CASMO-4/SIMULATE-3/MCNPX Analysis of a Reactor Pressure Vessel Scraping Test

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Abstract

To respond to current-day increased requirements on the quality of neutron fluence estimations, an up-to-date methodology for 3D fast fluence evaluation for light water reactors is under development at the Paul Scherrer Institute, centered around the MCNP(X) code using continuous-energy neutron data libraries.

An essential part of the verification and validation of the entire calculation route covering the core-follow and neutron transport simulation tools - CASMO/SIMULATE/ MCNPX - is the analysis of available experimental data on the fast neutron fluence at the inside of the reactor pressure vessel. The fluence estimations are based on actual reactor operation history data. The reference measurement-based fluence estimates were obtained from evaluations of pressure vessel scraping data that have been performed previously at the Paul Scherrer Institute.

The paper describes the general features of the developed and applied methodology and particular modeling options which were selected through accompanying comprehensive sensitivity and optimization studies. Also presented are the results of the calculations and their comparison with measurements.

Very good agreement is found between the calculated results and the evaluated experimental data, indicating a high level of accuracy in the fixed-source, ex-core neutron transport calculations.

KEYWORDS: Fast neutron fluence, CASMO-4/SIMULATE-3, MCNPX, verification

1. Introduction

To date, the in-house, two-dimensional deterministic transport code BOXER [1], together with its associated group-wise neutron data library, have been used at the Paul Scherrer Institute (PSI) for the analysis of the fast neutron fluence on the reactor pressure vessel (RPV) of the pressurized water reactor (PWR) “Kernkraftwerk Goesgen (KKG)” nuclear power plant. For this purpose, the BOXER code was verified against experimental fast neutron fluence data that were estimated from the RPV scraping test performed at the KKG in 1989, after ten cycles of reactor operation [1].

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Currently, the implementation and validation of an advanced CASMO-4 [2]/ SIMULATE-3 [3]/ MCNPX-2.4.0 [4] calculation route, utilizing a set of modern analysis tools necessary for accurate ex-core neutron transport calculations, is in progress at the PSI as a part of the STARS project [5]. The well-recognized requirements for methodology qualification [6] include comparison with measurements from an operating reactor. In this respect, the KKG scraping test represents a very valuable and almost unique data source for such validation. Indeed, benchmarks usually offered do not provide the reactor operation data that would allow the proper determination of the neutron source, rather specifying it as an independently evaluated input specification. Furthermore, such benchmarks test only the neutron transport code with the fixed-source option and an associated cross-section library in a stand-alone set-up, rather than evaluating the whole calculational chain.

The CASMO/SIMULATE/MCNPX calculation results have been verified against the scraping test data that provide estimates of the fast fluence (E>1MeV) spatial distribution at the KKG RPV inner wall after the first 10 fuel cycles [1]. All required CASMO/SIMULATE models for KKG, as well as the data from the scraping test, were already available at PSI. The original 2D lattice depletion calculations with CASMO-4 were performed using the JEF-2.2 70-group neutron data library [2] to generate the homogenized 2-group cross-section data. These are used in a standard fashion by the 3D nodal diffusion code SIMULATE-3. The JEF-2.2 continuous-energy neutron data library [7] has been used for the MCNPX-2.4.0 neutron transport calculations.

Very good agreement is obtained between the results of the new calculations and the experimental data. The improvement over the previous BOXER analysis is the result mainly of an accurate geometrical modeling, much more detailed account of the reactor operation history, the detailed specification of the variation of the neutron source in function of time, space and energy, and the continuous-energy Monte Carlo solution of the neutron transport problem.

2. Description of the methodology

2.1 General

A central feature of the present Monte Carlo based methodology for fast fluence modeling is the transfer of results from the CASMO-4/SIMULATE-3 core-follow calculations (power distribution and fuel compositions) to the MCNPX model for the specification of the 3D volumetric (axially distributed pin-by-pin) fission source. To that aim, a linking tool has been developed to automatically perform this transfer that directly produces the required MCNPX input cards for any burnup step or for reactor conditions averaged over some specified time interval, *i.e.* reactor cycle(s). Since, at PSI, the core models of the Swiss nuclear power plants are periodically updated and verified against plant measurements, the present fast fluence evaluation methodology benefits from qualified core data.

Prior to final elaboration of the described calculational approach, it should be mentioned that modern trends and well-recognized recommendations related to an accurate fast fluence modeling, as summarized in e.g. [6], have been taken into account when defining the PSI-methodology. It is important to note, however, that these general findings were derived from the analysis of past studies which applied different methodologies and computational tools and where the particular treatment of various phenomena and modeling options were subject to large variation.

Accordingly, rather than simply applying the recommendations directly, these have been evaluated by means of extensive sensitivity and optimization studies on the basis of the KKG reactor model and a consistent set of modeling options has been arrived at.

2.2 Sensitivity and optimization studies

The optimization studies have, in particular, aimed at reducing the efforts of computation associated with the fast neutron flux modeling without significantly sacrificing accuracy and precision of the calculations. In the framework of the present study, an effect (bias) was considered as significant if it is greater than the precision of a result in terms of the relative statistical error [4] of practical MCNPX calculations. An attempt was made to account for all relevant phenomena and modeling details which could affect the fluence estimates on the inner surface of the RPV by more than 0.2% and by more than 2% for the individual surface segment (Δz (height) $\approx$ 15cm; $\Delta\alpha$ (angle) = 2.5degree) of a tally.

With this approach based on a single calculation route and a single reactor model, using precise continuous-energy Monte Carlo calculations, a consistent set of model and parameter choices was arrived at. Investigations to determine the relative importance of the following phenomena and modeling details were performed:

- Detailed elaboration of specifications related to the problem geometry and the included materials:
  - Radial modeling (number of modeled fuel assemblies) and mesh-based Weight-Windows variance reduction;
  - Axial modeling (including account of regions, axially located outside the core; influence of core formers);
- Detailed time-spatial modeling of the coolant density (temperature) distributions (*i.e.* account of cycle-to-cycle variations and axial heating profile);
- Influence of account of the actual irradiated fuel composition (here - only with respect to neutron cross-sections);
- Influence of thermal expansion of the materials, especially causing the geometrical changes of the water gaps between the core baffle and the RPV wall;
- Neutron source specification:
  - Neutron source strength: account of spatial distribution of the actual irradiated fuel composition, affecting both the ν and E_R values (see next subchapter for definitions);
  - Neutron source spectrum: importance of modeling of spatially distributed fission neutron spectra of the individual nuclides (versus applying a core-averaged spectrum);
- Optimization of the neutron flux integration procedure:
  - Integration over a fuel cycle;
  - Integration over reactor life-time.

2.3 Application of the CASMO/SIMULATE core-follow calculations for the neutron source specification

The approximate form of the neutron source $S(\mathbf{r},E)$ (1) reconstruction on the basis of the core-follow calculation data, which has been implemented by default into the code, linking the CASMO-4/SIMULATE-3 system and the MCNPX-2.4.0 code, is following (2)-(4):

$$S(\mathbf{r},E) = S(\mathbf{r})\ \chi(\mathbf{r},E) \approx S_m\ \chi_m(E)\ ; \qquad (1)$$

$$S_m = P_m \frac{\nu_m}{E_{R\,m}\, C}\ ; \qquad (2)$$

$$\chi_m(E) = \sum_i \chi^i(E) \frac{\nu^i\, \sigma_f^i \bar{\rho}_m^i}{\sum_i \nu^i\, \sigma_f^i\, \bar{\rho}_m^i}\ ; \qquad (3)$$

$$\nu_m = \sum_i \nu^i \frac{\sigma_f^i \bar{\rho}_m^i}{\sum_i \sigma_f^i \bar{\rho}_m^i}\ ;\ E_{R\,m} = \sum_i E_R^i \frac{\sigma_f^i \bar{\rho}_m^i}{\sum_i \sigma_f^i \bar{\rho}_m^i}\ ; \qquad (4)$$

where "*m*" is a fuel assembly (FA) identifier, "*i*" is a fissionable nuclide; P_m is the power, released in the *m*-th FA; $\bar{\rho}$ - average nuclide atomic density within the *m*-th FA [at/(cm^3)]; σ_f - microscopic fission cross-section [barn (10^{-24}cm^2)]; ν and E_R are correspondingly the number of neutrons (n) per fission and the recoverable energy per fission, [eV]; C=1.6019·10^{-19} is the energy unit converter constant; [J/eV].

At present the tabulated σ_f^i data for monoenergtic thermal neutrons are used, consistent with the fission neutron spectrum approximation as used in the CASMO-4 code, where thermal fission cross-sections are determined for all nuclides (except ^{238}U) as $g^i \cdot \sigma_f^i\big|_{v=2200\ m/s}$; g is the non- 1/v factor [2]. σ_f^{238} is determined from test calculations [2].

Along with the 2D fuel assembly level neutron source map, the axial distribution for each FA is represented by a fuel-rod average axial power profile. Only ^{235}U, ^{238}U, ^{239}Pu and ^{241}Pu are included in the fixed neutron source definition since all other fissionable nuclides generated with burnup have negligible contributions to total fissions. The actual data for σ_f and ν , E_R for the considered nuclides were selected from references [2] and [8] and are reproduced in Tab. 1.

Table 1: Important properties of the fissionable nuclides.

Nuclide	σ_f, [barn]	ν [n]	E_R. [MeV] [(a)]
^{235}U	566	2.430	201.7
^{238}U	1.5	2.810	205.0
^{239}Pu	781	2.871	210.0
^{241}Pu	1060	2.969	212.4

(a) These values represent averages over both whole-core and fuel life-time [8].

2.4 General methodology overview

The major features of the current methodology, elaborated on the basis of the specified optimization studies, are as follows:

- The neutron transport calculations are performed with the MCNPX code using both a continuous energy neutron data library and a volumetric fixed neutron source.
- The problem specific mesh-based option of the MCNPX Weight Windows is utilized as the major variance reduction tool.
- The neutron source representing the fission neutrons is determined based on the CASMO-4/SIMULATE-3 core-follow calculations results (power and fuel composition time-spatial distributions).
- A dedicated linking tool is used for automated transfer of the SIMULATE-3 calculation results into the format of the MCNPX neutron source specification cards.
- The neutron source of the MCNPX model is specified as:
  - Synthesis of the 3D pin-by-pin source strength probability specification:
    - 2D FA-level source strength distribution for the core periphery;
    - 1D FA-level axial source strength distribution for each peripheral FA (40 axial layers were used for the KKG model according to SIMULATE models);
    - 2D pin-by-pin source strength distribution within each peripheral FA.
  - 2D FA-level fission neutron spectrum distribution for the core periphery: Individual specifications of the neutron spectrum and fission rates for the fissionable nuclides ^{235}U; ^{238}U; ^{239}Pu and ^{241}Pu for each peripheral FA.
  - Spatial distribution of the FA-average recoverable fission energy and effective number of neutrons per fission, caused by the spatial non-uniformity of the fuel burnup, is accounted for in the neutron source definition;
  - Reactor cycle specific MCNPX models are used with the corresponding cycle-averaged neutron source specifications.
- The default core pattern includes two peripheral FA rings such that even diagonally there are no paths with less fuel (neutron source) than two fuel assemblies present in any direction from the core shroud inside the core. When the domain of the neutron flux analysis is restricted by the RPV inner surface axial slice within the core region level, the structures situated axially outside the core could be effectively modeled as homogeneous regions or even neglected.
- The material compositions and densities (also averaged over the cycle(s) length) as obtained from the core-follow code system CASMO/SIMULATE are specified together with the neutron source in the MCNPX model.
- The reactor model explicitly represents the core periphery (at the pin-by-pin level), core baffle, core barrel, core formers and reactor pressure vessel. Several (7 in the present study) axial layers of the coolant are specified, each with different moderator densities.

In general, the overall complexity of the reactor calculation model (mostly, the detailed elaboration of the geometry and materials specifications) should be reasonably balanced with respect to the practically achievable statistical precision of the Monte Carlo fast fluence estimations and the quality of evaluated reactor operation history data including the neutron source estimations.

3. Calculation models

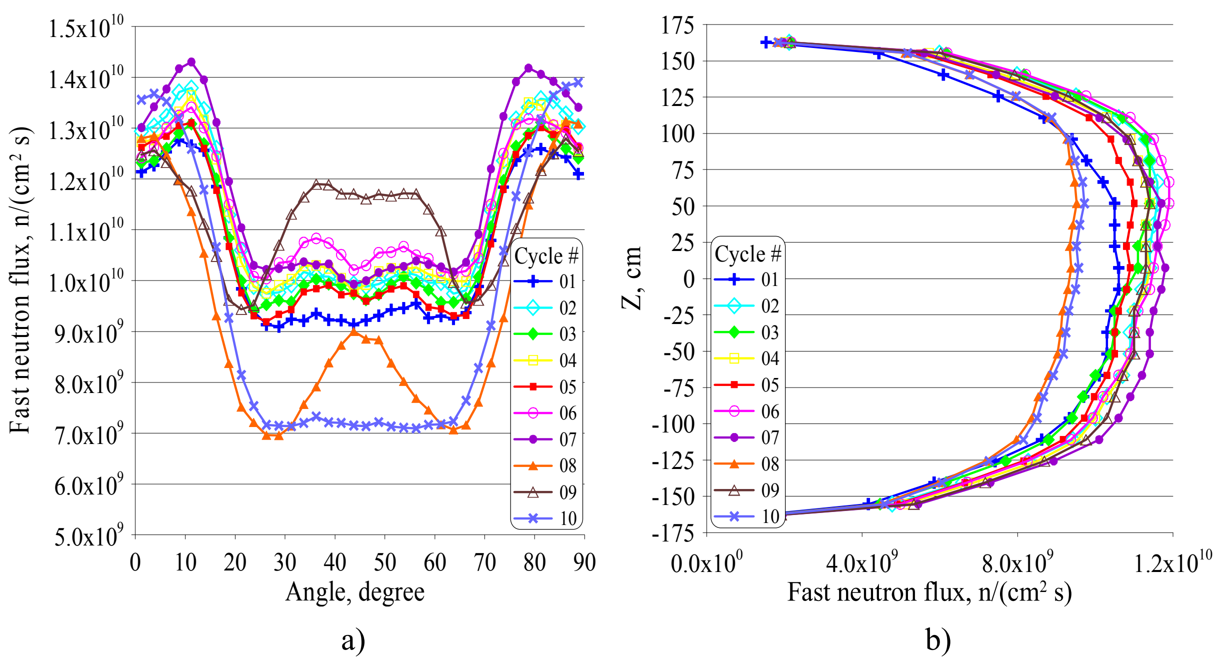
The 3D MCNPX calculation models for each cycle of the KKG reactor have been elaborated on the basis of the plant-provided drawings and operation conditions data. The domain of the present neutron flux analysis was restricted by the RPV inner surface axial slice within the core region level. The actual fuel compositions, extracted from the SIMULATE-3 calculation results, were used for the neutron source time-spatial-energy distributions, as described above. The one-energy-group, one-dimensional, cylindrical mesh-based weight windows were used in the MCNPX model as the major variance reduction tool. The "F2" MCNPX surface flux tallies were utilized for the neutron flux estimations at the RPV inner surface wall.

4. Calculation results

4.1 Cycle-by-cycle results on fast neutron flux

Calculation results on the cycle-by-cycle evolution of the fast neutron flux distribution at the KKG inner surface are presented on Fig. 1. The statistical uncertainties of the MCNPX results, which are discussed above, are omitted in the plots.

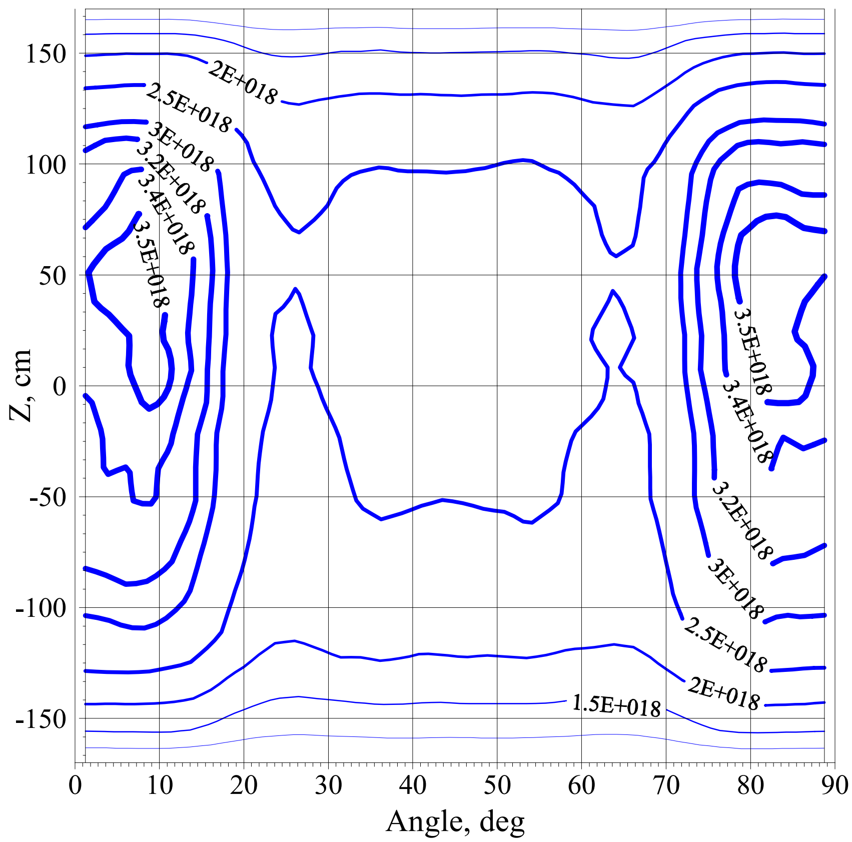
Figure 1: Cycle-by-cycle azimuthal fast neutron flux distribution at KKG RPV mid-plane (a) and axial distribution of average azimuthal flux (b).



4.2 Analysis of the fast neutron fluence distribution

The resulting fast neutron fluence estimations are presented in Fig. 2. The azimuthal behavior of the fluence is explained by the neutron source distribution, which in turn is affected by the azimuthal non-uniformity of neutron leakage from the core. The axial non-symmetry of the fluence is caused by the water density reduction along the core height and by the axial power profile, gradually shifted with burnup towards the upper core end.

Figure 2: Fast neutron fluence at the inner surface of the KKG RPV after ten fuel cycles.



5. Analysis of the scraping test

Reference [1] presents the original analysis of the KKG RPV scraping samples. The relative error of the fluence estimations is declared as ~10%.

To get the experimental verification of symmetry of the azimuthal fluence distribution, the steel samples were taken from the KKG RPV from two diagonally opposite sectors: from 90 to 180 and from 270 to 360 degrees. For the present analysis, like in the previous analysis using the BOXER code, it was simplistically assumed that the KKG reactor model is 90°- symmetric and therefore only the symmetry sector was modeled with the MCNPX code.

Keeping with this assumption, the experimentally estimated data on the fast neutron fluence at sectors from 90 to 180 and from 270 to 360 degrees were averaged according to (5), providing reduced uncertainties, $\langle\sigma\rangle$, of the weighted average fluence estimations comparing to the initial data:

$$F_{\mathrm{exp}} = \left\langle F_{\mathrm{exp},\,n} \right\rangle = \frac{1}{w} \sum_{n=1,2} w_n F_{\mathrm{exp},\,n}\;; \quad \langle\sigma\rangle = \frac{1}{\sqrt{w}}; \quad w = \sum_{n=1,2} w_n\;; \quad w_n = \frac{1}{\sigma_n^{\;2}}\;; \qquad (5)$$

The calculation results, obtained with the CASMO-4/SIMULATE-3/MCNPX, are presented in Tab. 2 and in Fig. 3, which gives comparison of the current results with the evaluated experimental neutron fluence data, together with the previous BOXER results.

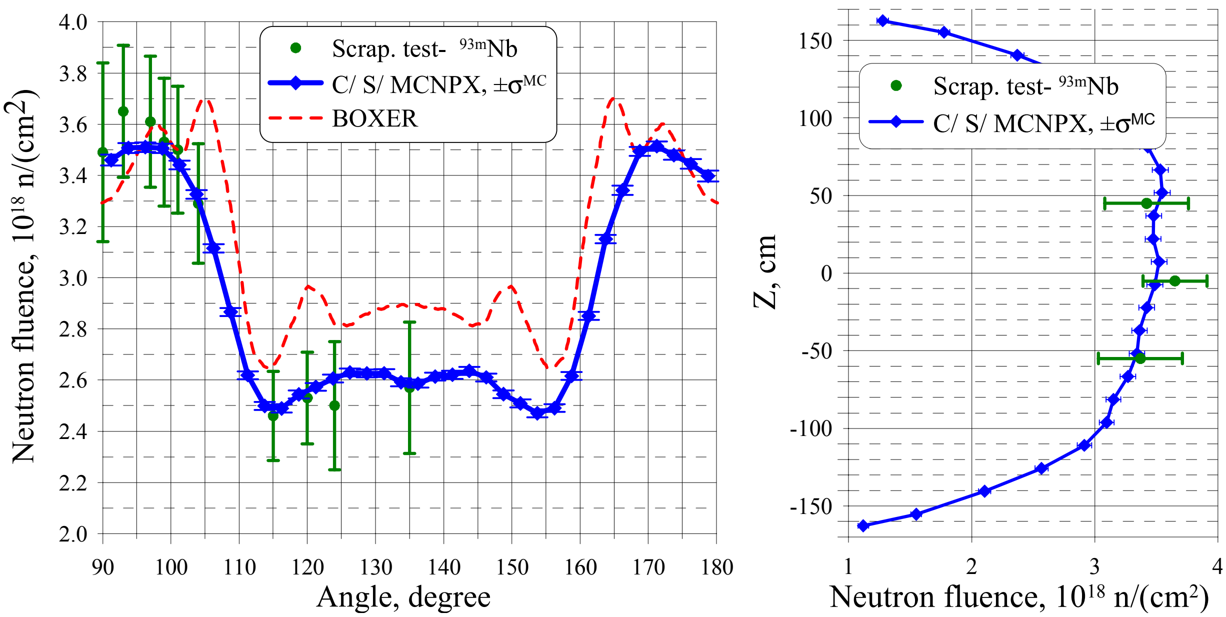
Table 2: Comparison of the calculated and measured neutron fluence data.

Axial position; z, [cm]	Azimuthal position; α, [deg.]	F_{exp}, 10^{18} [1/cm^2]	σ_{exp}, 10^{18} [1/cm^2]	F_{calc}[a], 10^{18} [1/cm^2]	F_{calc} / F_{exp}	$\sigma_{(calc / exp)}$[b], %
165	90	3.49	0.349	~3.44	0.986	10.0
	93	3.65	0.258	3.49	0.956	7.1
	97	3.61	0.256	3.51	0.972	7.1
	99	3.53	0.250	3.50	0.992	7.1
	101	3.50	0.248	3.44	0.983	7.1
	104	3.29	0.233	3.32	1.009	7.1
	115	2.46	0.174	2.49	1.012	7.1
	120	2.53	0.179	2.56	1.012	7.1
	124	2.50	0.250	2.61	1.044	10.0
	135	2.57	0.257	2.59	1.008	10.0
115	93	3.37	0.342	3.33	0.988	10.2
215	93	3.42	0.337	3.51	1.026	9.9

(a) Linear interpolation (extrapolation at 90 degrees) of data from Fig. 3;

(b) Defined as $\sigma_{calc / \exp} = \left(\frac{F^{calc}}{F^{\exp}}\right)_n \sqrt{\left(\frac{\sigma^{\exp}}{F^{\exp}}\right)^2 + \left(\frac{\sigma^{calc}}{F^{calc}}\right)^2}$; $\sigma_{calc} \approx 0.6\%$.

Figure 3: Analysis of the KKG RPV scraping test with the CASMO-4/SIMULATE-3/MCNPX: azimuthal distribution at z=165 cm (a), and axial distribution at α=93° (b).



a) b)

6. Discussion of the results

All calculation results for the fast neutron fluence obtained using the CASMO-4/SIMULATE-3/MCNPX route lie within the experimental uncertainty band (see Fig. 3); in fact, the results lie uniformly within approximately ±5% of the measurement data (as compared to ±15% for the BOXER analysis [1]). The new calculation results also predict the location of the maximum fluence perfectly well. Based on this good performance, it can be concluded that no significant biases were introduced with the present modeling, and the nature of the observed deviations between calculated and measurement results could be explained by the random uncertainties of both MCXNP-based modeling and the measurements.

Comparing the obtained results with those from the previous BOXER analysis, one may note in as mentioned that the BOXER results differ generally much more from the experimental data. The 'fine structure' observed with the BOXER results can probably be attributed to the rectangular-mesh based definition of the reactor geometry, thereby approximating the cylindrical geometry outside of the core.

The current modeling approach does have certain (although limited) deficiencies, e.g. neglecting the radial distribution of the moderator temperature within the core, neglect of any deviation from the nominal fuel geometry such as fuel-rod bending, uncertainties in the radial or axial within-assembly neutron source distribution or the axial distribution of the fuel composition. Such limitations may be causing the underestimation of the fast neutron flux at the RPV at ~93 azimuthal degrees and simultaneously an overestimation of the flux at ~124 degrees.

These effects, believed to be of second-order importance, should be further investigated in future studies. In any case, the results obtained so far are very promising with respect to the currently accepted level of accuracy for state-of-the-art neutron fluence evaluation (about ±20% in general [6]).

7. Conclusions

A Monte Carlo based methodology for 3D fast neutron fluence modeling for LWRs, utilizing CASMO-4/SIMULTE-3 core-follow calculation results for the neutron source definition in a MCNPX neutron transport reactor model, is being developed at PSI within the STARS project. The major features of the present study are the utilization of a modern Monte Carlo code for full-scale fast neutron fluence analysis using point-wise neutron data libraries (JEF-2.2 in the present case), and extensive complementary sensitivity and optimization computations. Modern high-performance computing hardware allows for results with low statistical variance.

The validation of the entire calculation route has been performed on the basis of estimates of the azimuthal and axial distributions of neutron fluence (E>1MeV) on the inner surface of the KKG RPV, evaluated from the scraping tests performed after ten reactor cycles.

Very good agreement between the calculated and experimental data has been found, suggesting:

- good performance of the developed methodology and utilized tools;
- high quality of the core-follow data and the fixed-source ex-core neutron transport calculations.

All calculation results fall within ±5% of the experimentally evaluated data and lie well within the evaluated experimental uncertainties. Some improvements of the applied methodology are already envisaged, among them an improved approximation of the axial distribution of the water density in the core bypass region.

It should be noted that, despite the known advantages of the Monte Carlo neutron transport codes in comparison with deterministic codes (*e.g.* with respect to the spatial-angular-energy approximations in the neutron transport modeling) and although Monte Carlo codes are already being applied for some practical ex-core neutron transport and dosimetry calculations, routine usage of these codes for full-scale 3D neutron fluence modeling is still considered a bit of a computational challenge. Nevertheless, deterministic codes, being very effective for routine applications, can produce fast fluence estimations associated with notable uncertainties caused mainly by approximate angular neutron transport treatment, usage of multigroup libraries and geometry simplifications [9].

Thus, the present methodology, focused on precise Monte Carlo calculations, accurate reactor conditions modeling and elimination of calculation biases associated with geometry, material and/or neutron source simplifications, can be characterized as a very modern approach.

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