LOW TEMPERATURE EFFECTS ON PWR FUEL ASSEMBLY CRITICALITY CALCULATIONS

Matthias Behler, Volker Hannstein, and Fabian Sommer

Gesellschaft für Anlagen- und Reaktorsicherheit (GRS) gGmbH
Boltzmannstraße 14, 85748 Garching, Germany

Matthias.Behler@grs.de, Volker.Hannstein@grs.de, Fabian.Sommer@grs.de

ABSTRACT

One of the parameters affecting the neutron multiplication factor k_{eff} of a system containing fissile material is the system temperature. Therefore, the effect of temperature on criticality safety analyses is an area of international interest. In this context, the Working Party on Nuclear Criticality Safety (WPNCSS) of the OECD Nuclear Energy Agency (NEA) formed a subgroup to define and execute a code-to-code comparison benchmark to investigate the effect of temperature on k_{eff} for PWR fuel assemblies. Two configurations of a generic water-moderated PWR fuel assembly were analysed at different temperatures between 233 K and 588 K, and with different assembly burnups. Based on this benchmark, GRS performed an additional study to investigate the impact of the moderator densities, the neutron reaction cross sections and the thermal scattering data on k_{eff} separately.

The benchmark results show the expected decrease of k_{eff} with temperature and a considerable jump in k_{eff} at the phase transition of the moderator. The additional investigation demonstrates that the jump in k_{eff} is mainly caused by the change of the moderator density due to the phase transition. The change of the thermal scattering data due to the phase transitions leads to a similar but smaller jump in k_{eff} . Furthermore, the actual impact of the different parameters on k_{eff} depend strongly on the considered fuel assembly configuration.

KEYWORDS: criticality safety, neutron multiplication factor, thermal scattering data, temperature effect

1. INTRODUCTION

In criticality safety analyses of fissile material, the most unfavourable configurations need to be analysed considering normal and credible abnormal conditions. Typically, such an analysis is based on the determination of the neutron multiplication factor k_{eff} . One of the parameters affecting k_{eff} is the temperature, since the temperature influences material densities and phases, as well as neutron reaction cross sections and thermal scattering data. Hence, an appropriate temperature range needs to be considered. For example, the IAEA Transport Regulation SSR-6 [1] requires the consideration of ambient temperatures from -40°C to 38°C (unless the Competent Authority specifies otherwise). Therefore, the effect of temperature on k_{eff} is an area of international interest. Especially, temperatures below 273 K are currently under investigation [2]. For instance, thermal scattering data of hydrogen bound in ice was recently included in the newest releases of nuclear data libraries, e.g. ENDF/B-VIII.0 [3] or JEFF-3.3 [4].

In this context, the Working Party on Nuclear Criticality Safety (WPNCSS) of the OECD Nuclear Energy Agency (NEA) formed a Sub Group to define and execute an code-to-code code comparison benchmark to investigate the effect of temperature on k_{eff} for PWR fuel assemblies [5, 6]. In this benchmark attention was paid to temperatures below 273 K to investigate the impact of the reaction cross sections and of the change in the thermal scattering data of bound hydrogen in this temperature region. Hence, the k_{eff} of two configurations of a generic water-moderated PWR fuel assembly were analysed at temperatures between 233 K and 588 K.

Based on this benchmark, GRS performed an additional study on the effect of the temperature on k_{eff} to investigate the temperature-dependent impact of the reaction cross sections, the thermal scattering data and the moderator density on the neutron multiplication factor separately, while the OECD/NEA benchmark analysed only the combined effect. Both, the GRS contribution to this benchmark and the additional investigations are described in this paper.

2. OECD/NEA BENCHMARK

2.1. Benchmark Specifications

In the OECD/NEA benchmark [5] two configurations of a generic water-moderated PWR fuel assembly were analysed: a single water-reflected fuel assembly (Single Unit) and an infinite array of identical fuel assemblies (Infinite Array). In both cases the same generic 17x17-25 PWR fuel assembly was used, see Fig. 1. In the first case the single fuel assembly was surrounded by a 1 m water reflector, while in the second case the infinite array of the fuel assemblies was built without any water gap between the fuel assemblies. Both configurations were considered infinite in the axial direction, i.e. two-dimensional models were used. The configurations were analysed at five different temperatures (233 K, 253 K, 293 K, 333 K and 588 K) considering three different fuel compositions with an initial enrichment of 4.5 wt-% of ^{235}U : fresh fuel as well as irradiated fuel with burnups of 30 GWd/t and 45 GWd/t, respectively. The irradiated fuel compositions were taken from a previous OECD/NEA burnup credit criticality safety benchmark [7].

For each analysed combination, the reaction cross sections, the thermal scattering data and the moderator density were adjusted according to the chosen temperature. The moderator was assumed to be ice instead of water for the temperatures of 233 K and 253 K. For temperatures up to 333 K normal pressure was

Figure 1. Generic water-moderated 17x17-25 PWR fuel assembly reflected by water.

assumed, and for 588 K a typical PWR moderator pressure was applied. In contrast to the moderator, the parameters of the water reflector in the case of the single fuel assembly were kept constant at their values of 293 K. The detailed description of the benchmark can be found in [5].

2.2. GRS Benchmark Results

GRS calculated the requested neutron multiplication factors with three different Monte Carlo codes: KENO-V.a of the SCALE package version 6.2.2 [8], OpenMC version 0.9.0 [9] and MCNP version 6.1 [10]. For all three codes, the nuclear data were taken from the latest ENDF/B-VIII.0 library [3, 11], which contains scattering data of hydrogen and oxygen bound in ice. The nuclear data in the so-called ACE format required by MCNP were taken directly from a library made available by the Los Alamos National Laboratory [11]. This library is based on the corresponding ENDF-files provided by the National Nuclear Data Center (NNDC) at Brookhaven National Laboratory (BNL) [3]. This ACE formatted data was also used for OpenMC after converting it to the OpenMC specific HDF-5 format. The ENDF/B-VIII.0 data in the so-called AMPX format required by the SCALE package were generated from the ENDF-files provided by the NNDC using the AMPX code system [12] (included in the SCALE package). Since the ENDF/B-VIII.0 thermal scattering data of hydrogen in water included in this ENDF-files caused an unexpected error during the conversion process, the thermal scattering data of hydrogen in water of the ENDF/B-VII.1 library was used instead to generate the AMPX formatted data.

Hence, the thermal scattering data of hydrogen bound in ice were used for the temperatures of 233 K and 253 K to take the moderator phase correctly into account. In the case of MCNP, the required temperature-dependent reaction cross sections were constructed by mixing two sets of nuclides with the respective nearest temperatures given the ENDF/B-VIII.0 library. However, the thermal scattering data were applied without interpolation. For the temperatures of 333 K and 588 K, for which no scattering data are included in the in ENDF/B-VIII.0 library, the scattering data of the temperatures 324 K and 600 K were used instead. This leads to a small error in the calculated k_{eff} of less than 70 pcm ($1 \text{ pcm} = 10^{-5}$) [13]. In the case of KENO-V.a and OpenMC, their internal methods to adjust the reaction cross sections and scattering data were applied.

Figure 2. Calculated neutron multiplication factors k_{eff} of the benchmark cases.

The calculated neutron multiplication factors k_{eff} of the different benchmark cases using the different codes are given in Fig. 2. For the temperatures above and below the phase transition of the moderator, the results show the well-known temperature-dependent behaviour, i.e. k_{eff} decreases with temperature. In contrast, the phase transition of the moderator leads to a jump in k_{eff} . The increase in k_{eff} by changing the temperature from 253 K (with ice as moderator) to 293 K (with water as moderator) varies from about 2700 pcm (fresh fuel) to 2000 pcm (45 GWd/t) in the case of the single fuel assembly. In the case of the infinite fuel assembly array, this increase in k_{eff} is about 700 pcm and almost independent of the fuel composition.

The results of the different codes are reasonably similar. The differences $\Delta k_{\text{eff}} (= k_{\text{eff,KENO/OpenMC}} - k_{\text{eff,MCNP}})$ between the KENO-V.a and MCNP results, and between the OpenMC and MCNP results as well as the statistical uncertainties of Δk_{eff} are given in Fig. 3. In the case of the single fuel assembly Δk_{eff} is mostly less than 100 pcm and statistically compatible with zero. Hence, the differences between the corresponding neutron multiplication factors are mostly insignificant. However, the largest discrepancies up to about 200 pcm exist between the KENO-V.a and OpenMC results at 233 K. For the infinite fuel

Figure 3. Differences Δk_{eff} in the neutron multiplication factors between KENO-V.a and MCNP, and between OpenMC and MCNP, respectively.

assembly array, the results of the different codes show somewhat larger discrepancies. In many cases Δk_{eff} is still compatible with zero, but it reaches also values up to 200 pcm. As before, the largest differences up to 300 pcm exist between the KENO-V.a and OpenMC results at 233 K.

The benchmark results show the combined impact of the temperature-dependent parameters on k_{eff} , but they do not provide enough information to draw any detailed conclusions about the quantitative impact of each single parameter on k_{eff} . Therefore, further investigations were performed based on these benchmark specifications.

2.3. Comparison with other Benchmark Contributions

In total, more than 30 benchmark contributions were submitted including six contributions from GRS [6]. Several combinations of codes and nuclear data libraries were used to perform the submitted results. In addition to the GRS contributions discussed above, the other three GRS contributions utilized KENO-V.a and the ENDF/B-VII.1 library in different energy group structures, but without thermal scattering data of hydrogen bound in ice. Other benchmark participants also utilized the codes TRIPOLI-4, MORET 5, MVP3, HELIOS 2 or different versions of MONK, as well as the nuclear data libraries JEF-2.2, JEFF-3.1.1, JEFF-3.1.2, JEFF-3.3 or JENDL-4.0.

A preliminary evaluation of these contributions has already been published in [6]. It demonstrates, that for each analysed configuration the vast majority of the calculated neutron multiplication factors vary not more than 600 pcm. The largest variation appears at the temperature of 588 K, while the variation is considerably lower at all other temperatures. Only two contributions result in systematic larger variations in k_{eff} , but without any clear explanation so far. However, the GRS contributions are compatible with the vast majority of the contributions, i.e. the calculated neutron multiplication factors are within the mentioned variation in k_{eff} of 600 pcm.

3. IMPACT OF EACH TEMPERATURE-DEPENDENT PARAMETER ON k_{eff}

Instead of varying reaction cross sections, thermal scattering data and moderator density with temperature simultaneously, the impacts of these parameters on k_{eff} were studied separately. For this purpose, only one single parameter was varied with temperature at a time, while all other temperature-dependent parameters were fixed at 293 K.

For this study the benchmark models were used as described above (see chapter 2.1.). Only the temperature range was reduced to 233 K – 350 K and k_{eff} was calculated for more temperatures to focus the analysis on a temperature region around the moderator phase transition. The temperatures considered to calculate k_{eff} were chosen identical to the temperatures of the thermal scattering data sets provided in the ENDF/B-VIII.0 library. In this way, the thermal scattering data of hydrogen bound in ice or water of the ENDF/B-VIII.0 library could be used without any correction or imposing any error on k_{eff} . These calculations were performed using MCNP only, since MCNP provides the required functionalities to include reaction cross sections and thermal scattering data separately at different temperatures in a user-friendly way.

The performed parameter variations show that only the variations of the moderator density, of the thermal scattering data of hydrogen and of the reaction cross sections of the fuel have a significant temperature-dependent impact on k_{eff} . Variations of the reaction cross sections of the moderator as well as of the thermal scattering data of all nuclides excluding hydrogen lead to no significant changes in k_{eff} in the analysed temperature range. In Fig. 4 the variations in k_{eff} due to the first three mentioned parameters are presented for the fresh fuel cases, with $\Delta k_{\text{eff}} = k_{\text{eff}}(T) - k_{\text{eff}}(293 \text{ K})$.

Figure 4. Temperature-dependent impact of the moderator density, the thermal scattering data of hydrogen ($S_{\alpha,\beta}$) and the reaction cross sections (XS) of the fuel on k_{eff} .

As shown in Fig. 4, the impact of the moderator density and of the reaction cross sections of the fuel on k_{eff} show a qualitatively similar behaviour for both analysed fuel assembly configurations. However, their quantitative effects are significantly different. In the case of the infinite fuel assembly array the variations in k_{eff} due to the temperature-dependence of the reaction cross sections are about twice as large as the variations in the case of the single fuel assembly. In contrast, the temperature-dependence of the moderator density causes considerably smaller variations in k_{eff} in the case of the infinite fuel assembly array than in the case of the single fuel assembly. This leads to the fact, that for the infinite fuel assembly array, both parameters have a similar quantitative impact on k_{eff} . For the single fuel assembly, the temperature-dependence of moderator density leads to much larger variations in k_{eff} compared to the variations caused by the reaction cross sections. Also, the jump in k_{eff} due to the change of the moderator density at the phase transition differs significantly between both configurations. In the case of the single fuel assembly this jump in k_{eff} is about 2800 pcm for fresh fuel and decreases to 2400 pcm and 2200 pcm considering the 30 GWd/t and 45 GWd/t fuel compositions, respectively. Instead, it varies only between 850 pcm and 1050 pcm in the case of the infinite fuel assembly array.

In contrast to the impact of the moderator density and of the reaction cross sections, the impact of the thermal scattering data of hydrogen on k_{eff} shows complementary behaviours for both analysed fuel assembly configurations, see Fig. 5. In the case of the single fuel assembly the temperature-dependence of the thermal scattering data of hydrogen causes a decrease in k_{eff} with temperature, while it results in an increasing k_{eff} in the case of the infinite fuel assembly array. Similarly, the change of the thermal scattering data due to the phase transition of the moderator from ice to water leads to an increase in k_{eff} in the case of the single fuel assembly, but to a decrease in k_{eff} in the case of the fuel assembly array. Furthermore, the results show a dependency of the jump in k_{eff} on the fuel composition. However, also this dependency behaves contrarily for both fuel assembly configurations.

4. CONCLUSIONS

The effect of the temperature on the neutron multiplication factor for PWR fuel assemblies was analysed. In the OECD/NEA benchmark the combined effect of the temperature-dependent parameters on k_{eff} was studied. The benchmark calculations performed by GRS show the expected temperature-dependent

Figure 5. Temperature-dependent impact of the thermal scattering data of hydrogen ($S_{\alpha,\beta}$) and the reaction cross sections (XS) of the fuel on k_{eff} for the different fuel compositions.

behaviour of k_{eff} , i.e. k_{eff} decreases with temperature, and the moderator phase transition leads to a jump in k_{eff} . The results calculated with the codes KENO-V.a, OpenMC and MCNP are in good agreement.

An additional study investigated the effects of the temperature-dependent parameters on k_{eff} separately. This investigation confirms the well-known effects of the temperature-dependent variations of moderator density and cross sections on k_{eff} . The temperature-dependence of the neutron multiplication factor is dominated by these two parameters. Especially, the jump in k_{eff} at the phase transition of the moderator is mainly due to the change of the moderator density. Furthermore, the investigation demonstrates that the temperature-dependent variations of the scattering data have a relatively small impact on k_{eff} . Especially, the change in the scattering data of bound H at the moderator phase transition leads to a jump in k_{eff} , which is much smaller compared to the one caused by the change of the moderator density.

However, the actual impact of each parameter on k_{eff} depends strongly on the analysed configuration. In particular, the impact of the scattering data of bound hydrogen on k_{eff} shows a complementary behaviour for both analysed fuel assembly configurations.

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