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Review calculations for the OECD/NEA Burn-up Credit Criticality Safety Benchmark

José J. Herrero [a,*], Alexander Vasiliev [a], Marco Pecchia [a], Hakim Ferroukhi [a], Stefano Caruso [b]

[a] Laboratory for Reactor Physics and Systems Behavior, Paul Scherrer Institut (PSI), 5232 Villigen PSI, Switzerland
[b] National Cooperative for the Disposal of Radioactive Waste (NAGRA), Hardstrasse 73, 5430 Wettingen, Switzerland

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ABSTRACT

A calculation methodology for criticality safety evaluations related to medium term dry storage, e.g. interim storage, and long term waste disposal, e.g. deep geological repository, is under development at PSI.

In that sense, the performance of present decay and criticality safety codes has to be evaluated for this kind of applications, with code to code, and data to data, comparison as a very first step. In this article, the Burn-up Credit Criticality Safety Benchmark Phase VII organized by OECD/NEA has been employed to evaluate decay calculations results for the codes CINDER and SERPENT2. The computed isotopic compositions have then been used for the assessment of the criticality calculations with MCNP6 and SERPENT2, while employing the most recent available cross sections libraries from ENDF/B-VII.1, JEFF-3.2 and TENDL-2014.

Results show overall a good agreement for all the options listed, while differences are pointed out and their origin is discussed.

1. Introduction

The Swiss National Cooperative for the Disposal of Radioactive Waste (NAGRA) plans to submit a general license application for the site of a deep geological repository for the disposal of spent fuel and high-level waste by 2022. One of the requirements to be accomplished for the design of the repository is the safety of the installations (encapsulation facility and repository) from the point of view of a possible criticality excursion on the time span when the concentration of actinides in the fuel is supposed to lead to the formation of a critical mass.

In this article, the Burn-up Credit Criticality Safety Benchmark - Phase VII organized by the Expert Group on Burn-up Credit Criticality Safety of the OECD/NEA Working Party on Nuclear Criticality Safety (Radulescu and Wagner, 2012) has been employed to evaluate decay calculations performances for the codes CINDER 1.05 and SERPENT2. The decay data was taken from ENDF/B-VII.1 or JEFF-3.1.1 for SERPENT2, and from ENDF/B-VI.2 in the CINDER data library. The different results are compared in the article.

After evaluation of the decay calculations, the set of isotopic compositions computed with SERPENT2 and the ENDF/B-VII.1 decay library have then been used for the assessment of the criticality calculations with the Monte Carlo codes MCNP6 and SERPENT2, employing the most recent cross sections libraries ENDF/B-VII.1, JEFF-3.2 and TENDL-2014.

Results show overall a good agreement for all the options listed, differences from one result to another are pointed out and the reasons for such deviations are discussed in the article.

2. Burn-up credit Phase VII benchmark specification

The objective of the benchmark was "to study the ability of the computer codes and the associated nuclear data to predict spent fuel isotopic compositions and *k*-eff values in a cask configuration over the time duration relevant to SNF disposal" (Radulescu and Wagner, 2012).

Participants performed decay and criticality calculations at 30 post-irradiation time steps, out to one million years. Although isotopes important to public dose were also considered, here the attention is focused on the criticality results and therefore only the isotopes considered for these calculations will be compared. Also the fresh fuel composition *k*-eff values were reported.

From all the participants' results, an averaged value for each compared quantity (with 4 significant digits) together with its standard deviation was included in the final report. These average

* Corresponding author. Tel.: +41 56 310 2802; fax: +41 56 310 2327.
E-mail address: jose-javier.herrero@psi.ch (J.J. Herrero).

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Table 1
Actinides only burn-up credit nuclides.

U-233	U-234	U-235	U-236	U-238	Pu-238
Pu-239	Pu-240	Pu-241	Pu-242	Am-241	

values will be used for the comparison to our results. The initial discharge composition is representative of a PWR assembly with an initial enrichment of 4.5 $^{w}/_{0}$ of U-235 and 50 GWd/MTU burn-up. The *k*-eff values will be computed taking credit only for actinides (11 isotopes) or for actinides plus fission products (19 additional isotopes), and including the O-16 (stable) present in the compositions. The isotopes considered for each type of calculation are listed in Tables 1 and 2.

The cask is loaded with 21 intact standard 17 × 17 fuel assemblies, all the dimensions for the fuel pins and the guide tubes are described in the final report (Radulescu and Wagner, 2012). The assemblies are situated in a borated stainless steel basket inside a stainless steel (SS304) cask forming an array. The cask is flooded with water and the temperature of the cask is supposed to be 293 K. All the material compositions are given and the isotopic compositions for each metallic species were taken from an IUPAC Technical Report (Berglund and Wieser, 2011) when needed.

3. Methodology

3.1. Decay codes

Two codes have been considered during the decay calculations, CINDER 1.05 and the decay module inside SERPENT2.

The characteristics of these codes should facilitate also a future coupling to the fuel burn-up sequence for the Swiss power plants and the sensitivity and uncertainty analysis methodologies under development.

3.1.1. CINDER 1.05

CINDER 1.05 is the latest version of CINDER available from the OECD/NEA Databank, it was compiled with the highest precision available. CINDER's method of resolution is based on the linearization of the Markov chains plus an automatic procedure to simplify the chains depth depending on a user given accuracy parameter (Wilson et al., 2008). The decay data used by CINDER cannot be easily changed and it is based on ENDF/B-VI.2, plus other sources when ENDF/B values were not available.

For the benchmark, two calculations were performed; one including only the original time positions whose results were included in the benchmark; another one halving these time steps by including intermediate points in the original time mesh. The results showed deviations in term of relative errors below 10^{-3}, so the method is quite independent on the time step. Also, some sensitivity study to the error tolerance for the convergence parameters was performed. In summary, default parameters can be considered adequate.

3.1.2. SERPENT2

SERPENT2 comes with a decay calculation module used in principle for burn-up calculations. The default decay calculation in SERPENT uses "an advanced matrix exponential solution based on the Chebyshev Rational Approximation Method (CRAM)", which has shown to be fast and accurate (Pusa, 2013) when coupled to the transport solution for core burn-up calculations.

More recently, the effect of the order of approximation in the calculation of the coefficients of the rational function was studied in connection with the use of very large time steps in decay calculations (Pusa, 2014), it indicates a limit to the time step to be used with the present approximation order.

The code can be instructed to run only the decay calculation without predictor/corrector transport calculations in between. In this case, the classical Transmutation Trajectory Analysis (TTA) or linear chains method is activated internally (Isotalo, 2013), this is the same method used by CINDER and the differences with this code should then come only from the decay data employed. In practice, the code was also instructed to use the CRAM to compare both algorithms, and no differences were encountered between both methods.

Unlike CINDER, here the user can choose the ENDF decay data library to be employed, which permits to investigate the effect of using different sources of data. Thus, the decay libraries from the ENDF/B-VII.1 evaluation and the JEFF-3.1.1 evaluation, including the spontaneous fission yields files, were employed in the decay calculations. The differences between the solutions from both libraries were minor as reported in next sections.

3.2. Criticality codes

Given the geometry to be modelled and the possible complexity in the material composition and distribution when more realistic configurations could be considered; and also to allow the possibility of using continuous energy and the most up to date cross sections libraries; Monte Carlo neutron transport codes have been chosen for these calculations. Among them, MCNP6 and SERPENT2 were studied as candidates.

MCNP-6.1 (Goorley et al., 2013) was released by merging together the MCNP5 and MCNPX codes. Its extensive validation and large number of users ensure constant development and improvement, MCNP is an important reference code for criticality calculations.

SERPENT2 is a neutron transport code directed towards calculation of models typical of reactor physics problems (Leppänen, 2007), version 2 is beta testing. A main difference with MCNP6 is that it is based on the Woodcock delta-tracking method instead of the track-length estimator (Leppänen, 2010).

3.3. Nuclear data

The nuclear parameters employed in the calculations are as important as the codes benchmarked. In this case, three distributions have been considered: ENDF/B-VII.1, JEFF-3.2 and TENDL-2014. In this way, it is expected to obtain at least a first estimation of the agreement of these libraries for waste disposal problems.

3.3.1. ENDF/B

The decay and neutron cross sections library files of version VII.1 (Chadwick et al., 2011) have been obtained through two paths. One is the data coming directly bounded to the MCNP6 distribution which includes neutron cross sections in ACE format, and the decay data contained in the CINDER data file (which is from ENDF/B-VI.2 mainly). The other way is through the files posted in

Table 2
Actinides plus fission products burn-up credit nuclides.

U-233	U-234	U-235	U-236	U-238	Np-237	Pu-238	Pu-239	Pu-240	Pu-241
Pu-242	Am-241	Am-242m	Am-243	Mo-95	Tc-99	Ru-101	Rh-103	Ag-109	Cs-133
Nd-143	Nd-145	Sm-147	Sm-149	Sm-150	Sm-151	Sm-152	Eu-151	Eu-153	Gd-155