained for the Phase II-E configurations and the case of partial non-coverage of the fuel zones are as set forth below:

- In general, the reactivity behaviour of spent PWR UO$_2$ fuel differs from the reactivity behaviour of un-irradiated fuel PWR UO$_2$ (e.g. in case of partial non-coverage of the fuel zones the reactivity behaviour of spent fuel cannot be derived from the reactivity behaviour of un-irradiated fuel).

- The end effect strongly depends on:
  - the depletion conditions, (in particular, on the CR insertion history during irradiation);
  - the asymmetry and “local asymmetry” of the axial burn-up profile (catchword: “bounding profile”, see Section 1.3.1.1) chosen to analyse the end effect;
  - the design of the spent fuel management system of interest.

- The end effect has to be controlled. If the end effect is negative the uniform burn-up of the average burn-up of the analysed axial burn-up profile is the bounding profile.

**Figure 1.42. Top end of fuel zone juts out of absorber channel**
1.3.8 Bounding depletion parameters

As stated in Section 1.3.4, the task of estimating a loading curve for the S/INF management system of interest implies the need for looking for a bounding irradiation history given by those core operation conditions leading, at given initial enrichment and given burn-up, to the highest reactivity of the S/INF under the conditions of the system of interest. Thus, the depletion parameters for the depletion analysis of the S/INF of interest (see Sections 1.2.2.1 through 1.2.2.8) have to be bounding with respect to the reactivity of the S/INF under the conditions of the S/INF management system of interest. Therefore, all the lessons learnt from the criticality calculation benchmarks described in Section 1.3.6 have to be taken into account.

As for the choice of bounding depletion parameters, the lessons learnt from Phase II-C through Phase II-E and from Section 1.3.7 are of particular interest. Since the neutron multiplication factor of a spent fuel management system, the design of which complies with the lesson learnt in Section 1.3.7, is virtually solely determined by the top end region of the active zone of the fuel assemblies, the depletion parameters to be chosen for the depletion analysis have to cover the depletion conditions in the top region of the core of interest. This pertains in particular the parameters:

- fuel temperature;
- moderator temperature and related density;
- use of fixed neutron absorbers, control rod insertion histories in particular;
- integral burnable absorbers initially present in the fuel.

An example for determining bounding depletion parameters without forgetting the remarks made in Section 1.2.2.8 is given in [49].

1.3.9 Generation of bounding axial burn-up profiles

Procedures for generating bounding axial burn-up profiles have to be based on the lessons learnt from Phase II-C under consideration of the lessons learnt from Phase II-E. In addition, since the axial end effect depends, as mentioned in Section 1.3.3.1, on the active length of the fuel assemblies, one will not derive bounding axial burn-up profiles from profile databases using normalised active lengths.

An example for a procedure that is completely based on the Phase II-C observations summarised at the end of Section 1.3.6.3.1 and which provides a bounding axial burn-up profile as a continuous function of the average burn-up (see Section 1.3.4) is described in [71]. Overviews on different procedures all complying with the lessons learnt from Phase II-C are given in [26], [28], and [30-32].
1.4 Uncertainty analysis

It is an indispensable part of a criticality safety analysis of a nuclear fuel system performed using numerical methods for calculating the neutron multiplication factor $k_{\text{eff}}$ of the system to determine the confidence that one has in the numerical result obtained for $k_{\text{eff}}$. It is necessary to determine this confidence in order to be able to demonstrate that the probability that the neutron multiplication factor $k_{\text{eff}}$ of the system, calculated by means of a specific criticality calculation procedure adequately chosen with respect to the system, exceeds the maximum allowable neutron multiplication factor $k_{\text{max}}$, is not greater than an administratively established margin $\gamma$, i.e. meets the following inequality:

$$
\pi_S = P((k_{\text{eff}} + \Delta k_B) > k_{\text{max}} | S) \leq \gamma.
$$

(10)

$S$ stands for the nuclear fuel system of interest; $\pi_S$ is the probability $P((k_{\text{eff}} + \Delta k_B) > k_{\text{max}} | S)$ that $k_{\text{eff}} + \Delta k_B$ is greater than $k_{\text{max}}$ given by an adequate administrative margin $\Delta k_m$ according to:

$$
k_{\text{max}} = 1 - \Delta k_m;
$$

(11)

and $\Delta k_B$ denotes the bias in $k_{\text{eff}}$ characteristic of the employed criticality calculation procedure with respect to the system $S$.

As explained in [59], the exact value of the probability $\pi_S$ usually remains unknown. Only a probability $(1 - \alpha)$ that inequality Equation (10) is met can be calculated [59] and [67]:

$$
P(\pi_S \leq \gamma) = (1 - \alpha)
$$

(12)

This expression is the criticality safety acceptance criterion, i.e. the criterion for deciding whether sufficient subcriticality is ensured. For both probabilities, $\gamma$ and $\alpha$, the value of 0.05 is usually prescribed by the relevant criticality safety regulations or standards.

The proof that the criticality safety acceptance criterion is met has to consider all the uncertainties coming along in a criticality safety analysis. According to the successive steps to be taken in a criticality safety analysis there is a certain hierarchy of the uncertainties which has strictly to be observed in the proof that the criticality safety acceptance criterion is met. Figure 1.43 depicts the hierarchy of uncertainties for BUC CSA. Complete uncertainty analysis tools for BUC CSA strictly observing the hierarchy of uncertainties are described in [48] and [67].
Figure 1.43. Hierarchy of uncertainties

The term "uncertainty" is understood as related to the covariance matrix of the respective parameters.
References

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2. MOX PWR Summary

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2.1 Physics of burn-up credit

2.1.1. Fuel composition

The Phase IV benchmarks considered the effect of burn-up, cooling time and initial MOX composition (MOX plutonium content and initial plutonium vector) upon both the pin cell and fuel assembly reactivity.

For the Phase IV-A Benchmark, consideration was given to the impact of the initial MOX composition using three different initial MOX fuels, which were chosen to represent the range of current interest in MOX fuel:

- Case A: Reference MOX fuel composition appropriate to a typical plutonium vector for material derived from the reprocessing of thermal reactor UO₂ fuels, often referred to as “first generation” MOX.
- Case B: MOX fuel composition appropriate to the disposition of weapons plutonium in MOX.
- Case C: MOX fuel composition appropriate to future MOX fuels that might be produced using plutonium recovered from the reprocessing of irradiated MOX, for example “later generation” MOX fuel from a plutonium recycling strategy.

The above-mentioned compositions are not truly equivalent to real MOX fuel, in terms of their lifetime performance in the reactor, however as their initial fissile plutonium contents are broadly the same (see Tables 2.1-2.3), it was judged acceptable to make comparisons in the analysis between their various components of reactivity.

The pin cell geometry for the Phase IV-A Benchmark and the spent fuel compositions for each burn-up were generated by the benchmark co-ordinator. Hence, each participant used the same fuel compositions to calculate the various $k_{\text{eff}}$ eigenvalues requested. Differences between the participants’ $k_{\text{eff}}$ results were therefore expected to be due only to the calculation codes and nuclear data libraries used.

The fresh MOX fuel compositions for the Phase IV-B benchmark were similar to those used for the Phase IV-A Benchmark except that Case C was not included (see Tables 2.1-2.3); this omission was to ensure that the calculation burden on the participants was minimised:

- Case A: Reference MOX fuel case, appropriate to a typical plutonium vector for material derived from the reprocessing of thermal reactor UO₂ fuels, often referred to as “first generation” MOX.
- Case B: MOX fuel case appropriate to the disposition of weapons plutonium in MOX.

The plutonium isotopic composition of Case B (weapons disposition MOX) was identical for the two benchmarks. However, there were slight differences in the $^{239}$Pu and $^{241}$Pu fissile fractions between the two benchmarks for Case A (first generation MOX). This was because
more up-to-date information became available for this MOX fuel composition and was therefore included in the later Phase IV-B benchmark.

Furthermore, since fuel assembly and super-cell (multiple assemblies) models were considered in the Phase IV-B benchmark, it was necessary to derive three different plutonium vectors related to high, medium and low plutonium content fuel pins so that the plutonium distribution within the MOX fuel assemblies was appropriately represented. Since in reality, the MOX fuel would be irradiated in a mixed UO₂-MOX PWR core, i.e. alongside UO₂ fuel assemblies, a typical UO₂ fuel composition with an initial enrichment of 4.3 w/o ²³⁵U/U was also defined for the UO₂ fuel assembly. In all cases, the uranium oxide component of the MOX was assumed to be depleted, with a ²³⁵U content of 0.25 w/o ²³⁵U/U (typical of current MOX fuel fabrication).

In contrast to the Phase IV-A Benchmark, each participant for the Phase IV-B benchmark calculated the fuel compositions as a function of burn-up and cooling time using their own nuclear physics codes and based on these fuel compositions, k_{eff} eigenvalues for the system were determined. Differences between the participants’ k_{eff} results were expected to be larger than for the results of the Phase IV-A Benchmark as there was more scope for errors due to the numerous depletion methods and nuclear data libraries used by the participants.

2.1.1.1. Phase IV-A Benchmark

The burnt up major actinides and major fission products generated for the Phase IV-A Benchmark show typical depletion and accumulation behaviour for LWR MOX fuel. During the cooling time of the fuel, ²⁴¹Pu decays and accumulates into ²⁴¹Am. In addition, the inventory of all the curium isotopes increase with burn-up, however, the ²⁴²Cm nuclide with a relatively shorter half live, vanishes during five years of cooling time. The inventory of major fission products does not change significantly during fuel cooling time except for the ¹⁴⁷Sm and ¹⁵⁵Gd nuclides which increase significantly. These two fission products are the main contributors of the burn-up credit gained by extending the cooling time from 1 to 5 years.

The reactivity worths of the major actinides for the later generation MOX fresh fuel composition are presented in Table 2.5; this MOX fuel case was chosen as it contained the largest plutonium content. It can be clearly seen from this table that, as expected, ²³⁹Pu gives the largest positive worth followed by ²⁴¹Pu. The largest negative worth is due to ²⁴⁰Pu followed by ²³⁸U. It is therefore considered that the extent of burn-up credit gain will be dominated by these four isotopes. Although not shown here, the reactivity worth of the curium isotopes was also estimated and it is recommended that they are included in the spent fuel composition of MOX fuel due to the positive reactivity worth of the ²⁴⁵Cm isotope. Inclusion of curium isotopes in MOX fuel can increase the reactivity of the system by up to 1000 pcm.

The results and analysis for the reactivity prediction benchmark, Phase IV-A (infinite arrays of PWR MOX fuel pin cells), will now be discussed. Based on the k_{eff} results of the 63 specified calculation cases, the components of the burn-up reactivity credit are shown in Table 2.6 below. It should be noted that the fuel was burnt up to a maximum of 60 GWd/teHM and the burn-up reactivity credit calculated for the major actinides and major fission products includes a one-year cooling time credit.

By taking into account all the reactivity components, total burn-up reactivity credits of approximately 24%, 32% and 20% dk/k can be obtained for first generation MOX, weapons disposition and later generation MOX fuels, respectively. In particular, the largest burn-up credit gain can be seen for weapons disposition MOX fuel. For all three MOX fuels, the contribution of the major fission products and cooling time (extending from 1 year to 5 years) to the total burn-up credit was found to be around 9-11 % and 6 % dk/k, respectively.
In addition, a closer observation of the relative contribution to the total reactivity credit reveals that the major fission products contribute more than 40% for the first and later generation MOX fuels and slightly less than 35% for weapons disposition MOX fuel. Furthermore, the contribution of the major actinides is always less than that of the major fission products for the first and later generation MOX fuels but is larger for the weapons disposition MOX fuel. This is attributed to the depletion behaviour of weapons disposition MOX fuel where the $^{239}$Pu nuclide is the predominant fissile isotope ($^{239}$Pu/Pu content of 93.6w/o) and depletes relatively faster than in the other MOX fuel cases.

2.1.1.2. Phase IV-B Benchmark

As already observed in the Phase IV-A Benchmark results, the two fission products, $^{147}$Sm and $^{155}$Gd, increase significantly during the cooling time. In particular, the increase of the $^{155}$Gd nuclide in the Phase IV-B benchmark (from 0 to 5 years) is an order higher than the increase observed in the Phase IV-A Benchmark (from 1 to 5 years). This difference can be explained by the fact that in the Phase IV-A Benchmark, the initial one-year cooling time results in a significant reduction of the short-lived nuclide $^{155}$Tb (electron capture) to $^{155}$Gd. Thus, it is during the first year of cooling where the majority of in-growth of $^{155}$Gd occurs. However, a cooling time of one year does not significantly increase in the amount of $^{147}$Sm because its precursor, $^{147}$Pm, has a half-life of 2.6 years (beta decay).

The results and analysis for the reactivity predictions of the Phase IV-B benchmark (MOX fuel depletion calculations) will now be discussed. Based on the six calculation cases presented in the benchmark specification, the components of burn-up reactivity credit for fuel pin cell model are shown in Table 2.7 below. It should be noted that the burn-up reactivity credit for all the actinides and major fission products shown in the table do not include the first cycle burn-up credit. This is because the benchmark specification did not require the participants to calculate the $k_{\text{eff}}$ of the BOC (beginning of cycle) for the first cycle. Therefore, the actual burn-up reactivity swing from BOC to EOC (end of cycle) for the first cycle cannot be directly determined. However, to be consistent with the results of the Phase IV-A Benchmark and to allow an assessment of the total burn-up credit, the burn-up reactivity credit from 0 to 48 GWd/teHM can be estimated as follows:

$$\Delta \rho(0 \rightarrow 48) \approx \frac{3}{2} \times \Delta \rho(16 \rightarrow 48)$$

This approximation is considered to be acceptable as it was seen that the burn-up reactivity swings for each cycle were approximately the same.

By taking all the reactivity components into account, a total burn-up reactivity credit of about 20 % and 30 % $\Delta k/k$ can be obtained for first generation MOX and weapons disposition MOX fuels, respectively. As already found in the Phase IV-A Benchmark results, the largest gain in reactivity credit was obtained for weapons disposition MOX fuel (Case B).

Despite the same initial fresh fuel composition, the difference in the burn-up credit for weapons disposition MOX fuel between the Phase IV-A and Phase IV-B benchmarks is thought to be mainly attributed to the difference in the final fuel burn-up (60 GWd/teHM as opposed to 48 GWd/teHM) and to a lesser extent to the slightly different fuel pitches used in each benchmark. For both MOX fuels, the contribution to the total reactivity burn-up credit was found to be 15-27% $\Delta k/k$ for all the actinides plus major fission products and 4-5% $\Delta k/k$ for the five-year cooling time.

A closer observation of the results reveals that the actinides plus the major fission products contribute 74% to the total reactivity credit for the first generation MOX fuel case and 89% for
the weapons disposition MOX fuel case. From Table 2.6, it can be seen that for the Phase IV-A Benchmark, the actinides and major fission products also contribute 74% to the total reactivity credit for the first generation MOX fuel case and 81% for the weapons disposition MOX fuel case.

The results of the burn-up reactivity credit calculations for the fuel assembly model are shown in Table 2.8. The results show similar reactivity components consistent with those of the pin cell model presented in Table 2.7. Slight differences are thought to be attributed to the existence of the 24 guide tubes included in the fuel assembly model.

The results of burn-up reactivity credit for the super-cell model are shown in Table 2.9. It should be noted though that the burn-up reactivity credit values shown in the table correspond to 1 MOX plus 3 UO$_2$ fuel assemblies and are not due to a single MOX fuel assembly. Taking into account all the actinides plus the major fission products along with the five-year cooling time, produces a total burn-up reactivity credit of about 27% and 33%dk/k for the first generation MOX and weapon disposition MOX fuel cases, respectively. The combination of 1 MOX plus 3 UO$_2$ fuel assemblies gives no significant reactivity credit improvement for weapons disposition MOX fuel but moderate credit improvement can be observed for first generation MOX fuel, which is mainly due to the actinides and major fission products. It can be seen for the super-cell model that a minimal amount of burn-up reactivity credit can be obtained from cooling the fuel.

**Table 2.1. Geometry and non-fuel material descriptions for Phase IV Benchmarks**

<table>
<thead>
<tr>
<th>Phase IV-A</th>
<th>Phase IV-B</th>
</tr>
</thead>
<tbody>
<tr>
<td>MOX Pin Cell Model</td>
<td>MOX Pin Cell Model</td>
</tr>
<tr>
<td>r=0.412 cm</td>
<td>r=0.412 cm</td>
</tr>
<tr>
<td>R=0.475 cm</td>
<td>(900K)</td>
</tr>
<tr>
<td>P=1.33 cm</td>
<td>Zircaloy</td>
</tr>
<tr>
<td></td>
<td>Boron 500 ppm</td>
</tr>
<tr>
<td>MOX Assembly Model</td>
<td>MOX Assembly Model</td>
</tr>
<tr>
<td>17x17 array</td>
<td>24 guide tubes</td>
</tr>
<tr>
<td>MOX-UO$_2$ Supercell Model</td>
<td>MOX-UO$_2$ Supercell Model</td>
</tr>
<tr>
<td>1 MOX assembly (centre)</td>
<td>3 UO$_2$ assemblies (outer)</td>
</tr>
</tbody>
</table>

$r$, $R$, and $P$ denote pellet, clad outer radii and fuel pin pitch.
Table 2.2. Fresh fuel composition descriptions for Phase IV Benchmarks

<table>
<thead>
<tr>
<th>Composition</th>
<th>Pu Content (w/o)</th>
<th>Fissile Pu Content (w/o)</th>
<th>Composition</th>
<th>Pu Content (w/o)</th>
<th>Fissile Pu Content (w/o)</th>
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</thead>
<tbody>
<tr>
<td>Case A (First Generation MOX)</td>
<td>5.6</td>
<td>3.987</td>
<td>Case A (First Generation MOX)</td>
<td>8.866</td>
<td>5.692</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>High</td>
<td>8.866</td>
<td>5.692</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Medium</td>
<td>6.206</td>
<td>3.984</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Low</td>
<td>4.894</td>
<td>3.142</td>
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<tr>
<td></td>
<td></td>
<td></td>
<td>Average</td>
<td>8.000</td>
<td>5.136</td>
</tr>
<tr>
<td>Case B (Weapons Disposition)</td>
<td>4.6</td>
<td>3.756</td>
<td>Case B (Weapons Disposition)</td>
<td>4.377</td>
<td>4.110</td>
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<td></td>
<td></td>
<td>High</td>
<td>4.377</td>
<td>4.110</td>
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<tr>
<td></td>
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<td></td>
<td></td>
<td>Low</td>
<td>2.416</td>
<td>2.269</td>
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<td></td>
<td></td>
<td>Average</td>
<td>3.950</td>
<td>3.709</td>
</tr>
<tr>
<td>Case C (Later Generation MOX)</td>
<td>8.0</td>
<td>3.840</td>
<td></td>
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</tr>
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</table>

Table 2.3. Plutonium isotopic composition in fresh fuel for Phase IV Benchmarks (w/o)

<table>
<thead>
<tr>
<th>Pu vector</th>
<th>Phase IV-A</th>
<th>Phase IV-B</th>
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</thead>
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<tr>
<td>238Pu</td>
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<td>2.5</td>
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<td></td>
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<td>0.1</td>
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<tr>
<td>239Pu</td>
<td>59.0</td>
<td>54.7</td>
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<td></td>
<td>93.6</td>
<td>93.6</td>
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<td>240Pu</td>
<td>23.0</td>
<td>26.1</td>
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<tr>
<td></td>
<td>6.0</td>
<td>6.0</td>
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<tr>
<td>241Pu</td>
<td>12.2</td>
<td>9.5</td>
</tr>
<tr>
<td></td>
<td>0.3</td>
<td>0.3</td>
</tr>
<tr>
<td>242Pu</td>
<td>4.0</td>
<td>7.2</td>
</tr>
<tr>
<td></td>
<td>0.1</td>
<td>0.1</td>
</tr>
</tbody>
</table>
### Table 2.4. Evaluation conditions for Phase IV Benchmarks

<table>
<thead>
<tr>
<th>Evaluated Parameters</th>
<th>Phase IV-A</th>
<th>Phase IV-B</th>
</tr>
</thead>
</table>
| Burn-up              | 0 (fresh), 20, 40, 60 GWd/teHM | Cycle 1: 420 FPD, EOC burn-up = 16 GWd/teHM; Downtime 30 days.  
Cycle 2: 420 FPD, EOC burn-up = 32 GWd/teHM; Downtime 30 days.  
Cycle 3: 420 FPD, EOC burn-up = 48 GWd/teHM; Downtime 0 years. |
| Cooling time         | 1 and 5 years | 5 years |
| Fuel composition     | FP + Major Actinides  
Major Actinides  
All Actinides | FP + All Actinides |

1) FP: 15 major fission products (large absorption cross-sections)  
2) Major Actinides: 12 major actinides (U, Pu isotopes, 241Np, 241Am, 243Am)  
3) All Actinides: major actinides plus 242Cm, 243Cm, 244Cm and 245Cm.  
4) FPD – Full Power Days.  
5) EOC – End of Cycle.

### Table 2.5. Reactivity worth of major actinides from fresh fuel of later generation MOX (Case C) for Phase IV-A Benchmark

<table>
<thead>
<tr>
<th>Nuclide</th>
<th>Reactivity worth (% dk/k)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{234}$U</td>
<td>0.02</td>
</tr>
<tr>
<td>$^{235}$U</td>
<td>0.58</td>
</tr>
<tr>
<td>$^{238}$U</td>
<td>-15.25</td>
</tr>
<tr>
<td>$^{238}$Pu</td>
<td>-1.43</td>
</tr>
<tr>
<td>$^{239}$Pu</td>
<td>28.17</td>
</tr>
<tr>
<td>$^{240}$Pu</td>
<td>-21.86</td>
</tr>
<tr>
<td>$^{241}$Pu</td>
<td>10.51</td>
</tr>
<tr>
<td>$^{242}$Pu</td>
<td>-3.16</td>
</tr>
</tbody>
</table>

1) Calculated by MONK8A code with JEF-2.2 library.
Table 2.6. Reactivity components of burn-up credit for Phase IV-A Benchmark (in % dk/k)

<table>
<thead>
<tr>
<th>MOX Fuel Compositions</th>
<th>Major Actinides 1)</th>
<th>Major Fission Products 1)</th>
<th>Cooling Time (1-5 year) 2)</th>
<th>Total</th>
</tr>
</thead>
<tbody>
<tr>
<td>Case A (First Generation MOX)</td>
<td>8.2 (33.8%)</td>
<td>9.8 (40.5%)</td>
<td>6.2 (25.7%)</td>
<td>24.2 (100%)</td>
</tr>
<tr>
<td>Case B (Weapons Disposition)</td>
<td>14.8 (46.0%)</td>
<td>11.2 (34.8%)</td>
<td>6.2 (19.2%)</td>
<td>32.2 (100%)</td>
</tr>
<tr>
<td>Case C (Later Generation MOX)</td>
<td>4.5 (22.2%)</td>
<td>9.2 (45.1%)</td>
<td>6.6 (32.7%)</td>
<td>20.3 (100%)</td>
</tr>
</tbody>
</table>

1) 60 GWd/teHM; one-year cooling time burn-up credit included
2) 60 GWd/teHM; burn-up credit obtained by extending the cooling time from 1 to 5 years
3) Figures in parentheses show the relative percentage of the total burn-up reactivity

Table 2.7. Reactivity components of burn-up credit for fuel pin cell model of Phase IV-B Benchmark (in % dk/k)

<table>
<thead>
<tr>
<th>MOX Fuel Compositions</th>
<th>All Actinides + Major Fission Products 1)</th>
<th>Cooling Time (5 year) 2)</th>
<th>Total</th>
</tr>
</thead>
<tbody>
<tr>
<td>Case A (First Generation MOX)</td>
<td>10.1 [15.2] 4) (68.7%) [76.3%]</td>
<td>4.7 (32.0%) [23.7%]</td>
<td>14.7 [19.9] (100%) [100%]</td>
</tr>
<tr>
<td>Case B (Weapons Disposition)</td>
<td>18.2 [27.3] (84.3%) [88.6%]</td>
<td>3.5 (16.2%) [11.4%]</td>
<td>21.6 [30.8] (100%) [100%]</td>
</tr>
</tbody>
</table>

1) First EOC to third EOC (48 GWd/teHM); First BOC (beginning of cycle) to EOC burn-up credit is not included
2) Burn-up credit obtained by extending the cooling time from 0 to 5 years
3) Figures in ( ) parentheses show the relative percentage of the total burn-up reactivity
4) Figures in [ ] parentheses show the estimated reactivity or its percentage including first BOC to EOC burn-up credit

Table 2.8. Reactivity components of burn-up credit for fuel assembly model of Phase IV-B Benchmark (in % dk/k)

<table>
<thead>
<tr>
<th>MOX Fuel Compositions</th>
<th>All Actinides + Major Fission Products 1)</th>
<th>Cooling Time (5 year) 2)</th>
<th>Total</th>
</tr>
</thead>
<tbody>
<tr>
<td>Case A (First Generation MOX)</td>
<td>10.3 [15.5] 4) (68.2%) [76.3%]</td>
<td>4.8 (31.8%) [23.7%]</td>
<td>15.1 [20.3] (100%) [100%]</td>
</tr>
<tr>
<td>Case B (Weapons Disposition)</td>
<td>18.3 [27.7] (82.4%) [88.1%]</td>
<td>3.7 (16.7%) [11.9%]</td>
<td>22.2 [31.3] (100%) [100%]</td>
</tr>
</tbody>
</table>

1) First EOC to third EOC (48 GWd/teHM); First BOC to EOC burn-up credit is not included
2) Burn-up credit obtained by extending the cooling time from 0 to 5 years
3) Figures in ( ) parentheses show the relative percentage of the total burn-up reactivity
4) Figures in [ ] parentheses show the estimated reactivity or its percentage including first BOC to EOC burn-up credit
Table 2.9. Reactivity components of burn-up credit for super-cell model of Phase IV-B Benchmark (in % dk/k)

<table>
<thead>
<tr>
<th>MOX Fuel Compositions</th>
<th>All Actinides + Major Fission Products 1)</th>
<th>Cooling Time (5 year) 2)</th>
<th>Total</th>
</tr>
</thead>
<tbody>
<tr>
<td>Case A (First Generation MOX)</td>
<td>17.1 [25.7] 4) (91.0%) [93.8%]</td>
<td>1.7 (9.0%) [6.2%]</td>
<td>18.8 [27.4] (100%) [100%]</td>
</tr>
<tr>
<td>Case B (Weapons Disposition)</td>
<td>21.1 [31.7] (93.4%) [95.5%]</td>
<td>1.5 (6.6%) [4.5%]</td>
<td>22.6 [33.2] (100%) [100%]</td>
</tr>
</tbody>
</table>

1) First EOC to third EOC (48 GWd/teHM); First BOC to EOC burn-up credit is not included
2) Burn-up credit obtained by extending the cooling time from 0 to 5 years
3) Figures in ( ) parentheses show the relative percentage of the total burn-up reactivity
4) Figures in [ ] parentheses show the estimated reactivity or its percentage including first BOC to EOC burn-up credit

2.1.2. Burn-up distributions

In the Phase IV-A and IV-B benchmark specifications, calculations were not requested by the organisers that would allow an investigation into either the pin by pin or assembly by assembly radial burn-up distribution. However, a rough estimation can be performed based on the results entitled Benchmark Calculation of Power Distribution within Fuel Assemblies Phase II published in 2000. In this report, it can be seen that except for the outer water reflector, the core configuration is identical to the super-cell model geometry. Large differences are observed in the fission rates for the fuel pins located at the boundary between the MOX and UO₂ assemblies compared to fuel pins located in other parts of the assembly. This will consequently have an effect on the radial burn-up distribution. However, as the Phase IV-B benchmark specification only requested assembly average burn-up data, the effect of the radial burn-up distribution on burn-up credit cannot be estimated from the results.

Regarding the axial burn-up distribution, it is well known that for a typical PWR operation, the use of soluble boron absorber minimises the effect of the control rod cluster on the axial power distribution. Therefore, it is possible to use a constant flux/power distribution to assess the axial burn-up distribution although as the benchmark geometry was two-dimensional, it is not possible to investigate this.

2.1.3. Operating history effects

In the Phase IV-A and IV-B benchmark calculations, the effect of exposure history is inherently simulated in the depletion analyses, in particular for the Phase IV-B benchmark. However, it should be noted that the depletion analyses were conducted under a fixed concentration of soluble boron, the boundary conditions were always white and no control rod cluster was included. Therefore, no additional information can be derived regarding the operating history effects other than that mentioned in the discussion above regarding the main nuclides of the major actinides and the two major fission product isotopes (¹⁴⁷Sm and ¹⁵⁵Gd).
2.1.4. Cask/Flask storage conditions

The Phase IV-A and IV-B benchmark calculations did not model a cask/flask geometry so this issue cannot be investigated.

2.2. Calculating burn-up credit criticality

- modelling detail;
- source convergence issues;
- deterministic vs. probabilistic analyses;
- nuclear data.

Various deterministic and Monte Carlo codes were used for the reactivity and depletion analyses in the Phase IV benchmarks; these are summarised in Table 2.10. State-of-the-art reactor physics codes as well as the latest processed nuclear data libraries were used to perform the benchmarks, which covered both deterministic (mostly SN, collision probabilistic and characteristic methods) and stochastic methods (point wise as well as multi-group Monte Carlo).

The nuclear data libraries used in the codes for the Phase IV Benchmarks were ENDF/B (Version IV to VI), FOND (Version 2), JEF (Version 2.2) and JENDL (Version 3.2). The deterministic codes employed the multi-group approach while the stochastic codes employed both the multi-group and continuous-energy approaches. In the deterministic multi-group approach, some codes adopted an ultra-fine group structure for the resonance energy region. For stochastic multi-group codes, the pin cell and assembly geometries were treated almost without approximation, although a homogenisation step for the production of the effective group constants could be considered as an approximation.

As the MOX fuel compositions presented in the benchmarks may have been relatively new to some of the participants, it is possible that some could have had limited calculation experience with the nuclear data used. Even so, the pin cell modelling in the Phase IV-A Benchmark and certain cases of the Phase IV-B Benchmark was very simple and thus good agreement was expected for the $k_{\text{eff}}$ eigenvalues predicted by the participants. However, even for this simple pin cell model, it was necessary to select a proper boundary condition and the neutron group number/structure carefully.

For the Phase IV-B Benchmark, errors in the depletion calculation at early stages of burn-up will propagate to the successive stages and thereby influence the accuracy of the $k_{\text{eff}}$ at higher burn-ups. Unfortunately, it is these higher burn-ups which are of most interest to burn-up credit criticality assessments. This issue becomes more complicated since inaccuracies in the processed nuclear data library used will further amplify these errors. In some cases, it is also possible that these inaccuracies could be hidden due to error cancellation. Therefore, sensitivity analysis is needed to determine the source of the errors and to quantitatively determine their extent.

The spread of the participants’ calculation results around the corresponding average value will now be discussed in detail. Although the average value of the participants’ results does not necessarily indicate an accurate answer, the standard deviation of the spread around the average is a valuable quantity to know in order to assess the degree of confidence in the burn-up reactivity credit results mentioned in Section 3.1.
2.2.1. Phase IV-A Benchmark

Based on the results of the 63 specified cases, the relative spread of the $k_{\text{eff}}$ results for the first generation MOX and weapons disposition MOX fuel cases was approximately 2.0% with the spread for the later generation MOX fuel case being about 2.5%. In addition, the spread in the $k_{\text{eff}}$ results was not sensitive to either burn-up or cooling time implying that it even exists for the $k_{\text{eff}}$ calculation of fresh MOX fuel. Further investigations into the sources of the spread in the $k_{\text{eff}}$ results revealed that the use of the Wigner-Sietz cell modelling as well as nuclear data libraries with a group structure of less than 80 energy groups were the main contributors.

The Wigner-Sietz cell modelling contributes a reactivity error of approximately 500 pcm. Therefore, it is strongly recommended to avoid the use of Wigner-Sietz cell modelling. The use of nuclear data libraries which have a group structure of less than 80 energy groups is also discouraged.

Although it is difficult to estimate the contribution to errors in the $k_{\text{eff}}$ results from the nuclear data libraries used, two important conclusions can be drawn from an analysis of the results. First, inaccuracies in the participants’ nuclear data sets for the plutonium isotopes could contribute to errors seen in the $k_{\text{eff}}$ results for the fresh MOX fuel compositions. Second, for later generation MOX fuels burnt up in excess of 30 GWd/teHM, discrepancies in the nuclear data for the $^{241}$Cm and $^{243}$Cm lead to a greater spread in participants’ $k_{\text{eff}}$ results. In addition, it was seen that inclusion of the curium isotopes in the fuel inventory can lead to an increase in the reactivity of the system of up to 1000 pcm. However, this was observed for MOX fuel only and not UOX fuel. It is therefore recommended that curium isotopes are included in the spent fuel composition of MOX fuel.

2.2.2. Phase IV-B Benchmark

Three types of models were used for the Phase IV-B Benchmark. These were, in order of increasing complexity, the fuel pin cell model, the assembly model and the super-cell (multi-assembly) model. In the following discussion, only the results of the super-cell model are presented since they represent the most complicated and realistic calculation model.

As predicted, the standard deviation in the $k_{\text{eff}}$ results calculated by the participants was seen to increase with both burn-up and cooling time. The relative standard deviations of $k_{\text{eff}}$ for first generation MOX and weapons disposition MOX fuels at the end of five years cooling were found to be 1.12% and 1.40%, respectively.

Concerning the reactivity swing, which is of most interest to the burn-up credit evaluation, the standard deviations of the total reactivity swing of fuel burn-up plus cooling time were found to be 5.3% and 5.2% for the first generation MOX and weapons disposition MOX fuels, respectively. The main contributor to the standard deviation was the burn-up of the fuel rather than the cooling time.

In order to try and identify the source of the deviations between the participants’ results, additional analyses were conducted. The analysis concentrated on the inventory prediction of the most dominant nuclide, $^{239}$Pu. The results of the analyses on the reactivity effect of $^{239}$Pu concluded that the variation of $^{239}$Pu nuclide densities among the participants’ results (9-10%) yielded a spread in the $k_{\text{eff}}$ results in the range of 3 to 4% depending on the calculation models and initial fuel compositions. However, this spread did not appear to depend on either the geometry of the system (pin cell, MOX assembly or MOX-UO$_2$ super-cell) or the type of MOX fuel used for the depletion calculation (first recycle MOX fuel or MOX derived from weapons grade plutonium).
Additional calculations were then performed, which increased the number of radial burn-up zones in the calculation model from 1 to 5 zones, however, no significant change in the $^{239}$Pu nuclide density was observed. Furthermore, reducing the burn-up steps in the calculation from 4 GWd/teHM to 2 GWd/teHM did not significantly change the $^{239}$Pu nuclide density calculated. It was therefore concluded that differences in the $^{239}$Pu nuclide density calculated by the various participants were not due to these two calculation modeling issues.

The figures in Phase IV-B Benchmark report (see Figure B.1 on pp. 68-69) show a representative result of the inventory calculations in terms of the Two-times Relative Standard Deviation (TRSD, %) for the super-cell model with the first recycle MOX fuel composition. It can be seen from these graphs that $^{234}$U (in particular for first recycle MOX fuel), $^{238}$Pu (in particular for weapons disposition MOX fuel) from the major actinides, and $^{237}$Np from the minor actinides generally show relatively large deviations, in terms of percentage difference relative to the mean. However, the large TRSD of $^{234}$U was significantly reduced when one contribution was excluded.

From the graphs of the participants’ results, it can also be seen that large values for the TRSD were seen for the fission products $^{155}$Gd, $^{109}$Ag and $^{103}$Rh. However, good agreement could be obtained for $^{109}$Ag if one contribution was excluded.

Considering both the actinides and fission products which had dominant effects on the $k_{\text{eff}}$ of the calculation models and which gave rise to large discrepancies in the nuclide density results, further improvement in the nuclear data libraries for $^{238}$U, $^{239}$Pu, $^{240}$Pu, $^{241}$Pu, $^{242}$Pu, $^{244}$Cm, $^{245}$Cm, $^{155}$Gd, $^{109}$Ag and $^{103}$Rh is recommended.

**Table 2.10. Calculation codes and nuclear data sources used in Phase IV Benchmarks**

<table>
<thead>
<tr>
<th>Method</th>
<th>Phase IV-A</th>
<th>Phase IV-B</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Criticality Code</td>
<td>Groups</td>
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<td>Deterministic</td>
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<td>137</td>
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<tr>
<td></td>
<td>APOLLO2</td>
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<td>SRAC95</td>
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<td>WIMS7B</td>
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<td>Monte Carlo</td>
<td>Code</td>
<td>Literature</td>
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<td>------------</td>
</tr>
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<td>ENDF/B-V, JEF2.2, JENDL-3.2</td>
</tr>
<tr>
<td>MONK, MONK7B</td>
<td>Point</td>
<td>JEF2.2, UKNDL</td>
</tr>
<tr>
<td>MVP, MVP94.1</td>
<td>Point</td>
<td>JENDL-3.2</td>
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<tr>
<td>TRIPOLI-4</td>
<td>Point</td>
<td>JEF2</td>
</tr>
</tbody>
</table>
3. Validating Burn-up Credit Criticality Summary

Alain Santamarina, Jim Gulliford

3.1. General

Validation of code schemes used in BUC assessment has two main components:

- validation of the depletion calculation for fuel in the reactor;
- validation of the $k_{\text{eff}}$ calculation for the spent fuel configuration.

Note that the two components may also be calculated using the same method (even in the same step under some code schemes).

More generally, functional testing of codes and their nuclear data libraries is also made. This normally includes numerical checks to verify that the processed cross-sections accurately represent the basic nuclear data. Further verification may be made through comparison with reference methods, such as continuous-energy Monte Carlo. Here we address validation, which is the demonstration of code accuracy by comparison with experiment.

Validation of depletion methods for BUC applications is normally made through comparisons with Post-Irradiation Examination (PIE) data for spent fuel. These experiments provide information on the isotopic composition of the spent fuel along with sufficient data on the fuel design, reactor conditions and irradiation history to allow precise modelling of fuel burn-up.

The code designer, the core designer and the reactor operator approach to depletion validation of depletion methods for core behaviour, including $k_{\text{eff}}$ and reactivity effects, is to use all available measurements, many of which are available as part of reactor operations. This approach may also provide useful additional evidence for validation of BUC depletion calculations.

For criticality assessments on fresh fuel, validation of methods used to calculate $k_{\text{eff}}$ has been based on comparison with critical benchmark experiments. There is a wide range of such experiments available, covering various types of geometry, enrichment, fuel-to-moderator ratio, fissile species etc. These generally provide enough data to allow rigorous derivation of code bias and uncertainty. For burnt fuel, there are few, if any such benchmarks available and validation has been made by comparison with other types of experiment, including small sample reactivity measurements, fuel substitution and chemical assay data. Evidence from calculations of the reactivity swing during operation of power reactors has also been used to support claims of code accuracy for BUC applications.

Some of the difficulties associated with the provision of validation for BUC have been avoided by claiming credit for only a limited set of isotopes in the fuel. In particular Actinide-only credit is attractive because it requires validation of only a limited set of actinides (mainly uranium and plutonium isotopes) for which PIE data are available to validate the depletion calculation. Similarly, MOX lattice critical experiments are available to validate the $k_{\text{eff}}$ calculation.
Meetings of the WPNCS BUC Expert Groups have provided a useful forum for the exchange of information on experimental programmes. This exchange allows lessons learnt to be shared among participants so that, where possible, experimental programmes can be developed to address outstanding issues. Much of the following material has been synthesised from these types of discussion at many meetings of the WPNCS BUC Expert Group.

3.2. Validation of depletion calculations for individual nuclides

PIE programmes provide the main sources of data for the validation of depletion calculations. These generally consist of chemical separation followed by mass spectrometry to derive the spent fuel concentrations of a set of isotopes. If detailed information on the fuel design, reactor conditions and irradiation history are also available, the data may be formed into a benchmark such that the burn-up can be modelled and concentrations of various isotopes in the spent fuel calculated. Comparison of the calculated and measured concentrations provides a quantitative test of the calculation accuracy. The level of burn-up of the fuel may be derived from the irradiation history, but it is also useful to include measurements in the PIE programme, which can be used to accurately determine this parameter.

In the past this type of analysis has been limited mainly to the actinides (often uranium and plutonium) and a small set of fission products (usually $^{148}$Nd, a commonly used ‘marker’ of fuel burn-up).

The growth in interest in BUC has stimulated the development of PIE programmes to produce data for a wider range of nuclides, particularly for fission products. An early activity of the expert group was to establish a set of fission products which might prove amenable to validation. These are: $^{103}$Rh, $^{133}$Cs, $^{148}$Nd, $^{149}$Nd, $^{155}$Gd, $^{95}$Mo, $^{99}$Tc, $^{101}$Ru, $^{109}$Ag, $^{147}$Sm, $^{149}$Sm, $^{150}$Sm, $^{151}$Sm, $^{152}$Sm and $^{153}$Eu. These 15 nuclides provide over 75% of the total fission product absorption in spent fuel and are radioactively stable, except $^{99}$Tc, which has a 5000-year half-life. Experimental programmes have subsequently been developed to provide PIE data for all these nuclides.

As noted earlier, progress reports from various international and national programmes have been a regular feature of the WPNCS BUC Expert Group meetings. These have included several major PIE programmes specifically aimed at providing validation for BUC calculation methods. A summary of some of the international programmes is given in Table 3.1.
<table>
<thead>
<tr>
<th>Programme</th>
<th>Ref.</th>
<th>Lead Institute(s)</th>
<th>Participating Nations</th>
<th>Fuel Type</th>
</tr>
</thead>
<tbody>
<tr>
<td>CERES</td>
<td>1</td>
<td>AEAT/CEA/SNL</td>
<td>France, UK, US</td>
<td>PWR, BWR</td>
</tr>
<tr>
<td>ARIANE</td>
<td>2</td>
<td>BelgoNucleaire</td>
<td>Belgium, France, Germany, UK, Japan</td>
<td>PWR, BWR, MOX.</td>
</tr>
<tr>
<td>MALIBU</td>
<td>3</td>
<td>BelgoNucleaire</td>
<td>Belgium, France, Japan, Sweden</td>
<td>PWR, BWR, MOX</td>
</tr>
<tr>
<td>REBUS</td>
<td>4</td>
<td>SCK•CEN</td>
<td>Belgium, France, Germany, Japan, US</td>
<td>PWR, BWR, MOX</td>
</tr>
<tr>
<td>PROTEUS</td>
<td>5</td>
<td>PSI</td>
<td>Switzerland, Germany (AREVA)</td>
<td></td>
</tr>
<tr>
<td>SFCOMPO</td>
<td>6</td>
<td>JAERI</td>
<td>Japan, NEA</td>
<td>Various</td>
</tr>
</tbody>
</table>

Japan is conducting PIE of 9x9 BWR fuels of burn-ups about 35 and 55 GWD/t and intends to measure about 30 nuclides of rare earth and metal FPs with high accuracy.

SFCOMPO is an extensive database of PIE data collated from various national and international programmes. Originally developed by the Japanese Atomic Energy Research Institute (JAERI), the database is now available through the NEA Data Bank. In addition, the WPNCS has established an Expert Group on Assay of Spent Nuclear Fuel. This group coordinates the development of SFCOMPO, establishes a state-of-the-art report identifying best practice in PIE measurement techniques and develops a better understanding of sources of uncertainty.

Overall, the consensus seems to be that experimental techniques for the separation of uranium and plutonium isotopes are well established and the data may be used with confidence. Participants report difficulties for some fission products, with inconsistencies between results from different laboratories. Experience with rhodium indicates that chemical analyses for this element are delicate with the possibility of significant systematic errors.

To date, most BUC applications have been for PWR UO$_2$ fuels and experimental coverage is better for this fuel type, although the REBUS and MALIBU programmes will significantly extend the dataset for BWR and MOX fuels. REBUS, MALIBU and PROTEUS will also significantly extend the burn-up range to above 60GWd/t. The French national programme will also provide PIE for high burn-up samples.

Participants report that current BUC requirements are reasonably well covered. An exception is for VVER fuel for which there is very little benchmark quality PIE data available in Eastern Europe. Nevertheless, in 2005 the results of a PIE project, funded under #2670 ISTC, were released by the USNRC.

For PWR UO$_2$ fuel, it is generally reported that modern code/data packages appear to predict the most important BUC nuclides well. Results for fission products may be less consistent, but this may be due to systematic errors in some experiments. A tendency for
calculations using JEF 2.2 data to slightly overpredict residual fissile content in PWR fuel ($^{235}\text{U}$, $^{239}\text{Pu}$ and $^{241}\text{Pu}$) has been reported by several participants.

Validation of burn-up credit calculations necessarily tests both analytical methods and nuclear data. In the case of $k_{\text{eff}}$ calculations, it is generally considered that methods uncertainties can be made negligible relative to the nuclear data uncertainties. For example, methods uncertainties using modern continuous-energy Monte Carlo codes are considered to be much less than 100 pcm, whereas nuclear data uncertainties using modern evaluated nuclear data libraries are considered to be approximately an order of magnitude larger. These uncertainties can be reduced via the validation effort provided adequate integral experiment data are available, (as is generally the case for fresh fuel). In the case of depletion calculations, it is generally understood that neither the methods uncertainties nor the nuclear data uncertainties can be made negligible. Furthermore, the quantification of these uncertainties, particularly the uncertainties due to nuclear data are much more complicated due to the reactivity feedback resulting from the unknown (calculated) isotopic compositions which are space-, energy-, time-, and nuclear data-dependent. Increasingly, the major nuclear data evaluation projects have attempted to meet these data needs, as illustrated by the inclusion of the limited integral measurements on separated fission products in the validation of the modern nuclear data libraries.

Increasing interest in sensitivity/uncertainty methods and uncertainty quantification points to the additional need for quality cross-section covariance data in the modern evaluated nuclear data libraries. Sensitivity calculations can estimate the reactivity effects of the isotopic components in irradiated fuel. This is helpful in prioritising the data needs for both differential and integral data in support of burn-up credit. Modern nuclear theory is now concentrating on methods to generate high-fidelity covariance data as an integral part of nuclear data evaluation. Availability of these data would allow forward error propagation to quantify uncertainties in isotopic components for which integral measurements are not available.

The last decade has seen significant development in depletion calculation methods, notably with the application of Monte Carlo techniques. While still at an early stage in the context of application to NPP calculations these methods in principle provide a means of further improving the accuracy of depletion calculations and separating out the effects of some modelling approximations.

### 3.3. Validation of $k_{\text{eff}}$ calculations related to individual nuclides

Whereas validation of depletion calculations has been achieved through extension of existing PIE measurement techniques, validation of criticality calculations for burnt fuel presents a particular challenge. There are few, if any (but see comments on use of power reactor data, later) criticality benchmark experiments for burnt fuel. The execution of a clean, well-defined critical experiment on burnt fuel presents significant difficulties, i.e.

- modification of spent fuel into form suitable for use in critical facility;
- relatively large amount of fuel needed to form critical assembly (particularly for high burn-up);
- requirement for extensive characterisation measurements;
- expense of transport to critical facilities;
- handling problems at critical facilities not designed to deal with highly irradiated material potential requirement for experiments to cover a wide range of fuel type, burn-
up, spent fuel environment (e.g. cask, storage pond, long-term storage facility, repository).

The difficulty and expense involved in carrying out such a programme of experiments has been a significant driving factor in the development of actinide-only credit, where validation can be based on critical experiments using MOX fuel. Several such experiments are available in the ICSBEP Handbook. The representativity of such experiments to BUC validation can be investigated quantitatively through the use of Sensitivity/Uncertainty (S/U) codes. Some such studies for MOX experiments for validating Actinide-only BUC suggest that additional sources of measured data may be required. Validation for fuel with burnable absorber may also require use of S/U methods to more rigorously demonstrate the applicability of available experimental data.

Given the problems associated with full-core critical experiments on burnt fuel, validation has been derived from several other types of experiment. These include:

- subcritical experiments on small numbers of spent fuel elements [Japanese exponential experiment];
- reactivity perturbation measurements on small samples of burnt fuel/actinide/separated fission products (e.g., PROTEUS, CERES);
- fuel substitution measurements on small bundles of burnt fuel (e.g., REBUS);
- critical experiments with separated fission products (e.g. Valduc BUC Programme, Sandia National Laboratory Rh foil measurements).

There are various pros and cons associated with each and some discussion of these has been made at WPNCs BUC Expert Group meetings. A brief summary is given below.

Reactivity perturbation experiments provide a means by which a large number of samples can be measured in a wide range of neutron spectra. Samples can be readily constructed from irradiated fuel, separated actinides and separated fission products. This provides experimental data to perform a check on various contributions to BUC. The experiments are particularly useful in validating the nuclear data used in criticality calculations. A drawback is that the experiments are not easily analysed using Monte Carlo methods, which carry an inherent statistical uncertainty associated with the random sampling, so that direct validation of this type of commonly used criticality code is not always possible. This may be achieved through intermediate verification against the deterministic code used to carry out the analysis of the reactivity perturbation experiment.

Fuel substitution experiments aim to provide sufficient reactivity change such that the measurements can be analysed using Monte Carlo methods. By substituting burnt for fresh fuel pins in a critical configuration, it is possible to produce reactivity changes in excess of 1% $\Delta k$. Typically, a bundle of roughly 20 or more pins are substituted at the centre of the core. Criticality is re-established by compensating the reactivity change associated with the substitution with a change to some other core parameter such as water height or radial core size. In validating the code it is therefore important to establish that the effect of the

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29. Subcritical experiments are gaining increasing acceptance and the ICSBEP Handbook now includes this type of benchmark. They offer a means of avoiding the use of large quantities of material and (with some interpretation) provide a benchmark amenable to direct analysis using Monte Carlo methods. They may also provide validation evidence at $k_{en}$ values more commonly encountered in criticality safety assessment, i.e. <0.95. On the other hand the measured parameter is not $k_{en}$ and some interpretation of the experiment is required to create a benchmark open to analysis by most criticality codes.
compensating change is well predicted. Having done that, the level of agreement seen when modelling the benchmark can then be ascribed to the accuracy of the code in predicting reactivity changes associated with burn-up. Diagnostic information on the code’s performance may be obtained through additional measurements such as reaction rate distributions and spectral indices. Another aspect of this type of measurement is the variation in fuel burn-up from pin to pin and axially over the height of the core (typically about 1m). To form a useful benchmark these variations should be well defined so that a complete 3D model can be established. Note that the effect of axial variation in burn-up on the measurement has little connection with the “end effect” for real spent fuel configurations. This is due to the limited length of the fuel pins and that the axial flux distribution in the experiment will be close to a cosine shape, very different from the skewed peak in flux seen in most spent fuel configurations.

Several experimental programmes have included critical measurements on configurations which include significant quantities of “separated” fission products. For $^{133}$Cs and $^{103}$Rh which occur at 100% abundance in the natural element this approach is particularly feasible. By including sufficient quantities of the material in the experiment, modelling of the critical configuration can provide a test of the code/data package’s ability to predict the reactivity worth of several of the most important contributors to BUC. If enough nuclides are validated it is possible to derive an estimate of the overall accuracy of BUC calculation methods. As for the other types of experiment it is important to understand how the neutronic effects contributing to reactivity change with burn-up vary between the experiment and “real” spent fuel configurations. For example, the experiments may use much higher concentrations of fission product than found in real spent fuel so that self-shielding will be an important factor in analysing the benchmark but much less important in the real configuration.

An additional source of information regarding the accuracy of predictions of spent fuel reactivity is available from power reactors, where fuel management tools usually include code schemes for detailed modelling of fuel burn-up. The ability of such codes to follow the evolution of the core reactivity balance (e.g. by following the critical soluble boron concentration in a PWR) provides evidence on the accuracy of modern codes and data. If a suitable point in the restart sequence of a commercial power reactor can be defined with sufficient precision then this might form the basis of a test of code accuracy for irradiated fuel configurations. A significant difficulty in using this type of data arises from how well the “experiment” conditions are known, particularly the burn-up (hence composition) of the irradiated part of the core. It is also important to understand how the effects of burn-up in the reactor configuration relate to burn-up effects for spent fuel following discharge (e.g. how the presence of fresh fuel effects the reactor calculations).

3.4. Direct validation of depletion calculations for irradiated fuel systems

Direct validation of $k_{\text{eff}}$ calculation methods relies on the availability of benchmarks. Such benchmarks have either been proprietary or extremely complicated for application to CS assessment. Recent efforts (NRC/ORNL, Yucca Mountain Project) discuss available published reactor data. Currently on-going efforts (EPRI/Studsvik) involve simplification of proprietary PWR 3D depletion measurements to publicly available 2D lattice physics $k_{\text{eff}}$ benchmarks for irradiated fuel. Other efforts (TVO, Finland) have started for BWR irradiated fuel benchmark creation.
3.5. Summary of lessons learnt

Overall it is concluded that a significant body of evidence has been accumulated to support claims of code accuracy for BUC applications. Results of analysis of various benchmarks (many of which are proprietary) indicate that modern code/data packages provide reliable predictions of spent fuel reactivity. This is supported by the generally consistent results seen for the range of calculation methods applied to the theoretical benchmarks studied by this group. The level of code bias and uncertainty indicated by the validation data set is a function of many variables, particularly the code/data scheme, reactor/fuel type, enrichment and burn-up. Also the level of confidence which can be applied varies with the number of applicable data points. Since many of the experimental programmes are not yet in the public domain, mechanisms for disseminating results for the validation of commonly used code/data packages are very valuable. The Expert Group on BUC has been an important example of how this can be realised. The Working Party on International Nuclear Data Evaluation Co-operation and the JEFF Project also provide a forum for feeding back the lessons learnt from new validation programmes through improvements to nuclear data libraries. Discussions at IAEA Technical Meetings on Burn-up Credit are a further useful medium for dissemination, as are various conferences and journals covering criticality safety, notably the ICNC.

In discussing the information presented at meetings of the BUC Experts Group some specific “lessons learnt” have been identified:

- Design and evaluation of benchmark experiments – the advantage of “clean”, well defined benchmarks has been highlighted. In particular, the experiment should be amenable to calculation without significant modelling approximations or assumptions and should include a complete and rigorous assessment of experimental uncertainty. The benchmark evaluation process used in the production of data for the ICSBEP handbook is felt to be an example of good practice in this area.

- Fission Product PIE – there have been some examples of inconsistent PIE results for some fission products. Chemical separation of spent fuel is known to be a delicate process, particularly for metallic fission products. Independent cross-checks of PIE measurements are therefore desirable.
4. Burn-up Credit for PWR Fuel – A Nuclear Criticality Safety Control Summary

Dennis Mennerdahl

4.1. Introduction

Burn-up credit is by definition a nuclear criticality safety control. It is a management option whether to apply burn-up credit or not in design and normal operation (if it is required for licensing purposes, it is not optional). It can be applied to increase a safety margin or to replace other criticality safety controls. During emergency conditions, burn-up credit may be a mandatory requirement.

This text focuses on safety aspects, relying on other texts to cover technical information required to complete a burn-up credit implementation. Such technical information includes the nuclear fuel, power reactor, fuel management, reactor operation, measurement methods and calculation methods for estimation of fuel transmutation (neutron transport and radioactive decay) and $k_{\text{eff}}$ determination for a specific application scenario.

4.2. Terminology

**Burn-up**

Burn-up is expressed as a volume-averaged specific energy (e.g. in MWd/kgU) produced by the fuel during reactor operation. Two materials with the same burn-up may have very different nuclide inventories and thus reactivities. Burn-up is thus not a sufficient specification to characterise the irradiated fuel. The neutron energy spectrum during reactor irradiation is essential. It is often implied by information on the fuel irradiation history.

**Transmutation**

When the fuel contributes to the reactor energy production, it is changed due to neutron transport and radioactive decay. After the reactor is shut down, the changes are limited to radioactive decay. Transmutation is the term used here to account both for neutron transport and radioactive decay. The term depletion is still more common but it is not an accurate or complete term.

**Criticality safety controls and operational controls**

There are two general types of controls. Criticality safety relies on a combination of criticality safety controls. During the design phase, these controls are optional. During the licensing phase, various combinations of the selected controls become mandatory.

Each criticality safety control may rely on one or more operational controls. Specific operational controls on parameters, instruments, etc. may be safety-related but are not necessarily covered by the term criticality safety control since they may have other functions and may acceptably fail partly or completely under certain conditions.

Examples of differences between safety and operational controls are:
• The required minimum burn-up of fuel in a configuration. The safety control (burn-up credit) may account for 15 MWd/kgU while the operational control may be set to a minimum of 30 MWd/kgU. The safety control accounts for the overall fuel properties and accounts for other parameters than burn-up, including uncertainties in the evaluation, measurements and records.

• The required minimum burnable absorber presence in a fuel rod. The safety control (burnable absorber credit) may account for 2.0 wt.% Gd$_2$O$_3$ while the operational controls may be set to a minimum of 3.0 wt.% Gd$_2$O$_3$. The number of burnable absorber rods per assembly may vary as well.

4.3. Scientific basis for burn-up credit

A reduction in $k_{\text{eff}}$ due to extensive transmutation of the fuel during and after reactor operation, has been theoretically explained and experimentally confirmed, at least in the reactor environment.

It would be very complicated to base burn-up credit outside the reactor core on reactivity measurements. Methods to do that are, however, available. Burn-up credit is thus normally based on calculations, using validated methods and supported by various types of measurements.

Burn-up credit accounts for some of the expected reduction in $k_{\text{eff}}$. The required accuracy and reliability in the methods depend on the application. Burn-up credit is thus a safety concept and not a physics constant or variable.

4.4. A graded approach to criticality safety, accounting for burn-up credit

Burn-up credit is a criticality safety control among others. General criticality safety standards and philosophy are not changed. Graded approaches are normally applied to criticality safety control, e.g.:

• Inherent material property controls. After being verified, burn-up credit may provide such a control, $^{235}$U enrichment is another control. Burnable absorber credit based on peak reactivity also fits under this approach.

• Passive hardware geometry controls. Examples are structures to assure a minimum spacing of fuel assemblies in storage racks or in transport cask baskets. Storage boxes that prevent fuel rod lattice expansion in cases of dropped fuel or transport casks are other examples.

• Passive neutron absorber controls. These may include water or neutron flux traps consisting of water and steel. Various materials containing boron are common.

• Active technical controls. Moderation control may be considered. Soluble boron at some low concentration may belong to this approach as well since it requires monitoring. Measurements to confirm the fuel composition, its degree of irradiation and cooling time may be required. Often such measurements have been performed during previous operations and only need verification.

• Active administrative controls. All of the previous approaches rely on administrative controls, before the actual operation is started. Controls during the actual operation are covered here. The potential for misloading may require active administrative controls. Verification that previous measurements have been carried out as required is an
administrative control. It may be required also during the actual operation and would then be an active control.

The final combination of criticality safety controls to be applied at a specific site or for a transport package design is a management decision. The licensing process determines whether it is sufficient for the intended operations. More than one alternative may be selected and licensed.

Implementation of burn-up credit changes the evaluated system. Screening the fuel inventory from assemblies with no or low burn-up reduces \( k_{\text{eff}} \). If there are no other changes than burn-up credit, that system will have a higher safety margin. If the burn-up credit is implemented as a safety control that replaces some other safety control, the safety margin may be reduced, increased or remain essentially unchanged.

Burn-up credit as a safety control is similar to absorber credit and other safety controls. A fixed absorber may be present without being accounted for. In that case it is not a safety control. The same applies to the presence of irradiated fuel where irradiation (burn-up) is not accounted for. It is not a safety control and it may be disastrous to assume that there is an extra safety margin without really evaluating that properly.

4.5. Burnable absorber credit is not burn-up credit

Presence of burnable absorbers in PWR fuel may lead to an increase of \( k_{\text{eff}} \) due to the combined transmutation of the fuel constituents (fissile and fertile nuclides as well as burnable absorber nuclides).

Accounting for burnable absorbers is an established safety control, referred to as burnable absorber credit. This is usually associated with BWR fuel but applies to many PWR fuel types as well, in particular under emergency conditions. For fresh fuel, the burnable absorber credit, measured in \( \Delta k_{\text{eff}} \), is very large. Even if there is no increase in \( k_{\text{eff}} \) due to transmutation, this needs to be demonstrated, when credible.

Burnable absorber credit requires assurance that the absorber is not removed or damaged to an extent that it loses its absorption function. The burn-up level is irrelevant if peak reactivity is the basis for the credit.

Burnable absorber credit for fuel that may have been irradiated requires assessment of fuel transmutation. Burn-up credit is an optional accounting for fuel transmutation. Related to assessment of transmutation, the two control methods are thus fundamentally different.

Burnable absorber credit and burn-up credit assessment methods are often discussed together. The reasons are that transmutation is a complicated process and that the methods are similar. The two credit types may also be combined, typically applying burnable absorber credit for fresh low-burn-up fuel and burn-up credit for higher burn-up values.
4.6. Safety under emergency conditions

It may be conservative to over-estimate $k_{\text{eff}}$ in a safety report. However, under emergency conditions such conservative assumptions can cause substantial harm to humans and to the environment. Preparedness for assessment of realistic conditions should be considered at every site.

When burn-up credit is applied, some of the needed information is already available, both the actual fuel properties, the calculation methods and perhaps even results. Realistic evaluations are thus easier than if only fresh fuel has been accounted for.

Even if burn-up credit is not implemented, accurate information on the fuel nuclide inventory for each fuel assembly may become extremely valuable in an emergency situation. Being able to flood a spent fuel pool with unborated water, even though it is only designed to be subcritical for some minimum boron concentration, without any criticality concerns could be extremely valuable knowledge.

4.7. Dependence on administrative controls in burn-up credit applications

In criticality safety, dependence on administrative controls is often avoided, in particular during operation (active controls). Burn-up credit requires some administrative controls for verification of the fuel properties and for identification of the fuel, before being transferred to a new position. Any movement of the fuel may require such controls. If all the fuel has been verified to comply with the requirements, the active administrative controls may be reduced.

Maybe surprisingly to some criticality safety specialists, burn-up credit may thus reduce the need for administrative controls during operation. The number of different bounding fuel designs may decrease, enrichment control may become irrelevant, number of burnable absorber rods and their specifications may become irrelevant, fuel with removed or damaged rods may be a non-issue, etc. It may be sufficient to verify the fuel history and its identity before moving it to a new facility or transport cask.

Burnable absorber credit is most advantageous for fresh fuel and during the first reactor cycle with that fuel assembly. After that, burn-up credit can replace burnable absorber credit and reduce the administrative controls.

4.8. Reactivity prediction and not necessarily nuclide inventory determination

For burn-up credit in storage and transport of PWR fuel assemblies, the detailed nuclide inventory is not necessarily required. The material properties are needed, not the individual constituents. In technical terms, the macroscopic cross-sections for the material or lattice need to be adequate.

Further, heterogeneous lattices of fuel rods in a fuel assembly may be homogenised, using appropriate methods. That is not only a useful criticality safety approach but the normal procedure for reactor design, operation and safety assessment. That procedure is validated daily at all operating nuclear power reactors.

The selection of actinide nuclides to be accounted for may be based on element reactivity rather than the reactivities of individual nuclides. Of particular interest may be that the curium element in irradiated fuel may have a positive reactivity effect, e.g. for some PWR MOX fuel. This was observed in the NEA infinite fuel rod study of Phase IV-A [3].
4.9. Neutron energy spectrum

To evaluate the criticality safety of a scenario, the fuel properties must be simulated adequately by the calculation method. It is not sufficient to have $k_{\text{eff}}$ for benchmarks calculated accurately if the benchmarks and the analysed scenario are not very similar. An essential variable is the neutron flux spectrum during transmutation of the fuel in the operating reactor.

The calculation methods and their validation are described in other chapters. It is, however, essential for the criticality safety evaluator to understand the importance of this issue. New fuel designs or modified reactor operating procedures may change the fuel properties significantly. The impact on reactor operation may be small but the criticality safety impact may be large.

The main point here may be that burn-up, expressed as an integral specific energy (e.g. in MWd/kgU) produced by the fuel, is not a complete specification. Two materials with the same burn-up may have very different reactivities.

In some cases surrounding fuel assemblies and control rods have large effects on the fuel properties in a particular fuel assembly zone. One complication is if there is MOX (mixed oxides of plutonium and uranium) fuel in the neighbouring fuel assemblies. This is known to change the spectrum compared with a pure uranium fuelled reactor core.

There are many NUREG reports prepared by ORNL [4] as well as NEA studies [3] that demonstrate the influences of different neutron energy spectra during transmutation.

4.10. Axial and radial effects

Probably as long as burn-up credit has been considered, the axial variation has been noted. Burn-up credit applications, at least since the late 1970s, have been required to account for the influence of axial burn-up variations. Radial variations include overall assembly effects as well as local fuel pellet effects.

The reactivity effects of realistic axial burn-up distributions compared with an average burn-up distribution can be large. The effect is application-dependent. There is, however, no single axial profile that will be bounding for all scenarios if the total burn-up is preserved. An obvious example would be for dry storage where the only credible moderation scenario involves adding water to a quarter of the container height. A profile optimising the fuel reactivity at the top would then not be appropriate. Other scenarios may increase the importance of the central fuel region.

A conservative burn-up profile to be used for all evaluations could be prepared. In that case the total burn-up of that fuel assembly would be lower than the nominal burn-up. The burn-up values in different zones could be reduced and the profile obtained would be applied, without normalisation to the estimated integral burn-up value for the assembly.

There are many NEA studies [3], NUREG reports [4] and other studies that demonstrate the influences of different axial burn-up distributions.
4.11. Fission source convergence

This issue is more general than burn-up credit but has been observed during burn-up credit studies. It has also been observed in safety reports for spent fuel storage, applying fresh fuel assumptions.

During hot conditions at full power of reactor operation, the global neutron flux is quite flat over large regions. The neutron leakage at the top and bottom of the fuel reduces the burn-up in these regions. Higher water temperature at the top of the fuel hardens the neutron energy spectrum. The result is larger plutonium production and thus less burning of $^{235}$U for the same burn-up.

When such fuel is moved to fuel storage or transport casks under cold water conditions, the more reactive fuel regions near the top of the assembly may dominate the fission source completely.

Traditional calculation methods can solve such problems. The standard input parameters, however, may need to be modified to allow proper convergence of the fission source. In Monte Carlo calculations this means that more neutron histories need to be tracked to find an adequate source distribution. The “transient” phase of the calculation, before the source is converged, should not be included in the statistical compilation of results.

The NEA burn-up credit [3] and source convergence [5] expert groups have studied this issue quite extensively. A new Advanced Monte Carlo Techniques (AMCT) Expert Group continues with related studies. A major objective is to find recommendations for calculations of complicated problems, such as large power reactors.

A quote from the Foreword to the NEA Phase II-C report [6]:

*It is important to recognise that in a Monte Carlo calculation there are two types of convergence one needs to achieve. The first is fission source iteration convergence (colloquially referred to as source convergence) i.e. the convergence of outer iterations one achieves by skipping generations. Failure to converge the fission source results in a bias that depends on the initial source, since the effect of the outer iterations is to reduce the contamination of the fission distribution with the (necessarily) erroneous components of the initial source.*

This is basically correct; failure to converge the fission source, before starting the tally of fission sites, results in a bias due to contamination with the erroneous initial source. Unfortunately, the following paragraph of the Foreword rejects the most accurate results of the Phase II-C study:

*For the Phase II-C benchmark, zero estimates are very likely to be the result of poor statistical convergence (insufficient tracking), not incomplete fission source iteration convergence. This is imprecision, not a bias in the calculated result. As has been pointed out for this benchmark exercise, there is (physically) fission in all axial locations, however sparse or infrequent. A zero estimate could, in principle, be caused by non-convergence of either type.*

This conclusion is not correct. The benchmark model includes no fissions at all; it is a subcritical system with no neutron source from radioactive decay. The participants selected to use Monte Carlo methods with a few million neutron histories. The fission probability, normalised to one fission neutron, in some lower regions was sometimes $10^{-7}$ and below. With a few million total neutron histories, the expected number of fissions should be zero.
Other studies have later demonstrated that, for small regions, very loosely coupled to the fission source peak region, the number of fissions may of course be zero. The Phase II-C report instead contains evidence of contamination of the results by the initial source, (see Figure 4.1). Some results have large values for the fission numbers in regions where there should not be any in a converged calculation. The participants were not requested to and did not intend to provide accurate results for insignificant regions.

The Phase II-C report (appendix V) explains:

*Therefore, the recorded axial fission density distributions which show zero fission densities in some region of the fuel zone are not really converged and hence not acceptable for the investigation of the impact of the asymmetry of axial burn-up profiles on the fission density distribution. Consequently, only those of the recorded axial fission density distributions are considered which are different from zero in all axial zones over the full active length of the fuel.*

**Figure 4.1. NEA BUC results from Phase II-C contributors**

![Fission Density Distribution](image)

**Figure 4.2. Recalculations by the Phase II-C report author**

![Fission Density Distributions Related to the Axial Burn-up Distributions with 50\% of the Average Burn-up](image)
The best results (many initial generations skipped, many active generations) are thus rejected, while the worst (few initial generations skipped, few active generations) are retained. Figure 4.2 shows revised results by the author of the report, using slightly better statistics.

Appendix VII of the Phase II-C presents a reservation to the views presented in the report and in the Foreword. Figure 4.3 is based on 475 million active neutrons, with 25 million passive (skipped) neutrons. The skipped neutrons are more than the total number of neutron histories in any calculation in Figure 4.1. There were zero fission densities in some of the cases. Since the scale is logarithmic, the zero fission densities in the chart were set to one fission in that zone.

The fission density distribution of Figures 4.1-4.3 would not be credible in an operating power reactor. An overestimation of the fission density in a reactor simulation, intended to determine the transmutation in the fuel, may lead to a serious underestimation of the $k_{eff}$ in a criticality safety evaluation. The burn-up would be too high.

**Figure 4.3. NEA BUC Phase II-C: Results by (prompt) critical participant**

There are also convergence tests and other recommendations that express the need to avoid regions with zero fissions. Eventually the Phase II-C, as well as the mentioned tests and recommendations, need to be reconsidered. Zero fissions can always be obtained in any problem by dividing the geometry into smaller regions. That would not reduce the accuracy or convergence of the solution, rather the opposite (more information, related to the discussion on symmetry).

There are many studies and here the NEA Burn-up Credit Expert Group Phases II-B [7] and II-C [6] are of particular interest.

### 4.12. Reactivity equivalencing

Reactivity equivalencing is a common method in criticality safety. It can be based on measurements and such methods have been developed for burn-up credit purposes. Such measurement methods are usually too complicated and may involve additional radiation hazards. Validated calculation methods are often applied but reactivity equivalencing may still be a difficult approach for some systems.
Different fuel assemblies with identical reactor lattice $k_{eff}$ values may result in very different $k_{eff}$ values in a storage lattice scenario. Due to transmutation, no fuel assembly has an identical nuclide inventory as another assembly even if they were identical before irradiation. This should be considered in a safety evaluation.

Reactivity equivalencing, with the two examples of burn-up credit (Section 4.1) and IFBA credit (Section 4.2) are described in [1]. Two NRC documents [8,9] discuss recognised complications with reactivity equivalencing.

4.13. Mixing different fuel designs

This issue may be viewed as a special case of reactivity equivalencing. Two different fuel designs, in particular if they have significantly different outer geometry specifications, may have identical $k_{eff}$ values in the same storage facility. The larger fuel assembly design may be subcritical due to burn-up while the smaller design may be subcritical due to neutron flux traps (e.g. water combined with steel plates). In a mixed configuration, the neutron flux traps may lose some or even most of their function. The mixed configuration may be intentional, an incident or an administrative mistake.

The problem may apply to mixing of fuel designs having different $k_{eff}$ values as well if some kind of index method based on fraction of some subcritical value is applied. An established method used in transport of fissile material, the Criticality Safety Index (CSI) does not account for mixing of different designs. The CSI method is sometimes adapted to storage of fissile materials in facilities and that may have a questionable basis.

Problems with mixing different fuel designs have a lot in common with other reactivity equivalencing. A point in case is mixing fuel assemblies with different dimensions.

4.14. Combination of effects

Reactivity effects do not in general accumulate linearly. The combined effect may be smaller or larger than the sum (integral) of the reactivities. Several individual local variations may each shift the fission source distribution significantly without causing a large reactivity effect. If they shift the distribution in different directions the combined effect may be small. If each variation shifts the distribution in the same direction, the result may be much larger than the sum of each shift.

The NEA Burn-up Credit Phase II-B report [7] contains an Appendix IV that demonstrates a much larger total positive reactivity than the sum of the individual reactivities. That effect involved burn-up credit and an axial region with no neutron absorber.

The left model in Figure 4.1, with cases A and B, represents nominal Phase II-B cask geometry with irradiated PWR fuel. Case A has a uniform axial burn-up distribution while Case B has a typical axial burn-up shape. The right model in Figure 4.1, with cases X1 and X2, has a perturbation of the nominal geometry by having the boron removed from the top 20 cm of the active fuel region and above. The yellow pattern near the top of the fuel is just text specifying the fuel as PWR. Case X1 corresponds to Case A, by having a uniform axial burn-up profile, while Case X2 corresponds to Case B with a typical axial burn-up profile.

In the nominal geometry, the uniform burn-up (Case A) and the typical axial burn-up (Case B) distributions result in identical values of $k_{eff}$, (see Table 4.1). The removal of the boron alone (Case X1) increases the nominal $k_{eff}$ by 0.0374 (from 0.8900 to 0.9274) for the uniform burn-up distribution, (see Table 4.2). If the “end effect” conclusion from the nominal case was applied, the increase in $k_{eff}$ for the typical axial burn-up distribution in Case X2
should be the same, or 0.0374. The calculation result is an additional increase of 0.0766, or a total increase in $k_{\text{eff}}$ of 0.1140. It is easy to find larger effects.

Similar scenarios are credible in real applications. As soon as Appendix IV of Phase II-B was recognised, it caused within a year actual revisions of safety reports and procedures for some transport cask designs, previously internationally approved.

Figure 4.4. NEA BUC Phase II-B

Table 4.1. Phase II-B cases A and B

<table>
<thead>
<tr>
<th>Problem</th>
<th>$k_{\text{eff}}$</th>
<th>$\sigma$</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>0.8900</td>
<td>0.0020</td>
</tr>
<tr>
<td>B</td>
<td>0.8900</td>
<td>0.0008</td>
</tr>
<tr>
<td>$\Delta k$</td>
<td>0.0000</td>
<td>0.0022</td>
</tr>
</tbody>
</table>
Another scenario is a dropped PWR fuel assembly, causing the lower lattice region, between spacers (grids), to expand significantly in the storage or transport cask position. Applying burn-up credit, this would shift the fission source from the top to the bottom of the fuel. Even though the bottom part is slightly less reactive, the combination of burn-up credit and local fuel expansion may cause a significantly larger positive reactivity than the expansion of the same region for fresh fuel. This is also an example where an axial burn-up profile shifted towards the bottom may be non-conservative.

### Table 4.2. Phase II-B cases X1 and X2

<table>
<thead>
<tr>
<th>Problem</th>
<th>$k_{\text{eff}}$</th>
<th>$\sigma$</th>
</tr>
</thead>
<tbody>
<tr>
<td>X1</td>
<td>0.9274</td>
<td>0.0012</td>
</tr>
<tr>
<td>X2</td>
<td>1.0040</td>
<td>0.0012</td>
</tr>
<tr>
<td>$\Delta k$</td>
<td>0.0766</td>
<td>0.0017</td>
</tr>
</tbody>
</table>

4.15. Specific calculation method issues

- **Lumped fission products**: Traditional reactor core simulation has relied on cross-sections for lumped fission products rather than for individual fission products. The criticality safety specialists appear not to have adopted the idea of lumped fission products, as evidenced by NEA studies. Recent developments [11] (NRC SFST ISG 8 R3) has introduced a technique that is essentially equivalent to lumped fission products. The validation of the cross-sections is based on the integral bias and uncertainty of all nuclides. Large positive and large negative biases thus cancel each other out.

- **Symmetry in Monte Carlo calculation models**: Often calculation models of real systems with fissile material are symmetrical (reality is never perfectly symmetrical). Historically, there has been an advantage in accounting for the symmetry in Monte Carlo calculations by reducing the geometry along the symmetry lines. The advantage is that the calculation requires less computer memory. This reduced model is referred to below as the “symmetric model” while the complete model is referred to as the “full model”.

Recently, the notion that symmetry speeds up, or improves, convergence of Monte Carlo calculations has become popular. If the neutron tracking simulates reality correctly, every neutron collision in the symmetric model should be identical to that in the full geometry model.

The calculations are thus identical, the only difference is that the results for the full model are more detailed. If only the integral value of $k_{\text{eff}}$ is requested, the results should be identical, with identical uncertainties and convergence test results. If the average value of some reaction rate or ratio is requested over some specific regions (symmetric or not), the information is available in the full model results even if the average is not provided directly by the code. An asymmetric solution to a symmetric geometry can be observed and the adequacy of the solution can be checked.
For the symmetric model, the average value for symmetric regions may be provided by
the code but it is still identical to the average results from the full model calculations.
The asymmetric problems that could be observed in the full model calculations are
present in the symmetric model calculations but are much more difficult to observe, if
possible at all.

The conclusion is that, at least for criticality safety evaluation, use of a full geometry
model is preferable to a reduced model accounting for symmetry. Even for an infinite
lattice, e.g. fuel assemblies in a storage rack or an infinite number of transport packages,
inclusion of more than one unit is recommended to be able to recognise any unexpected
behaviour of the calculated neutron flux (not only fissions are of interest).

4.16. Reactivity benchmark measurements and fuel sample assay data verification

Burn-up credit for PWR storage and transport does not require accurate nuclide inventories.

Even if the detailed nuclide inventory and adequate microscopic cross-sections are
available, the macroscopic cross-sections are still needed to validate the burn-up credit method.
A burn-up credit benchmark needs to be integral rather than a combination of verifications and
reasoned argument.

Fuel sample radiochemical analysis is valuable as a complement to integral reactivity
measurements. For applications that may require individual nuclide validation, e.g. shielding,
final disposal, etc. the fuel sample assay data measurements are valuable. The reactor
operating history still needs to be documented and simulated adequately.

The sample burn-up and the average neutron energy spectrum during irradiation in the
reactor can perhaps be more accurately determined from the measurement results than from the
reactor history. This is not sufficient for application to burn-up credit when the fuel history is
based on reactor records. It is not so difficult to accurately calculate the fuel inventory of a
fraction of a fuel pellet if the burn-up and neutron energy spectrum are determined from the
same sample.

The use of radiochemical analysis results from irradiated fuel samples is perhaps similar to
the measurement of cross-sections. Cross-sections are measured and their uncertainties
(covariances) are determined. Calculation methods applying those cross-sections and
covariances are demonstrated to provide good results by comparing with calculations of $k_{eff}$
benchmarks based on integral experiments.

Nuclide abundances in several fuel samples are measured and the results are treated
statistically to determine best-estimate values and uncertainties. We can verify the
“microscopic” transmutation process, including cross-sections and decay data.

Simulation of irradiation of a fuel pellet fraction in a known neutron energy spectrum to a
specific burn-up level is basically a cross-section evaluation rather than a “macroscopic”
transmutation evaluation for the complicated operation of a nuclear reactor.

Reactivity measurements of irradiated fuel samples or of simulated irradiated fuel samples
are also valuable but limited to verification purposes.
For bounding, conservative burn-up credit applications verifications based on results of radiochemical analysis and sample reactivity measurements may be sufficient. For more realistic estimation of the influence of reactor transmutation of fuel on criticality safety margins, actual reactor operation measurements are required and the results need to be documented in an appropriate form.

4.17. Information on actual reactor operation and associated fuel histories

Burn-up credit is an option for design and routine operation of storage racks, transport casks, final disposal and other facilities. The better and more reliable information on the fuel that can be obtained, the more efficient the burn-up credit can be.

What is needed for best-estimate burn-up credit is integral measurement benchmarks of transmutation in nuclear power reactors. What information is required to simulate the transmutation and how well can it be simulated using that information? For criticality safety, we are interested in $k_{eff}$ of an application system and not necessarily in the detailed nuclide inventory of every region of a fuel assembly.

Even if best-estimate burn-up credit, accounting for uncertainties, is possible, it does not need to be applied.

To understand potential error sources, it is important to have information on past, current and planned reactor design and operation. What information is required to assure adequate safety under all credible conditions, including emergency conditions?

The reactor operator performs measurements and calculations, validated by measurements, which result in a fuel irradiation history that is recorded by the operator. A great advantage is that the measurements involve all fuel at all times. They are needed and applied to routine operation of the reactor. Some of them are also applied to demonstrate safe reactor operation to the regulator. How reliable and accurate are those records? Can they be improved to support burn-up credit even better?

Several efforts have been made by various organisations, e.g. the Yucca Mountain Project (YMP), Oak Ridge National Laboratory (ORNL) and the Electric Power Research Institute (EPRI), to obtain routine operation power reactor measurement data and to apply them as benchmarks for validation of burn-up credit methods.

In the past, the measurements and calculations of the reactor operator have been accounted for to validate the methods used in burnable absorber credit and in burn-up credit. Since reactor core physics methods have now become more widely available and can run on inexpensive computers, the need for measurement-based benchmarks for validation has become apparent.

The proprietary nature of the measurements is an obstacle. It is however possible to simplify the measurements into benchmarks that remove any proprietary information on fuel and reactor designs as well on reactor operation. The EPRI depletion reactivity benchmarks published in 2011 [12] are excellent examples of what can be done. Many of the “commercial reactor criticals” (CRCs) that have been publicly released and calculated by YMP and ORNL have required very large efforts to model. It should be possible to simplify those measurements to obtain accurate experiment benchmarks requiring less effort to model without losing information value. The IRPhE Handbook [13] may be a suitable target for such efforts.
In addition to the value of the benchmarks in themselves, the evaluations of the measurements provide extremely valuable information on power reactor operation. This is evident from reports on the EPRI depletion benchmarks.

4.18. New types of error sources in the use of calculation methods

Transmutation calculations (“depletion” and radioactive decay simulation) often result in a result for a fixed time after the shut-down of the reactor using that fuel assembly. The effect of radioactive decay can easily be calculated later for specific decay periods. An error that has been observed is the failure to remove $^{135}$Xe from the nuclide inventory at reactor shut-down when this is required by the method. There are other examples where “small” input errors or incorrect interpretation of the results can be serious to safety.

The most reliable methods for evaluating the transmutation of fuel in a reactor would be those that are applied and validated daily at various reactor sites. Deviations between measurements and calculation results would be investigated immediately, before criticality safety becomes an issue. When such methods are applied to criticality safety scenarios outside the reactor core, further validation and verification are needed.

An example of an observed problem (many years ago) is the use of a lattice physics code, developed for reactor core management, to evaluate a storage configuration. The lattice physics code had a fixed mesh (“hard-coded”) for the regions between the assemblies. This mesh was not adequate for the wider and more complicated regions in the storage configuration. Modern lattice physics codes do not have this limitation. A method that requires setting the $^{135}$Xe density to zero is referred to in [1].

4.19. Verification of the fuel nuclear properties

Burn-up credit requires determination and verification of some of the fuel nuclear properties. Unlike for fresh fuel, a direct determination is not practical, even though some measurements can be used to verify some parameters. Instead, the fresh fuel properties together with the fuel history (reactor design, operation, measurements, cooling time) can be used to determine the fuel properties.

Reactor operation and non-proliferation control require accurate identification of each fuel assembly from arrival to departure from the reactor site. Markings on the assemblies together with sophisticated accounting systems support correct selection of the intended assemblies.

Additional measurements on irradiated fuel, justified by burn-up credit only, involve hazards on their own. Measurements can also be justified for other purposes such as radiation protection, non-proliferation control, waste management and heat generation control.

Even when measurements have been performed, identification of each fuel assembly is required to avoid “misloading”, i.e. placing another fuel assembly than what is intended in a specific location. The NRC SFST ISG-8 Rev.3 [11] contains guidance on verification of fuel assemblies.
4.20. Misloading

Misloading fuel with low or no burn-up into positions where higher burn-up is required is a potential problem. This problem is different from the issue of determining fuel properties at some time after reactor operation. Misloading is not unique to burn-up credit, it applies to fresh fuel with different restrictions for different $^{235}\text{U}$ enrichments and to burnable absorber credit. Misloading fuel in a PWR reactor can also involve rotation of PWR fuel assemblies but this is normally accounted for in a criticality safety evaluation. The NRC SFST ISG-8 Rev.3 [11] contains guidance on misloading.

4.21. Safety experience from NEA burn-up credit studies

The NEA activities related to burn-up credit [3] are described elsewhere but some specific experiences related to safety, as opposed to method development and testing are mentioned here. The activities primarily involve exercises of comparison of calculation methods in different countries and organisations.

  - The United States around 1976 proposed two criticality safety topics for the Nuclear Energy Agency (NEA). Both topics were related to the need to evaluate the criticality safety during transport of spent nuclear fuel.
    - One topic was development of a “Standardised Cask-Analysis for Licensing Evaluation” (SCALE) calculation system for performing criticality, shielding and heat transfer analysis. The primary effort was directed towards safety analyses of nuclear fuel shipping containers. Even though burn-up credit was not yet proposed, methods to determine source terms for shielding and heat transfer were specifically requested. This project was not included in the NEA programme but was initiated and funded by the Nuclear Regulatory Commission (NRC). SCALE continues to be supported and many options for burn-up credit evaluation are maintained and new ones are being added. The other topic, proposed by the US Department of Energy (DOE), was a comparison of calculation methods for criticality safety evaluation of spent fuel casks. This was eventually accepted by the NEA and its Committee on Safety of Nuclear Installations (CSNI). It was carried out during 1980 and 1981.
  - Fresh fuel critical benchmarks were selected from published reports. Their quality and the error source correlations between the benchmarks were discussed. Theoretical spent fuel cask models, with 7 PWR fuel assemblies in water and with thick lead or steel walls, were selected for realistic simulation of transport casks.
    - Calculation methods included typical criticality safety methods as well as reactor core management methods. The 2D lattice physics code CASMO was used to generate homogenised regions for a diffusion code, DIXY. Another 2D lattice physics code PHOENIX was used to generate homogenised cross-sections for KENO. Homogenisation of quite large fuel assembly regions is applied in modern calculation methods for reactor core simulation.
      - The CASMO code was used as a “reactivity meter” in the EPRI depletion benchmarks evaluation [12] and the PHOENIX-P code (a development of the PHOENIX code referred to above) was used in [1].
A majority conclusion, after much discussion, was that diffusion theory codes were not appropriate for criticality safety application. That conclusion was not based on results of comparisons but on other experience by some of the participants. Diffusion theory for reactor core simulation was necessary at that time and continues to be used in modern calculation methods.

**NEA Initial burn-up credit studies, 1991-1993**

- An informal proposal to study burn-up credit was made by the working group chairman (Elliott Whitesides) during the June 1989 meeting. It was supported by many of the participants. The direct work with burn-up credit started in 1991. NEA support had shifted, from CSNI, via the Committee on Reactor Physics (NEA/CRP), to the Nuclear Science Committee (NSC) where it still belongs. The focus is on methods but general criticality safety considerations are covered, in co-operation with CSNI and other NEA committees.
- A conclusion from early studies was that the participants’ $k_{eff}$ results for fresh fuel often varied more than for irradiated fuel.
- The working group focused on determining the nuclide inventory rather than on reactivity. Some early industry participants used production methods, such as Studsvik using CASMO, which relied on lumped fission products. This was an established, validated and approved method for reactor design and safety. Due to the lack of some individual fission products, Studsvik was not encouraged to continue its participation.
- Following the recommendation from the initial 1980-1981 comparison study, diffusion codes and lumped fission products were not used by participants.

**Axial burn-up distribution studies 1994-2008**

- During the 1990s, the idea of a bias to account for the axial variation of burn-up and irradiation spectra, and thus also the nuclide inventory and reactivity (the “end effect”), was popular. Phase II-B [7] of the working group demonstrated that the use of a general bias would be difficult since it could be very large under certain conditions. Eventually, this bias idea appears to have been dropped and replaced by representative axial burn-up profiles.
- The Phase II-B resulted in essential information about the complications of obtaining source convergence in a large transport cask for spent fuel. The difference from hot operating reactor conditions to cold storage conditions was dramatic. Hot conditions in reactor geometry increase the coupling between fuel assemblies as well as between the top and bottom regions of the fuel. Under cold conditions and with fuel assemblies more separated than in the reactor, the local reactivity becomes dominant due to the axial burn-up distribution. The fission source in many scenarios becomes limited to a small region near the top of the fuel.
- A substantial contribution was made by the German industry for Phase II-C [6] by providing realistic axial burn-up profiles based on actual PWR measurements.
• Source convergence
  – The source convergence problem in Phase II-B [7] was one of the reasons for the creation of a new expert group on source convergence. It included some burn-up credit models in its studies.
  – Source convergence was a hot topic in the Phase II-C [5] study, some years later. With a fission source peak near the top of the fuel, how important is the fission source near the bottom of the fuel and how can convergence in that region be determined? The Monte Carlo methods used for these problems typically included a few million neutron histories.
  – This issue continues to be discussed in new NEA studies, e.g. in a recently started Expert Group on Advanced Monte Carlo Techniques.

• Burn-up credit benchmark experiments
  – NEA is involved in many studies related to burn-up credit, including benchmarks for use in burn-up credit and other areas requiring determination of irradiated fuel inventories. Three of the expert groups or projects supported by the NSC are covered here. In addition, many of the reactor and nuclear data studies are of direct interest for burn-up credit evaluation.
  – SFCOMPO and the Expert Group on Assay Data for Spent Nuclear Fuel (ADSNF) [3]. SFCOMPO started in the 1990s as a Japanese effort to compile published (open) fuel sample measurement results for PWRs and BWRs. SFCOMPO was after a few years offered to NEA where it was maintained. The new expert group created in 2006 is described separately. The ADSNF Expert Group has generated interest from the nuclear industry, leading to measurements, evaluation and publication for new irradiated fuel samples. Significant efforts are made to provide guidance and establish formats for documenting benchmark measurements.
  – The IRPhE Handbook [13] contains a modified version of the EPRI depletion reactivity benchmarks [12]. They are based on actual PWR operation and measurements, leading to much more reliable data than simple $k_{\text{eff}}$ benchmark experiments or irradiated fuel sample measurements. In addition to the benchmark themselves, the basis is valuable to describe measurement and calculation methods applied at PWRs. This will help to understand and accept records for the fuel irradiation history as well as to identify potential problems in such records or in the operations behind.
  – The IRPhE Handbook contains other measurements that may be useful in burn-up credit. The transition from hot reactor conditions to cold storage conditions is one of the areas where such benchmarks may be available. In 2014, a new evaluation of irradiated fuel sample oscillation measurements in the research reactor MINERVE at Cadarache was expected. Associated measurements at the UK research reactor Dimple are expected to follow soon. Both sets of measurements have been proprietary and are only now being released to the public.
4.22. IAEA, NRC and other burn-up credit efforts

IAEA workshops on burn-up credit held in 1997, 2000, 2002, 2005, 2009, 2011 provide essential information on burn-up credit methods and implementation in different countries.

4.23. Nuclear power industry support in burn-up credit benchmark efforts

- The EPRI benchmarks [12] provide a very important contribution to burn-up credit and serves as an example for what the industry can do when motivated. Radiochemical measurements of irradiated fuel samples are valuable as an additional support.

- The Finnish utility TVO has published [15] work on simplifying cold condition reactivity measurements typically made for BWR every year. It is not clear whether such benchmarks will be published but just the information that it is possible with reasonable efforts is valuable. Global Nuclear Fuel (GNF) has presented some ideas on similar benchmarks for BWRs. Benchmarks for BWRs may be directly applicable to some PWR validation, e.g. in the transition from hot to cold conditions.

- The German contribution (Neckarwestheim II and Siemens) of measured axial burn-up distributions for a large number of different PWR fuel burn-ups and operating conditions, made available for the NEA Phase II-C [6] burn-up credit study, provides an important basis for realistic studies.

4.24. ANS and ISO standards related to burn-up credit

In 2008, the ANSI/ANS 8.27 [16] burn-up credit standard was published after many years of discussion. It focuses on intact LWR fuel but may be applied to other scenarios.

In 2011, ISO published a different type of standard [17], directed towards PWR fuel burn-up credit. It is not restricted to intact fuel, covering reprocessing as well.

4.25. Experience of interest for burn-up credit applications

- Misloading in Damphierre reactor 2003 [18]

This event has been described in many published documents. The main source here is the paper presented at the ANS/NCSD Topical Meeting in Knoxville 2005.

- Boraflex panel (BFP) degradation in spent fuel pools, 198X-

This experience has been documented in several publications. In the US, EPRI has released substantial information since 1988 and NRC has released several Information Notices (starting 1987). The issue remains to be relevant at some LWR sites.

There may be a gap in essentially any axial position along the active parts of the fuel. If there is a known gap somewhere, this is an example where the axial burn-up profile needs to be selected to optimise $k_{eff}$ for the system being evaluated.
• Potential for active fuel being outside the neutron absorber region 198X

Several package designs for irradiated fuel contain baskets with neutron absorbers that do not cover the full length of the fuel positions. Spacers are required in each position, sometimes both under and above the fuel assembly, to prevent the active part of the fuel to be positioned outside the absorber region.

• All burnable absorber rods removed from many fresh fuel assemblies

This experience is documented in a telex from the Swedish licensing authority. There was no violation or missing safety restrictions since burnable absorber credit was not yet applied at the time (introduced in 1981) and the operation was accepted by the licensing authority. The event is important in showing that simultaneous removal of all burnable absorbers from a large number of fuel assemblies can be a credible event.

• Unintentional criticality – Japanese power reactor Shiga, 1999

This experience, a few months before the JCO accident, was not reported until many years later, in 2007. A control rod was intended to be inserted but instead three control rods were withdrawn, leading to a 15-minute criticality excursion. It was stopped by manual insertion of control rods.

• Failure to remove $^{135}$Xe from fuel composition

The irradiated fuel normally has its peak reactivity near zero cooling time, if the $^{135}$Xe is ignored. However, this may require extra input preparation. It can be missed by specialists who calculate the reactor core behaviour using the same method. At least, one documented case is known where the applicant corrected for such a mistake after the licensing application was submitted to the authority. It seems appropriate to build such considerations into the software to avoid mistakes.

• Source convergence – Local “hot spot” missed in fuel storage rack design

In the early 1980s, a licensing application for a large fuel storage rack included evaluation of the consequences of a partial contact between fuel in storage and fuel being moved. The storage rack assured 10 cm spacing between fuel assemblies in their storage positions but, while being moved, there could be contact between stored and moved fuel in less than 90 cm “active area” of the upper part of the rack. The limited number of neutron histories per generation and in total, as typically used at that time, did not provide source convergence. The underestimation in $k_{eff}$ was about 2%, resulting in a value above the limit after correction.

This experience was one of the reasons for starting the Expert Group on Source Convergence [5].

4.26. Summary

Burn-up credit is a criticality safety concept. It is a safety control that can be an addition or a replacement to other criticality safety controls. Burn-up credit is optional in design and normal operation but may be mandatory during emergency conditions. The efficiency and reliability of burn-up credit depends on the ability to:

• operate the reactor under full control;
• measure and simulate the fuel reactivity properties during operation;
• identify each fuel assembly at all times before, during and after reactor operation;
account for all credible events (including those originating in the human factor);
• evaluate all information and convert it to safe and reliable limits and procedures;
• implement the limits and procedures.

Methods for application to burn-up credit have been available as long as man-made nuclear fission reactors have existed. Validation under reactor conditions has been possible for those with access to such benchmarks (including routine measurements). The large accumulation of used fuel in the world has increased the potential value of applying burn-up credit.

Powerful calculation methods and computers are available at low cost to criticality safety specialists involved in burn-up credit. A complication for the general criticality safety specialist, not having access to reactor operation information, is the lack of full benchmarks for validation of the transmutation of the fuel in the reactor. The industry can provide such benchmarks and this is what is occurring now. Another complication is the difficulty in assuring that only the intended fuel assemblies are moved to locations where burn-up credit is applied. The potential for relying on reactor records of fuel irradiation history and the development of benchmarks based on reactor measurements are related.

It is interesting to note that some of the methods applied by reactor physicists, such as diffusion theory, few-group cross-sections, homogenisation of lattices and lumped fission products have been rejected by many criticality safety specialists since 1980. Recently, with the need to evaluate burn-up credit, the criticality safety specialists are again using such “primitive” methods. The Polaris code [19] being developed for SCALE [20] is an example.

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