ICONE23-1685

UNCERTAINTY ON FEEDBACK COEFFICIENTS AND KEY CORE PARAMETERS FOR A PRESSURIZED WATER REACTOR DUE TO NUCLEAR DATA UNCERTAINTIES

D.F. da Cruz
Nuclear Research and Consultancy Group NRG,
Petten, The Netherlands

D. Rochman
Nuclear Research and Consultancy Group NRG,
Petten, The Netherlands

A.J. Koning
Nuclear Research and
Consultancy Group NRG,
Petten, The Netherlands

ABSTRACT

The last years the use of the so-called best estimate codes is increasing for the safety analysis required during the licensing process, and are even gradually being prescribed by the regulatory authorities. The use of BE codes have to be coupled with uncertainty and sensitivity analysis.

This paper discusses the uncertainty analysis on reactivity feedback coefficients and other important key reactor parameters for a typical PWR core as a result of uncertainties in $^{235,238}U$, ^{239}Pu and ^{1}H nuclear data. A typical Westinghouse 3-loop reactor design fuelled with UO_2 fuel with 4.8% enrichment has been selected. The Total Monte-Carlo method was applied using the deterministic transport code DRAGON, to generate cross sections and kinetic data for the reactor code PANTHER. The nuclear data used in this study is from the JEFF3.1 evaluation, except for the ENDF nuclear data files for $^{235,238}U$, ^{239}Pu, and thermal scattering data for ^{1}H in water (randomized for the generation of the various DRAGON libraries) which were taken from the nuclear data library TENDL. The total uncertainty on the reactor parameters calculated from the results of the PANTHER code has been split into different components (different isotopes) and the main sources of uncertainties were identified.

1. INTRODUCTION

An important and integral part of the safety analysis required for the license of new reactors and upgrading of current reactors is a thorough analysis of transients, which are considered relevant and realistic for the particular design. Nowadays there is an increasing acceptance and tendency of using best estimate codes (BE) to quantify the effect of these transients, coupled to a comprehensive uncertainty and sensitivity analysis of the results (IAEA, 2009), instead of the traditional methods applying conservative codes and models.

One of the most recent proposed methods to quantify the uncertainties due to nuclear data is the total Monte-Carlo (TMC) method (Koning 2008; Koning 2012), which has been successfully applied to core calculations during both steady-state (da Cruz 2014a) and transient conditions (da Cruz 2014b). The TMC method is a Monte-Carlo based technique developed at NRG that relies on the higher computational power available nowadays. It involves a large number of calculations for the same model performed with different nuclear data in each of them, and therefore bypassing the various covariance processing codes required in the more traditional deterministic approach (Salvatores 2008).

The main goal of the paper is to quantify the uncertainty on key reactor parameters, in special the most important feedback coefficients of reactivity, due to uncertainties in nuclear data. These coefficients are important operational parameters, and are directly related to the stability of the reactor. The paper is organized as follows: Section2 describes the PWR core model using in this work, Section 3 and 4 present the code systems and methodology used respectively, Section 5 summarize the results, and the conclusions and prospects for future work are included in Section 5.

2. PWR core model

The model used in the core calculations are based on a Westinghouse 3-loop PWR loaded with assemblies with 4.8% enriched UO_2 fuel. The main data used for this reactor model are included in Table 1.

Table 1 - Parameters of PWR core model

Nominal thermal power [MWth]	2800
Nr. of loops	3
Power density [W/gHM]	39
Number of Assemblies	157
Assembly configuration	17x17
Assembly pitch [cm]	21.5
Core inlet temperature [°C]	286
Core outlet temperature [°C]	323
Core average temperature [°C]	305
Coolant mass flow [kg/s]	13250
Coolant pressure [bar]	155

The assemblies contain fuel rods arranged in a 17x17 square lattice configuration with pitch of 1.26 cm, and does not contain any burnable absorbers either integrated in the fuel or in the 25 guide tube positions. Therefore, a relatively short fuel cycle is obtained. The core is fueled with 157 fuel assemblies with an assembly pitch of 21.5 cm. Table 2 includes the main parameters used for the fuel assemblies. A 4-batch loading scheme is adopted where the fresh fuel assemblies are placed mostly at the outer boundaries of the core (low-leakage configuration).

Table 2 - Parameters of PWR assembly

Configuration	17x17 lattice
Nr. of guide tubes	25
Cladding material	Zirconium
Clad outer diameter [cm]	0.95
Clad thickness [cm]	0.06
Pellet diameter [cm]	0.82
Active stack [cm]	365
Pin pitch [cm]	1.26

3. Code systems

Most results presented further on in this paper were obtained with the neutronic code PANTHER which contains the full 3D reactor core model. This code uses input data contained in nuclear databases, generated with the lattice code DRAGON based on a single assembly model and a microscopic cross section library. This input library was generated in its turn with the nuclear data processing code NJOY, which takes its data directly from the evaluated nuclear data files in ENDF format. These three code systems will be described in more detail in the coming paragraphs.

3.1 NJOY

NJOY (MacFarlane 1994) is a modular code for processing of nuclear data, read from the evaluation nuclear data files (ENDF). It processes the data at different temperatures and dilution levels, collapses the nuclear data in a few-groups energy grid, and writes the data into a format recognized by the lattice code, in our case the code DRAGON. In this study the DRAGLIB format was chosen. The external module DRAGR, compiled with the standard version of NJOY takes care of editing the necessary information in the DRAGLIB format. The automation of the generation of nuclear data in DRAGLIB format for the different isotopes is taken care by

the code PyNjoy, written in the PYTHON language. This script is also included in the DRAGON code package. The resulting nuclear data libraries used in this study contain data in 172 energy groups (XMAS energy structure).

3.2 DRAGON

The lattice cell code DRAGON (Marleau 1993) can simulate the neutron transport in several types of geometry (1-D up to 3-D), for both thermal and fast spectrum systems. Several algorithms can be used to solve the neutron transport equation including: method of collision probabilities, interface-current method, or the long characteristics method. Other modules are available for interpolation of microscopic cross sections, resonance shielding calculations, editing of condensed and homogenized nuclear quantities, depletion calculations, and sensitivity analysis. Different formats of the microscopic library are supported, besides its native DRAGLIB format. The code DRAGON version 4.0.6 was used in this work. For the nuclear data base generation required by the neutronic code PANTHER, a set of DRAGON runs were required, to deplete the fuel up to a maximum burn-up level and at different reactor conditions. UNIX shell scripts were used to automate these runs. An octant of a fuel assembly is modelled. More details on the modelling in DRAGON were described in a previous publication (da Cruz 2014c).

3.3 PANTHER

PANTHER (Hutt 1991) is a 3-D nodal reactor code for steady-state, fuel management and core transient analyses, and includes an internal thermal-hydraulics module. No modelling is available in this module for the azimuthal and axial conduction. Each channel is treated separately and no account is made for flow redistribution between the channels. The model used cannot predict the propagation of shock waves or choking. Boiling of the coolant is allowed and the code treats it as a vapor/liquid mixture with the possibility to account for sub-cooled boiling and steam-water slip. The user has full control over the material data, including the conductivity and specific heat capacity, which can be provided as function of temperature, irradiation and rating. The conductivity data originates from an expression for UO_2 used in the ENIGMA fuel performance code.

Each assembly (and reflector regions) is represented in PANTHER as a homogenized block (with possible sub-divisions in all three Cartesian directions). PANTHER reads as input a nuclear database for one (or several) fuel type(s), and for each of the reflector types (radial, axial top, and axial bottom). The nuclear database contains mainly macroscopic cross sections (like absorption, fission, scattering and power cross sections), kinetic parameters, isotope concentrations and microscopic cross sections for important fission products. These data are given in a broadband energy structure (2 energy groups, with group boundary at 0.625 eV), and are tabulated as a function of the fuel burn-up and reactor parameters like: fuel and coolant temperature, coolant density, boric acid concentration, and control rod state.

4. Methodology

The uncertainty quantification of important reactor parameters at steady-state conditions due to uncertainties in nuclear data was carried out using the TMC method. The method consists in the repetition of the same calculation (in this case a core simulation with PANTHER) a large number of times varying in each calculation the basic nuclear data used. The nuclear data are changed at the ENDF level, therefore at the input of the NJOY code. Figure 1 shows schematically the total calculation flow.

The different nuclear data files (in ENDF format) are obtained by changing randomly nuclear model parameters within some pre-defined boundaries, at the input of the TALYS nuclear reaction code system (Koning 2012). A total of 20-30 theoretical parameters are varied simultaneously (and independently), with the addition of random resonance parameters. Therefore, nuclear reactions from thermal energy up to 20 MeV are covered. The resonance parameters for a given resonance are varied in a correlated way, taking into account the resonance area.

The resulting random nuclear data files were generated for the following isotopes: ^{235,238}U, ^{239}Pu, and ^{1}H (only thermal scattering data in H_2O); these are considered to yield the largest contribution to the total uncertainty. The following parameters were included in the random ENDF's: cross sections, ν-bar, energy per fission, angular and energy distributions, resonance information, etc. The generation of the random data files for thermal scattering for ^{1}H in H_2O are discussed in a dedicated paper (Rochman 2012).
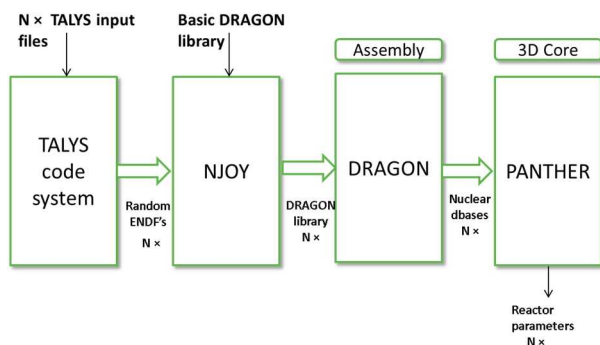

Figure 1 - Calculation scheme for determination of uncertainties in reactor parameters due to nuclear data

Around 450 random nuclear data evaluation files (for each considered isotope) were used to create the same number of microscopic cross section libraries for the lattice code DRAGON. The microscopic cross sections were generated with the processing code NJOY. One basic DRAGON library was used in the process to create the random DRAGON libraries, and it is fully based on JEFF3.1 data. The random data for the chosen isotopes (^{235,238}U, ^{239}Pu, and thermal scattering data for ^{1}H in H_2O) were appended to this basic library. The random data are taken from the nuclear data library TENDL-2011.

For the same number of DRAGON libraries, nuclear databases for the code PANTHER were generated according to the procedure described in section 3.2. The PANTHER runs represent the last stage of the calculation flow, that yields the results for key core parameters during the

equilibrium cycle. The equilibrium core was obtained through simulation of the first 12 cycles, where fresh assemblies are loaded at the beginning of each cycle, and resident assemblies are shuffled according to the loading scheme discussed in Section 2. The first core implemented in the PANTHER model is loaded with fuel of different compositions and enrichment dependent on the batch number. With all control rod banks removed from the core the burn-up of the core is followed at small time steps. The boric acid concentration (with natural boron isotopic composition) in the coolant is adjusted at each time step to keep the core critical, until the end of the natural cycle. From the results of cycle 12 the parameters characterizing the equilibrium cycle were analyzed. The PANTHER results presented in this paper were obtained by varying the nuclear data at cycle #1, and therefore keeping consistent the data used to achieve the equilibrium cycle. By performing statistical analysis of the final results (parameters which characterize the steady-state calculations) obtained separately for each of the available 450 nuclear databases, the different moments (average, standard deviation, skewness, and kurtosis) can be determined and thus infer the final uncertainties in the studied parameters, as a first approximation to the solution of the likelihood equations.

Correlation Analysis

To complement the statistical analysis of the PANTHER results, a correlation analysis of some results was carried out. A set of dedicated scripts calculated the Pearson correlation coefficient (therefore assuming a linear dependence) between particular reactor parameters and the microscopic cross sections for the isotopes of interest. The Pearson correlation coefficient is a measure of the degree of linear correlation between two random variables. The microscopic cross sections for a particular isotope were extracted directly from the random ENDF's and stored in files for further processing.

5. Results

The partial contributions of the different isotopes was quantified for steady-state conditions. These results are presented separately in the following sections.

5.1 General reactor parameters

The contribution of each of the four isotopes to the final uncertainty on the different key quantities were obtained using independent PANTHER runs. The runs for the large number of random nuclear databases were performed, where the nuclear data of only one of the four isotopes were varied at a time. Therefore about 400-450 PANTHER runs were performed for each of the four isotopes. The key quantities chosen to characterize the reactor behavior during steady-state conditions were: critical boron concentration (B_{critic}), maximum power density (P_{max}'''), peaking factors ($F_{\Delta H}$ and F_Q), maximum fuel temperature (T_{fuel}), and maximum fuel burnup. The maximum quantities were calculated over the whole core, and the fuel temperature represents the central temperature of the hottest fuel pin.

In Figure 2 below we show in graphical form the time evolution of the absolute uncertainty in all six parameters, and for each of the four isotopes.
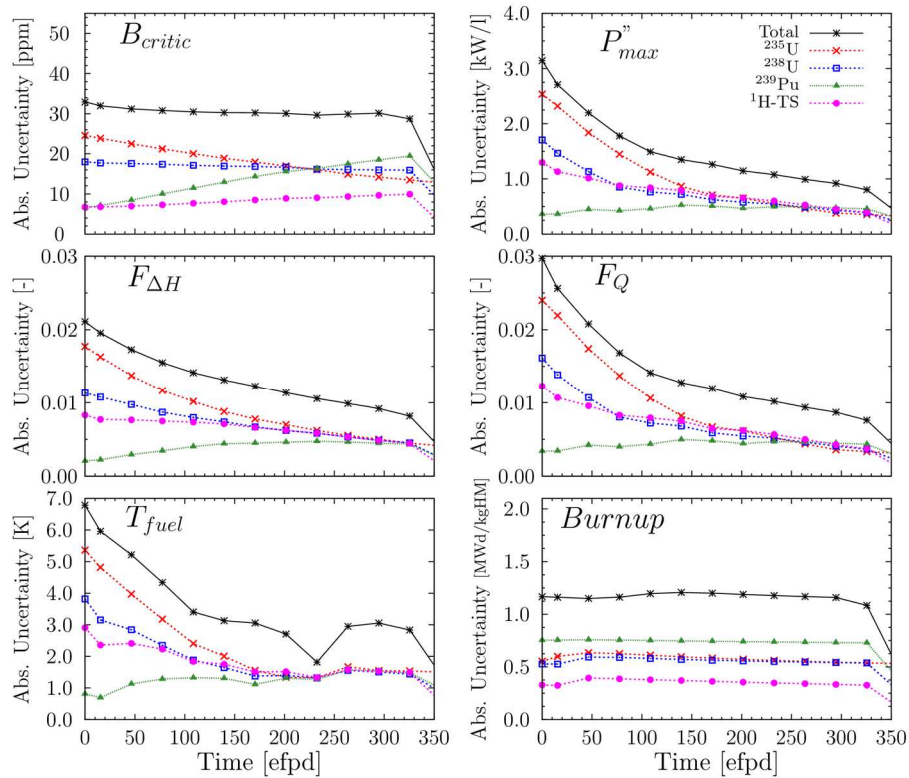
Figure 2 – Time evolution of absolute uncertainty in key reactor parameters, when varying separately nuclear data of the main isotopes (^{235,238}U, ^{239}Pu, and ^{1}H), and for simultaneous variation of all isotopes ("Total"). Critical boron concentration (B_{critic}), maximum power density (P_{max}"), peaking factors ($F_{\Delta H}$ and F_Q), maximum fuel temperature (T_{fuel}), and maximum fuel burnup

Table 3 - Feedback coefficients of reactivity (val.) and relative uncertainties [σ], and main contributor (isot.). DTC- Doppler temperature coefficient, MTC – Moderator temperature coefficient, TPC – Total power coefficient, and Bworth – Boron worth.

	BOC			MOC			EOC		
	val	*σ [%]*	*isot.*	*val*	*σ [%]*	*isot.*	*val*	*σ [%]*	*isot.*
DTC [pcm/K]	-2.34	3.2	U8	-2.52	3.0	U8	-2.62	2.9	U8
MTC [pcm/K]	-27.3	6.3	U5/U8	-46.5	3.7	U8	-66.5	2.1	U8
TPC [pcm/%]	-17.0	3.5	U5	-22.1	2.6	U8U/5	-28.5	1.9	U8/U5
Bworth [pcm/ppm]	-6.36	0.85	U5/8	-6.70	0.96	U8/H1	-7.36	1.1	H1/U8

Also shown is a curve which represents the simultaneous variation of all four isotopes. The average parameters and its time evolution are shown in Figure 3, exclusively for the nuclear databases where the nuclear data for all four isotopes were changed simultaneously. Also included, for the sake of comparison, is a curve correspondent to the nuclear database generated with nuclear data from JEFF3.1 evaluation for all isotopes. The results shown are from cycle #12, and represent therefore the equilibrium cycle results.

The uncertainty in B_{critic} is virtually constant during the cycle and amounts to about 30 ppm, correspondent to 2% relative at BOC. As one could expect, the main contribution at BOC comes from ^{235}U (followed by ^{238}U at the second place), and at EOC ^{239}Pu is the main contributor followed closely by ^{238}U and ^{235}U (in this order). Regarding P_{max}''', the uncertainty is about 3 kW/l at BOC (about 1.4% relative) and decreases monotonically towards the EOC. The largest contribution at BOC is attributed to ^{235}U followed by ^{238}U, whereas at EOC all four isotopes are found to be equally

important.

The peaking factors ($F_{\Delta H}$ and F_Q) show a similar behavior as for the power density, with a monotonic decrease of the uncertainty towards the EOC, and a relativity uncertainty of about 1.2-1.4% at BOC. The main contributors are identical to those for P_{max}'''. The maximum fuel temperature, T_{fuel} also shows a similar behavior, with an absolute uncertainty of 7 K at BOC (0.6% relative).

The maximum fuel burnup increases from a value of 50 MWd/kgHM to about 62 MWd/kgHM towards the EOC. The absolute uncertainty remains virtually constant and amounts to about 1.2 MWd/kgHM (2.5% relative at BOC). Different than for the other five quantities, ^{239}Pu represents the main contributor over the whole cycle, followed by ^{235}U and ^{238}U.

One interesting observation is that for the four quantities: P_{max}''', $F_{\Delta H}$, F_Q, and T_{fuel}, the effect of the uncertainties in ^{1}H thermal scattering data prevails over the ^{239}Pu contribution during a large part of the cycle.
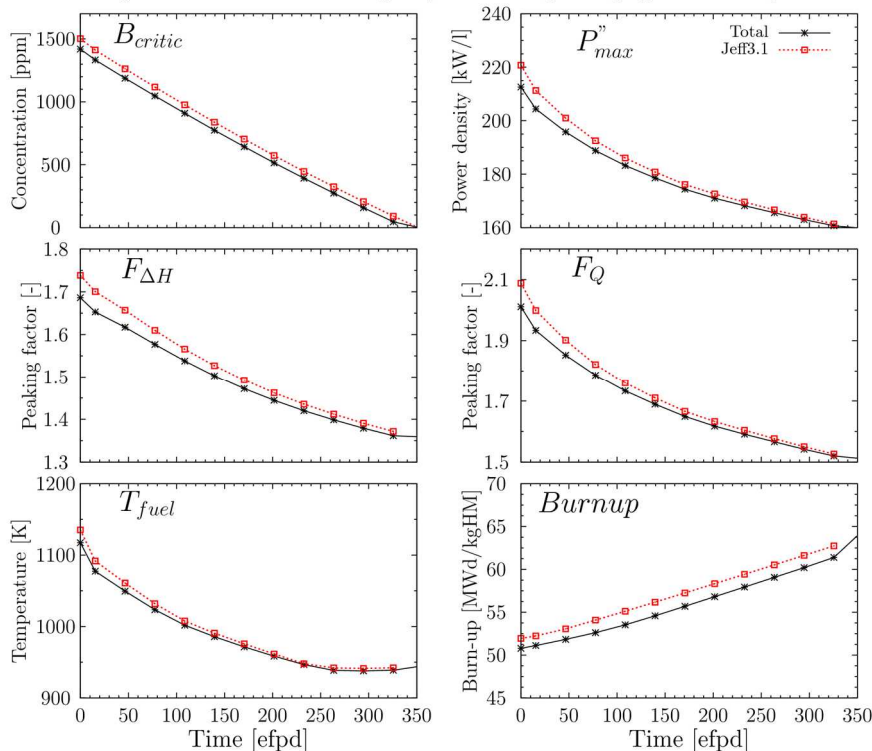

Figure 3 - Time evolution of average key parameters ("Total"). Also included is a curve correspondent to a database fully based on JEFF3.1 data

5.2 Feedback coefficients of reactivity

The following reactivity feedback coefficients were analyzed:

1. DTC – Doppler temperature coefficient
2. MTC – Total moderator temperature coefficient
3. TPC – Total power coefficient
4. Bworth – Boron worth

These coefficients and correspondent uncertainties were calculated according to the procedure described above, and

for three time steps during the cycle: BOC, MOC and EOC. The values presented are for cycle number 12.

Table ?? includes the results for the feedback coefficients. For each of the three time steps the table gives the central value (*val*), the relative uncertainty (σ), and the isotope that gives the largest contribution to the total uncertainty (*isot.*). When more than one isotope is quoted in the table, the second label denotes the second isotope that follows closely the main contributor. The following labels are used: U8 - ^{238}U, U5 - ^{235}U, P9 – ^{239}Pu, and H1 – thermal scattering of ^{1}H in H_2O.

For the DTC, the maximum uncertainty is observed at

BOC and amounts to about 3.2%. The nuclear data of ^{238}U (the main fertile material in the fuel) is the main source of uncertainty, throughout the whole cycle.

The MTC shows a large decrease in central value towards the EOC, and the maximum uncertainty is about 6% at BOC. The main contribution at BOC is attributed to ^{235}U, followed by ^{238}U. At MOC and EOC the contribution of ^{238}U data dominates. Correlation studies of the MTC values with the energy-dependent microscopic cross sections show some significant correlation factors. When correlated with ^{235}U data, the correlation factor with elastic (σ_{el}) and fission (σ_f) cross section at BOC amounts to about -0.5 and -0.6 respectively, for neutron energies below 10 eV. The correlation factor with (σ_f) shows some peak structure correspondent to some resonances. Correlation with the capture cross section (σ_c) shows a peaking behavior, with positive correlation factors for energies below 10 eV with peaks that amounted to up to 0.8. When correlated with ^{238}U data, the most significant correlation is found for σ_{el} with a value of about -0.5, virtually constant for energies below 20 keV, except for some resonant peaks. The correlation factor with σ_c is the second most significant and amounts about -0.4 for energies above 20 keV.

The TPC also shows a monotonic decrease towards the EOC, with a maximum value of -17 pcm/%, and a maximum relative uncertainty of 3.5% at BOC. The main contributors to the final uncertainty are ^{235}U and ^{238}U, dependent on the considered time step. At BOC the ^{235}U nuclear data are the main source of uncertainty, as shown as well by the correlation studies. Similar as for MTC, the correlation factors with σ_{el} and σ_f for ^{235}U are significant and negative for energies below 10 eV, and amount to about -0.5 and -0.7, respectively, at BOC. The correlation with σ_c shows a peak behavior, and with positive correlation factors that can reach up to 0.75. The correlation factors with ^{238}U σ_{el} data, show a constant negative value of about -0.45 at MOC and EOC at energies below 20 keV, except for some peaks in the energy range 10-300 eV.

The boron worth also decreases towards the EOC, with a maximum value of -6.36 pcm/ppm observed at BOC. The maximum relative uncertainty is found at EOC and amounts to about 1.1%. The main contribution to the total uncertainty at BOC can be attributed to ^{235}U (followed by ^{238}U), whereas for MOC the major contribution comes from ^{238}U data and ^{1}H thermal scattering data. At EOC thermal scattering of ^{1}H is the main source of uncertainty.

6. CONCLUSIONS

The Total Monte-Carlo (TMC) method was applied to quantify the uncertainty in reactor parameters due to uncertainties in nuclear data of the main isotopes: ^{235,238}U, ^{239}Pu, and ^{1}H (only thermal scattering data in H$_2$O). Key reactor parameters for a typical PWR core were calculated using the reactor code system PANTHER, for steady-state conditions. These included general core parameters: critical boron concentration, maximum power density, peaking factors, maximum fuel temperature, and maximum fuel burnup; and the main feedback coefficients of reactivity (DTC, MTC, TPC, and boron worth). The study also identified the isotopes that contribute the most to these uncertainties. The following conclusions could be taken:

1. The relative uncertainty in the main general parameters are within 0.6%-2.5%, and the largest uncertainty is found for the maximum fuel burnup values and critical boron concentration. For most parameters nuclear data of ^{235}U represent the largest source of uncertainty, except for fuel burnup for which ^{239}Pu is the main contributor.

2. All four feedback coefficients are negative all over the cycle, and show a decreasing trend towards the EOC. The uncertainty in these values are in the range 0.85%-6.3%, and the largest values are observed for MTC at BOC. For all coefficients the uncertainties decrease towards the EOC, except for the boron worth which displays an opposite trend. The main source of uncertainty at BOC is attributed to ^{235}U for all coefficients, but for boron worth which has ^{238}U data as the main contributor. At EOC the nuclear data of ^{238}U is the main source of uncertainty for all coefficients, except for boron worth for which the contribution of ^{1}H thermal scattering data.

We also show that correlation studies can be used to try to identify the reaction channels that mostly contribute to the uncertainty in feedback coefficients. However, because the resonance parameters in the TMC method are varied consistently, some reaction channels are highly correlated at the resonance energy range, which can pose some difficulties in the interpretation of the results.

In a follow-up of this work, the same approach will be applied to study the uncertainties (and their main sources) during important core transients.

REFERENCES

IAEA, 2009, "Best estimate safety analysis for nuclear power plants: uncertainty evaluation", Safety Report Series, No. 52, International Atomic Energy Agency, Vienna (2008).

A.J. Koning and D. Rochman, 2008, "Towards sustainable nuclear energy; Putting nuclear physics to work," Annals of Nuclear Energy, Vol. **35**, 2024-2030 (2008)

A.J. Koning and D. Rochman, 2012, "Modern nuclear data evaluation with the TALYS code system," Nuclear data sheets, Vol. **113**, 2841-2944 (2012).

D.F. da Cruz, et. al., 2014a, "Total Monte-Carlo method applied to the assessment of uncertainties in a reactivity-initiated accident," Proceedings of Pacific Basin Nuclear Conference (PBNC 2014), Vancouver, Canada, 2014 August 24-28.

D.F. da Cruz, et. al., 2014b, "Propagation of nuclear data uncertainty for a control rod ejection accident using the Total Monte-Carlo method", Proceedings of PHYSOR-2014 Conference, Kyoto, Japan, 2014 September 28 – October 3.

M. SALVATORES et al., 2008, "Uncertainty and Target Accuracy Assessment for Innovative Systems Using Recent Covariance Data Evaluations," a report by the Working Party on International Evaluation Cooperation of the NEA Nuclear Science Committee, NEA0WPEC-26, Vol. 26, Nuclear

Energy Agency, Organization for Economic Co-operation and Development – 2008.

R. MacFarlane and D.M. Muir, 1994, "The NJOY Nuclear Data Processing System, version 91", Report LA-17740, Los Alamos National Laboratory (1994).

G. Marleau, R. Roy, and A. Hebert, 1993, "DRAGON: A Collision Probability Transport Code for Cell and Supercell Calculations", Report IGE–157, Ecole Polytechnique de Montreal (1993).

D.F. da Cruz, et. al., 2014c, "Uncertainty Analysis on Reactivity and Discharged Inventory due to ^{235,238}U and ^{239,240,241}Pu and Fission Products: Application to a Pressurized Water Reactor Fuel Assembly", Nucl. Technol., **185**, 174 (2014).

P.K. Hutt, 1991, "The UK code performance package," Nucl. Energy, Vol. **30**, 291-298 (1991).

D. Rochman and A.J. Koning, 2012, "Random adjustment of the H in H_2O neutron thermal scattering data," Nucl. Sci. and Eng., Vol. **172**, 287-299 (2012).