Uncertainties of Reactivity Calculations with Respect to Nuclear Data for the Canadian SCWR

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Abstract

The Canadian supercritical water-cooled reactor (SCWR) is a pressure tube reactor using heavy water moderator, similar to conventional pressurised heavy water reactors (PHWR). However, it is intended to operate with a coolant pressure of 25 MPa and temperatures of 350ºC (inlet) to 625ºC (outlet). Other novel features include PuO_2/ThO_2 based fuel and advanced fuel bundle and fuel channel designs. This paper presents results of the sensitivity of reactivity calculations such as coolant voiding and fuel temperature coefficients to nuclear data along with contributions to uncertainties of calculation for a radially reflected, axially finite fresh fuel SCWR.

1. Introduction

The high temperature and pressure of supercritical light water (SCW) coolant produce demanding conditions for materials in the Canadian SCWR. Balancing the durability of materials and gains in thermodynamic efficiency against losses due to increased material neutron absorption is a major challenge in SCWR development. Additional challenges to current modelling techniques include large gradients in coolant temperature and density between the inlet and outlet of SCWR fuel channels.

Reliability of reactor physics calculations for the SCWR depends on detailed knowledge of the nuclear data for the materials and range of conditions being modelled. As accuracy of the nuclear data limits the accuracy of the calculations, assessing the quality of nuclear data for SCWR requires that the sensitivity of the calculations to the data as well as the quality of the data itself be considered [1] [2]. A study of the effect of uncertainties in actinide cross sections in advanced systems for transmutation of nuclear waste [3] or the use of the ERANOS code to examine uncertainties in modeling of advanced fast reactors [4] are among the few nuclear-data-related studies pertaining to GEN-IV systems. A previous study on nuclear data sensitivity of the Canadian SCWR was a comparative study [5] of nuclear data libraries.

In this paper TSUNAMI (Tools for Sensitivity and Uncertainty Analysis Methodology Implementation) codes in SCALE (Standardized Computer Analyses for Licensing Evaluation) 6.0 [6] were used to gain understanding of the effects of nuclear data on calculations for SCWR fresh fuel. This study involves the neutron multiplication factor of the system (k), as well as the coolant voiding and fuel temperature reactivity coefficients. The

sensitivity of these calculations to nuclear data is examined as well as their uncertainties due to the uncertainties in the nuclear data. A radially reflected, axially finite lattice of fresh fuel was considered for simplicity; it facilitates the isolation of major contributions to uncertainties in *k* and reactivity coefficients without the complication of fission and activation products. Subsequent studies will include the examination of irradiated fuel in infinite lattices and a representation of the entire SCWR core. The data libraries used for this study are based on ENDF/B-VII data.

2. Theory

The TSUNAMI code modules used here consist of TSUNAMI-3D for sensitivity calculations of *k* calculations and TSAR (Tools for Sensitivity Analysis of Reactivity) for sensitivity calculations of reactivity parameters. These are described in more detail below.

TSUNAMI-3D is one of the functional TSUNAMI sequences that execute KENO V.a to generate forward and adjoint neutron transport solutions followed by SAMS (Sensitivity Analysis Module for SCALE) to produce sensitivity coefficients as described in [6].

SAMS determines a sensitivity profile consisting of a dimensionless quantity at each energy group, which is calculated as a fraction of the neutron multiplication factor, *k*. As will be discussed later, the contributions to sensitivity from selected isotopes are also dimensionless and expressed as fractions of *k*. The complete sensitivity including the implicit component from the resonance self shielding calculations and the explicit component of *k* due to perturbations of the nuclear data $\Omega^{i}_{x,g}$, (representing both the cross section data Σ and other nuclear data terms)can be defined as,

$$(S_{k,\Sigma^{i}_{x,g}})_{complete} = \frac{\Omega^{i}_{x,g}}{k}\frac{\partial k}{\partial \Omega^{i}_{x,g}} + \sum_{j}\sum_{h}\frac{\Omega^{j}_{y,h}}{k}\frac{\partial k}{\partial \Omega^{j}_{y,h}} \times \frac{\Omega^{i}_{x,g}}{\Omega^{j}_{y,h}}\frac{\partial \Omega^{j}_{y,h}}{\partial \Omega^{i}_{x,g}}, \qquad (1)$$

where the nuclear data component for process *y* of nuclide *j* in energy group *h* is denoted $\Omega^{j}_{y,h}$,.

The code also determines uncertainties in code results, such as *k*, that are due to cross-section uncertainties by combining the sensitivity results with the covariance matrix,

$$\sigma_k^2 = S_k C_{\alpha\alpha} S_k^T, \qquad (2)$$

where $C_{\alpha\alpha}$ is the nuclear data covariance matrix between all cross sections α,

$$C_{\alpha\alpha} = \left[\frac{COV(\alpha_m, \alpha_p)}{\alpha_m \alpha_p}\right], \text{ m = 1, 2... M; p = 1, 2... M,} \qquad (3)$$

and M is the number of nuclide-reaction pairs multiplied by the number of energy groups. The diagonal terms are the nominal cross section uncertainties for each nuclide, reaction and energy, whereas the off diagonal terms relate terms at different energies and in a few cases different reactions and/or nuclides. SAMS can provide the total uncertainty, or partial uncertainties in *k* due to the uncertainty in individual nuclides.

The TSAR code computes reactivity sensitivities based on the *k* sensitivities of two states. The reactivity sensitivity profile is calculated from the *k* sensitivity profiles S_k using

$$S_{\rho,\alpha} = (\lambda_2 S_{k_2,\alpha} - \lambda_1 S_{k_1,\alpha}), \quad (4)$$

for a particular nuclide reaction cross-section "α" where the reactivity change between the two states is (λ_1-λ_2) and $\lambda = 1/k$.

Because it uses the sensitivity profiles generated by SAMS and covariance data, TSAR can also be used to compute uncertainties in calculated reactivity coefficients due to uncertainties in the nuclear data. TSAR can provide the total uncertainty, or partial uncertainties in reactivity coefficients due to individual nuclide reaction uncertainty.

3. Models

Models were constructed for a radially reflected fresh fuel SCWR channel. The radial specifications for the bundle are based on those used in [8] and are shown in Table 1 and Figure 1. This is a 54 element bundle with a centre pin of zirconia. The channel then has a perforated steel liner, a porous zirconia insulator and a Zircaloy pressure tube.

Table 1
Specification for the 54-Element Bundle and HEC (High Efficiency Channel)

Parameter	Value
Elements per bundle	54
Elements in rings 1, 2, 3	12, 18, 24
Pitch circle radius, ring 1	2.8755 cm
Pitch circle radius, ring 2	4.3305 cm
Pitch circle radius, ring 3	5.8000 cm
Radius of central pin	1.94 cm
Outer radius of central pin cladding	2.00 cm
Radius of fuel in ring 1, 2 and 3	0.620 cm
Outer radius of ring 1, 2 and 3 pin cladding	0.680 cm
Lattice pitch	25 cm
Liner tube inner radius	6.8 cm
Liner tube thickness	0.1 cm
Insulator inner radius	6.9 cm
Insulator thickness	1.33 cm

Pressure tube inner radius	8.23 cm
Pressure tube thickness	1.4 cm

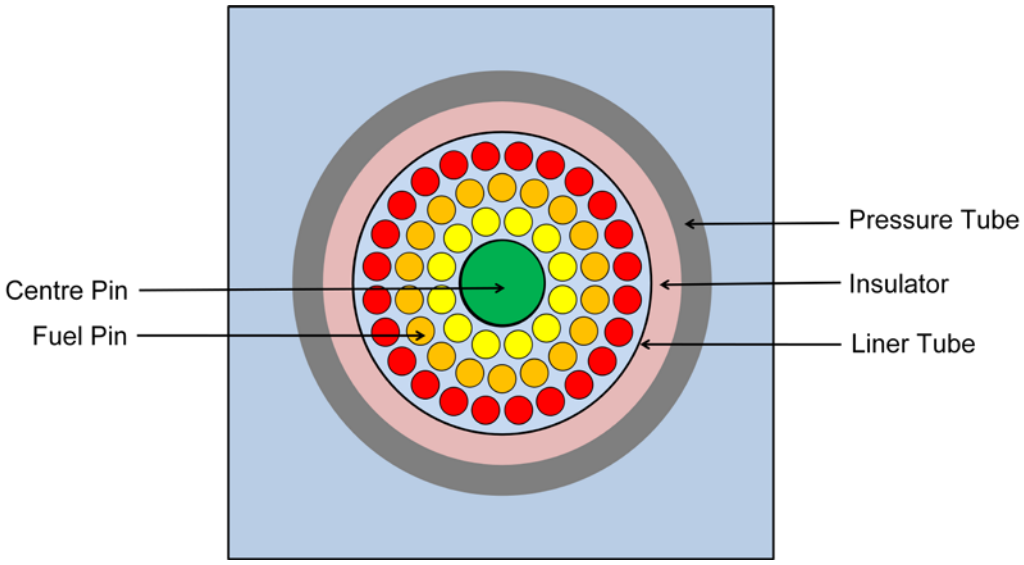

Figure 1 The SCWR Channel Cross section

The materials that were used in building the models are shown in Table 2. The fuel is 14% by weight PuO_2 in ThO_2 . The fuel cladding and perforated liner are made of modified 310 stainless steel (310 SS).

Table 2
Material Composition in Model

Material	Composition
Centre Pin	ZrO_2
Fuel Pins	14% by weight PuO_2 in ThO_2
Pin Cladding	Modified 310 SS
Perforated Liner	Modified SS with 50% by volume Coolant
Porous Insulator	ZrO_2 with 70% by volume Coolant
Pressure Tube	Zircaloy
Coolant	H_2O
Moderator	0.09% by weight H_2O in D_2O

Table 3
Material Temperatures

Axial Zone	Coolant Density (kg/m^3)	Coolant Temp (K)	Fuel Temp (K)	Clad Temp (K)	Liner Temp (K)	Insulator Temp (K)	Pressure Tube Temp (K)	Moderator Temp (K)
1	592.54	632.35	960.15	796.35	632.35	554.88	477.55	342.16
2	382.46	656.30	960.15	808.30	656.30	570.83	485.51	342.16
3	160.92	675.27	960.15	817.76	675.27	583.46	491.82	342.16
4	89.49	774.05	960.15	867.04	774.05	649.25	524.65	342.16
5	69.63	881.45	960.15	920.63	881.45	720.78	560.35	342.16

The temperatures for the materials at each nominal axial location are also taken from [8] and are shown in Table 3. The liner and insulator are modeled as volume percent mixtures with the metal and coolant.

The geometry of the models is a single channel, reflected in x and y and with a 30 cm layer of coolant at both axial ends. The coolant regions at the ends of the channel are of the same density of the coolant in the adjacent part of the channel and simulates the gross features of the coolant flow at either end of the channel. The fuel assembly in the channel is axially subdivided into ten subassemblies which are separated by nine plates that act as spacers/bundle ends, as well as plates at either end of the channel. These are 1 cm plates of 310 SS between the fuel and 0.5 cm plates on each end, comprising 2% of the total axial length of the channel. For modelling purposes, the channel is divided into 5 axial zones (see Figure 2), in each of which the temperatures and coolant pressure are held constant. This step-wise change in the material properties approximates the gradual change of conditions from the inlet to the outlet.

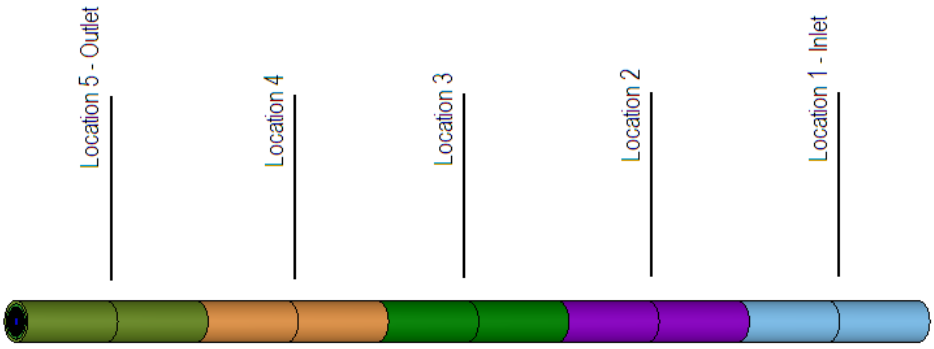

Figure 2 Axial Partitioning of Model

Each ring of fuel pins used different material designation numbers, though the material definitions were identical. In addition, each of the five temperature zones used separate material designation numbers. This allows for sensitivity results to be obtained as a function of both radial and axial location in the channel.

The base or reference case that was modeled for the KENO V.a /TSUNAMI-3D calculations has the temperature and coolant density properties indicated in Table 3. To examine sensitivities of reactivity cefficients to the nuclear data, perturbations in temperature and coolant composition were implemented as shown in Table 4. These calculated sensitivities for pairs of perturbations were used in TSAR to examine the sensitivities of the reactivity changes.

Table 4
Scenarios Modeled in TSUNAMI-3D and the Calculated Effective Multiplication Factor

Case Name	Description	KENO *k*
Reference	Cooled SCWR channel, nominal Moderator, Coolant and Fuel Temperature	1.2303 ± 0.0001
Voided	Coolant replaced with air	1.2269 ± 0.0001
Fuel Hot	Fuel Temperature Increased by 100 K	1.2275 ± 0.0001
Fuel Cool	Fuel Temperature Decreased by 100 K	1.2330 ± 0.0001
Fuel Hot while voided	Fuel Temperature Increased by 100 K and Coolant Replaced by Air	1.2239 ± 0.0001
Fuel Cool while voided	Fuel Temperature Decreased by 100 K and Coolant Replaced by Air	1.2300 ± 0.0001

4. Results

4.1 Reference Case

The effective multiplication factor calculated for the base case is shown in Table 4. The sensitivity of the calculation to nuclear data is shown in Table 5. A negative sensitivity indicates that the change in *k* is in the opposite direction than the change in the cross section (i.e. an increase in the cross section would lead to a decrease in *k*).

The sensitivities are calculated as a function of the reactions for each nuclide for each material. The highest ten sensitivities in this edit are on plutonium isotopes in the outer ring of fuel. The ^{239}Pu $\bar{\nu}$, fission and capture reactions are the most relevant. Because the model was built with each ring of fuel and each coolant density region having unique material numbers, this also indicates locations in the channel for which various materials have the most significant contribution to sensitivities. The results are center-peaked and approximately symmetrical along the channel, with the inlet and outlet materials making smaller contributions to the sensitivities. It is important to note that though the ten most sensitive

materials are listed here, this is an arbitrary cut-off. It is more relevant generally to make a cut on the uncertainty impact for calculations of interest.

Table 5
Top 10 Sensitivities by Reaction, Nuclide and Material

Material Number	Material Description	Nuclide	Reaction / Data	Sensitivity
231	Outer Ring Fuel in Location 3	^{239}Pu	$\bar{\nu}$	2.12E-01
331	Outer Ring Fuel in Location 4	^{239}Pu	$\bar{\nu}$	1.60E-01
131	Outer Ring Fuel in Location 2	^{239}Pu	$\bar{\nu}$	1.22E-01
231	Outer Ring Fuel in Location 3	^{239}Pu	fission	9.44E-02
331	Outer Ring Fuel in Location 4	^{239}Pu	fission	7.06E-02
231	Outer Ring Fuel in Location 3	^{241}Pu	$\bar{\nu}$	7.03E-02
231	Outer Ring Fuel in Location 3	^{239}Pu	n,γ	-5.91E-02
131	Outer Ring Fuel in Location 2	^{239}Pu	fission	5.40E-02
331	Outer Ring Fuel in Location 4	^{241}Pu	$\bar{\nu}$	5.34E-02
331	Outer Ring Fuel in Location 4	^{239}Pu	n,γ	-4.47E-02

The sensitivity of the *k* to nuclear data can be combined with a nuclear data uncertainty covariance matrix to estimate the uncertainty in *k* due to uncertainties in nuclear data. Here, the total uncertainty due to nuclear data is estimated to be 11.20 mk and is determined by the quadrature sum (the square root of the sum of squares, preserving negative signs) of the individual terms. This method uses first order perturbations and assumes that changes are linear. This is generally true if the perturbations are small enough. As the total of all perturbations to *k* come to less than 1% of the value of *k*, this assumption is reasonable.

The nuclides that make contributions to the uncertainty above 0.5 mk and the values of those contributions are shown in Table 6.

The summed uncertainty of the displayed terms is 11.15 mk, indicating that the important terms are captured. The uncertainty contributors are elements of the covariance matrix. Hence, there are two columns, though in most cases the diagonal term is the primary contributor. The negative contributions occur because of the cross terms between reactions in the covariance matrix, for example deuterium n,2n and elastic scattering.

It is important to note that largest contributors to the uncertainties do not necessarily correlate with the largest contributors to sensitivity. For example, the uncertainty contribution of ^{92}Zr n, γ is higher than ^{239}Pu n, γ contributions, yet the sensitivity of *k* to this reaction does not appear in the top sensitivities shown in Table 5. This may be explained by the relatively high cross-section uncertainty for zirconium, which increases the importance of zirconium in simulations of SCWR and similar applications. Also of note, the code does not have the ability to deal with differential scattering or angular components which may be important for terms such as deuterium scattering.

Table 6
Contributions to Nuclear Data Uncertainty in the Reference Case

Covariance Matrix		Contributions to Uncertainty Due to this Matrix (mk)
Nuclide Reaction	Nuclide Reaction	
^{239}Pu $\bar{\nu}$	^{239}Pu $\bar{\nu}$	8.84
^{239}Pu fission	^{239}Pu fission	2.78
^{92}Zr n,γ	^{92}Zr n,γ	2.65
^{2}H elastic	^{2}H elastic	2.47
^{239}Pu n,γ	^{239}Pu n,γ	2.38
^{91}Zr n,γ	^{91}Zr n,γ	2.02
^{2}H n,2n	^{2}H elastic	-2.01
^{239}Pu fission	^{239}Pu n,γ	1.92
^{90}Zr n,γ	^{90}Zr n,γ	1.71
^{2}H n,2n	^{2}H n,2n	1.58
^{240}Pu n,γ	^{240}Pu n,γ	1.48
^{93}Nb n,γ	^{93}Nb n,γ	1.34
^{232}Th n,γ	^{232}Th n,γ	1.29
^{56}Fe n,γ	^{56}Fe n,γ	1.17
^{241}Pu $\bar{\nu}$	^{241}Pu $\bar{\nu}$	0.91
^{242}Pu n,γ	^{242}Pu n,γ	0.88
^{241}Pu fission	^{241}Pu fission	0.81
^{58}Ni n,γ	^{58}Ni n,γ	0.68
^{239}Pu chi	^{239}Pu chi	0.66
^{53}Cr n,γ	^{53}Cr n,γ	0.62

4.2 Coolant Void Reactivity

The code module TSAR was used with sensitivity input from both cooled and voided cases. There were no other changes made to these models. The coolant void reactivity (CVR) calculations were performed assuming that a voided condition meant air in the channels. Other perturbations of interest may be of a channel uniformly filled with the lowest density light water coolant, or the highest; these will be examined in the future.

The value of the CVR worth according to the cooled and voided *k* calculations is 2.25 mk. The TSAR calculated sensitivities are shown in Table 7. The primary contributors to uncertainty are shown in Table 8, with the total uncertainty due to nuclear data assessed to be 1.12 mk, which is found by the same quadrature summing procedure as for k_{inf}. Absorption in zirconium is a high contributor here. However, it is not high on the list of sensitivities seen in

Table 7. The inclusion of these isotopes on the list of important uncertainties is due to the high nuclear data uncertainty assessed to them rather than them having high sensitivities.

Table 7
Top Ten CVR Nuclear Data Sensitivities Calculated by TSAR

Nuclide	Reaction	Sensitivity
^{2}H	elastic	44.0
^{1}H	elastic	-18.6
^{232}Th	n,γ	-13.2
^{1}H	n,γ	8.5
^{239}Pu	n,γ	7.8
^{241}Pu	$\bar{\nu}$	7.2
^{239}Pu	$\bar{\nu}$	-7.2
^{241}Pu	fission	2.9
^{56}Fe	elastic	-0.7
^{241}Pu	n,γ	-0.6

Table 8
Top Ten CVR Nuclear Data Uncertainties Calculated by TSAR

Covariance Matrix		Contributions to Uncertainty Due to this Matrix (mk)
Nuclide-Reaction	Nuclide-Reaction	
^{2}H elastic	^{2}H elastic	0.90
^{92}Zr n,γ	^{92}Zr n,γ	0.42
^{91}Zr n,γ	^{91}Zr n,γ	0.31
^{90}Zr n,γ	^{90}Zr n,γ	0.27
^{2}H n,2n	^{2}H elastic	-0.27
^{239}Pu n,γ	^{239}Pu n,γ	0.21
^{239}Pu fission	^{239}Pu n,γ	0.16
^{239}Pu $\bar{\nu}$	^{239}Pu $\bar{\nu}$	0.15
^{239}Pu fission	^{239}Pu fission	0.14
^{232}Th n,γ	^{232}Th n,γ	0.13

4.3 Fuel Temperature Coefficient

The TSAR code module was also used to examine the effect of fuel temperature coefficient (FTC). The fuel temperature was changed along with the fuel cladding. The coolant

temperature was not changed. The TSAR calculation looked at the reactivity difference between a state with the fuel temperature 100 K above the nominal conditions and one at 100 K below the nominal conditions. This effect was calculated for both a cooled and voided system, where the voided system is important for potential accident scenarios and the cooled system fuel temperature effects can give information relating to fuel feedback temperature changes during operation.

4.3.1 Fuel Temperature Coefficient in SCW Cooled Case

The reactivity worth of increasing the fuel temperature by 200 K in the cooled case is -3.63 mk, or -0.02 mk/K. The highest contributors to nuclear data sensitivity are shown in Table 9. Deuterium, plutonium and thorium reactions have high sensitivity here. The uncertainty due to nuclear data is assessed to be 0.07 mk or 3.5E-4 mk/K, with the ten most important components listed in Table 10. Here, deuterium scattering and absorption in ^{232}Th and ^{239}Pu are the most important.

Table 9
Cooled FTR Nuclear Data Sensitivities Calculated by TSAR

Nuclide	Reaction	Sensitivity
^{2}H	elastic	2.6
^{239}Pu	$\bar{\nu}$	2.5
^{239}Pu	fission	2.2
^{232}Th	n, γ	-1.9
^{1}H	elastic	-1.1
^{241}Pu	$\bar{\nu}$	0.8
^{241}Pu	fission	0.8
^{1}H	n, γ	0.7
^{239}Pu	n, γ	-0.5
^{16}O	elastic	-0.2

Table 10
Cooled Fuel Temperature Coefficient Uncertainties Calculated by TSAR

Covariance Matrix		Contributions to Uncertainty Due to this Matrix (mk/K)
Nuclide-Reaction	Nuclide-Reaction	
^{2}H elastic	^{2}H elastic	2.5E-4
^{232}Th n,γ	^{232}Th n,γ	1.5E-4
^{2}H n,2n	^{2}H elastic	-1.5E-4
^{239}Pu $\bar{\nu}$	^{239}Pu $\bar{\nu}$	1.0E-4
^{92}Zr n,γ	^{92}Zr n,γ	1.0E-4
^{239}Pu fission	^{239}Pu fission	0.5E-4

^{91}Zr n,γ	^{91}Zr n,γ	0.5E-4
^{232}Th n,n'	^{232}Th n,n'	0.5E-4
^{2}H n,2n	^{2}H n,2n	0.5E-4
^{90}Zr n,γ	^{90}Zr n,γ	0.5E-4

4.3.2 Fuel Temperature Coefficient in Voided Case

The reactivity worth of increasing the fuel temperature by 200 K in the voided case is -4.05 mk, or -0.02 mk/K. The highest sensitivity nuclide reactions are listed in Table 11. Changes in scattering data in the moderator have a positive effect on FTC, whereas capture in the fuel has a negative effect. The main difference seen from the cooled FTC sensitivities are that here the plutonium fission is much less important, whereas the deuterium scattering is more important.

Table 11
Voided FTR Nuclear Data Sensitivities Calculated by TSAR

Nuclide	Reaction	Sensitivity
^{2}H	elastic	4.2
^{239}Pu	$\bar{\nu}$	3.0
^{232}Th	n, γ	-1.9
^{239}Pu	n, γ	-1.5
^{239}Pu	fission	0.9
^{241}Pu	$\bar{\nu}$	0.7
^{240}Pu	n, γ	-0.5
^{241}Pu	n, γ	-0.2
^{241}Pu	fission	0.1
^{240}Pu	$\bar{\nu}$	0.1

Table 12
Voided Fuel Temperature Coefficient Uncertainties Calculated by TSAR

Covariance Matrix		Contributions to Uncertainty Due to this Matrix (mk/K)
Nuclide-Reaction	Nuclide-Reaction	
^{2}H elastic	^{2}H elastic	4.0E-4
^{239}Pu $\bar{\nu}$	^{239}Pu $\bar{\nu}$	1.5E-4
^{232}Th n,γ	^{232}Th n,γ	1.5E-4
^{2}H n,2n	^{2}H elastic	-1.0E-4
^{239}Pu n,γ	^{239}Pu n,γ	0.5E-4

^{239}Pu chi	^{239}Pu chi	0.5E-4
^{232}Th n,n'	^{232}Th n,n'	0.5E-4
^{242}Pu n,γ	^{242}Pu n,γ	0.5E-4
^{92}Zr n,γ	^{92}Zr n,γ	0.5E-4
^{240}Pu n,γ	^{240}Pu n,γ	0.5E-4

The uncertainty due to nuclear data is assessed to be 0.10 mk or 5.0 E-4 mk/K, with the ten most important components listed in Table 12. Following from the sensitivities, deuterium scattering and thorium absorption are high contributors to the uncertainty.

5. Conclusion

The *k* calculations show that in the fresh fuel case, plutonium and deuterium reactions are the highest contributors to the uncertainty arising from nuclear data. The most sensitive individual reactions are those involving plutonium in the outer fuel ring.

For CVR calculations, the nuclear data contributing the most to uncertainty are those for deuterium scattering, zirconium absorption and plutonium reactions. For FTC calculations, deuterium scattering is still important, as is absorption in both plutonium and thorium.

The next phase of this work will be to examine partly irradiated fuel (e.g. mid and end of cycle) in order to assess and compare the contributions to uncertainty of important nuclides in the irradiated fuel such as ^{233}U, ^{233}Pa, ^{234}Pa and various fission products.

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