Nuclear Data Sensitivity and Uncertainty for Fresh Fuel Assemblies in the Canadian SCWR

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Abstract

Accurate and complete nuclear data are a fundamental requirement for any nuclear reactor model. One major challenge to the modeling of advanced nuclear reactor systems is the lack of sufficient nuclear data for the operating conditions and materials relevant to the advanced systems. The Canadian supercritical water-cooled reactor (SCWR) is an advanced reactor concept which, like all advanced GEN-IV reactor concepts, differs significantly in operating conditions, fuel composition and non-fuel materials from conventional reactors. The Canadian SCWR is a pressure tube-based reactor with heavy water moderator and light water coolant, intended to operate with a coolant pressure of 25 MPa and temperatures ranging from 350 °C (inlet) to 625°C (outlet), with $(Pu,Th)O_2$ fuel, using advanced fuel bundle and fuel channel designs. Because of these differences from conventional heavy water (HWR) and light water (LWR) reactors, it is not clear whether presently-used core modeling methods or nuclear data libraries are adequate for SCWR modeling. In this paper, an idealized model of an SCWR fuel channel with fresh fuel is modeled in order to examine the nuclear data contributions to the sensitivity and uncertainties in the neutron multiplication factor, *k*, and various lattice reactivity coefficients.

Keywords: Nuclear Data, Sensitivity, Uncertainty, Reactivity, Supercritical Water-Cooled reactor, SCWR

Highlights:

- Simplified fuel channel model specifications are provided for the Canadian SCWR.
- Nuclear data-based sensitivities and uncertainties in reactivity are evaluated.
- Major sources of the uncertainties in *k* and reactivity coefficients are identified.

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1. Introduction

Advanced Generation-IV (GEN-IV) reactor concepts are being developed through an international collaboration, the GEN-IV International Forum (GIF), in order to provide future nuclear energy systems with enhanced safety, improved resource sustainability, improved economic benefit and enhanced proliferation resistance (U.S. DOE Nuclear Energy Research Advisory Committee, 2002). Canada's primary contribution to the GIF is the Canadian SCWR (Leung et al., 2011), which is a heavy water moderated, pressure tube reactor that uses supercritical light water (SCW) as a coolant. The use of SCW coolant significantly increases the thermodynamic efficiency of the SCWR over present heavy water reactors (HWR), from approximately 33% to as high as 48% efficiency. This increase is offset by the need for SCW-resistant in-core materials, which absorb more neutrons than traditional materials, and for batch (rather than online) refuelling (Pencer and Hyland, 2011). SCWR operating conditions and materials, therefore, present significant differences from conventional HWR and light water reactors (LWR). Since current reactor core physics modeling codes have been optimized for conventional HWR and LWR designs, the SCWR challenges current modeling methods.

The accuracy of calculations of reactivity parameters is limited by the nuclear data, and assessment of the nuclear data must consider the sensitivity of the SCWR calculations to the data as well as the quality of the data itself (Chang, 2003; Driscoll and Hejzlar, 2005; Forrest, 2010; Pelloni and Mikityuk, 2012). A study of the effect of uncertainties in actinide cross sections in advanced systems for transmutation of nuclear waste (Artisyuk et al., 2008), and the use of the ERANOS code to examine uncertainties in modeling of advanced fast reactors (Aliberti et al., 2006; Pelloni and Mikityuk, 2012) are among the few nuclear-data-related studies pertaining to GEN-IV systems. There have only been two previous studies on nuclear data sensitivities of the Canadian SCWR, a comparative study of nuclear data libraries (Kozier and Dyck, 2005) and a similarity study against previous and proposed experiments in the ZED-2 critical facility (Langton et al., 2012).

In this paper, the TSUNAMI (Tools for Sensitivity and Uncertainty Analysis Methodology Implementation) codes in SCALE (Standardized Computer Analyses for Licensing Evaluation) 6.0 (Oak Ridge National Laboratories, 2009; Reardon et al., 2011) are used to study the effects of nuclear data on calculations for SCWR fresh fuel. This study presents results for the neutron multiplication factor of the system (k), as well as coolant voiding, fuel temperature, coolant temperature and moderator 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 is considered for simplicity; it facilitates the isolation of major contributions to uncertainties in k and in reactivity coefficients without the complication of fission and activation products. This paper combines and expands upon studies presented at two recent conferences, the 3rd China-Canada Joint Workshop on Supercritical-Water-Cooled Reactors (Blomeley and Pencer, 2012a) and the 33rd Canadian Nuclear Society Annual Meeting (Blomeley and Pencer, 2012b).

2. Theory

As discussed above, the accuracy of any reactor model is limited by the uncertainties in nuclear data that form the basis of that model. The objective of this study is to determine the impact of these uncertainties in nuclear data on modeling of the SCWR. In this paper, the sensitivities of *k* and reactivity coefficients to nuclear data, and resultant uncertainties are determined using the TSUNAMI code set. The specific TSUNAMI code modules used were TSUNAMI-3D for sensitivity calculations of *k* calculations and TSAR (Tools for Sensitivity Analysis of Reactivity) for sensitivity calculations of reactivity parameters. The TSUNAMI code set, nuclear data library and nuclear data covariance data library used for this study were the versions distributed with SCALE 6.0 (Oak Ridge National Laboratories, 2009). The libraries and codes used are described in more detail below.

Calculations were performed using the 238-group ENDF/B-VII Rel. 0 library and the single, comprehensive cross-section-covariance data library distributed with SCALE 6.0. The covariance library combines evaluated covariance data from a number of sources (Reardon et al., 2011). The application of this set of covariance data is based on a number of assumptions (Williams et al., 2009), which will not be discussed here. Nevertheless, the uncertainties determined below depend directly on the covariance data and consequently, specific conclusions made based on those uncertainties should take into account the relevant assumptions made in the evaluations of the covariance data used.

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 (Oak Ridge National Laboratories, 2009; Reardon et al., 2011).

SAMS determines a sensitivity profile consisting of a dimensionless quantity at each energy group, which is calculated as the fractional change in the neutron multiplication factor, *k*, with respect to the fractional change in the macroscopic cross section, Ω, i.e.

$$sensitivity = \frac{\frac{\partial k}{k}}{\frac{\partial \Omega^{i}_{x,g}}{\Omega^{i}_{x,g}}}, \tag{1}$$

where the nuclear data component for process *x* of nuclide *j* in energy group *g* is denoted $\Omega^{i}_{x,g}$. The contributions to sensitivity from various isotopes discussed later 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,

$$(S_{k,\Sigma^i_{x,g}})_{complete} = \frac{\Omega^i_{x,g}}{k}\frac{\partial k}{\partial \Omega^i_{x,g}} + \sum_j \sum_h \frac{\Omega^j_{y,h}}{k}\frac{\partial k}{\partial \Omega^j_{y,h}} \times \frac{\Omega^i_{x,g}}{\Omega^j_{y,h}}\frac{\partial \Omega^j_{y,h}}{\partial \Omega^i_{x,g}}, \qquad (2)$$

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 *k* that are due to nuclear data covariances by combining the sensitivity results with the covariance matrix,

$$\sigma_k^2 = S_k C_{\alpha\alpha} S_k^T, \qquad (3)$$

where $C_{\alpha\alpha}$ is the nuclear data covariance matrix between all cross sections (and all other nuclear data terms) α,

$$C_{\alpha\alpha} = \left[\frac{COV(\alpha_m, \alpha_p)}{\alpha_m \alpha_p}\right], \; m = 1, 2 \ldots M; \; p = 1, 2 \ldots M, \qquad (4)$$

and *M* is the number of nuclide-reaction pairs multiplied by the number of energy groups. The diagonal terms are the nominal cross section variances (square roots of the covariances) 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 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

$$S_{\rho,\alpha} = (\lambda_2 S_{k_2,\alpha} - \lambda_1 S_{k_1,\alpha}), \qquad (5)$$

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

For this study, a radially reflected, axially finite lattice of SCWR channels containing fresh fuel assemblies was considered for simplicity; it facilitates the isolation of major contributions to uncertainties in neutron multiplication factor *k* and reactivity coefficients without the complication of fission and activation products. Although alternative SCWR bundle designs have recently been presented (McDonald et al., 2011), the specifications used in this study are based on those used in (Boczar et al., 2010; Magill et al, 2011) in order to facilitate

comparisons with other related studies (e.g. Harrison and Marleau, 2012; Shen, 2012). The bundle and channel specifications are shown in Table 1 and Figure 1. This is a 54-element bundle with a centre pin of zirconia. The channel has a perforated steel liner, a porous zirconia insulator and a Zircaloy pressure tube.

The materials that were used in the models are listed 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). The liner and insulator are modeled as homogeneous volume-weighted mixtures of coolant with liner material and insulator material, respectively.

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

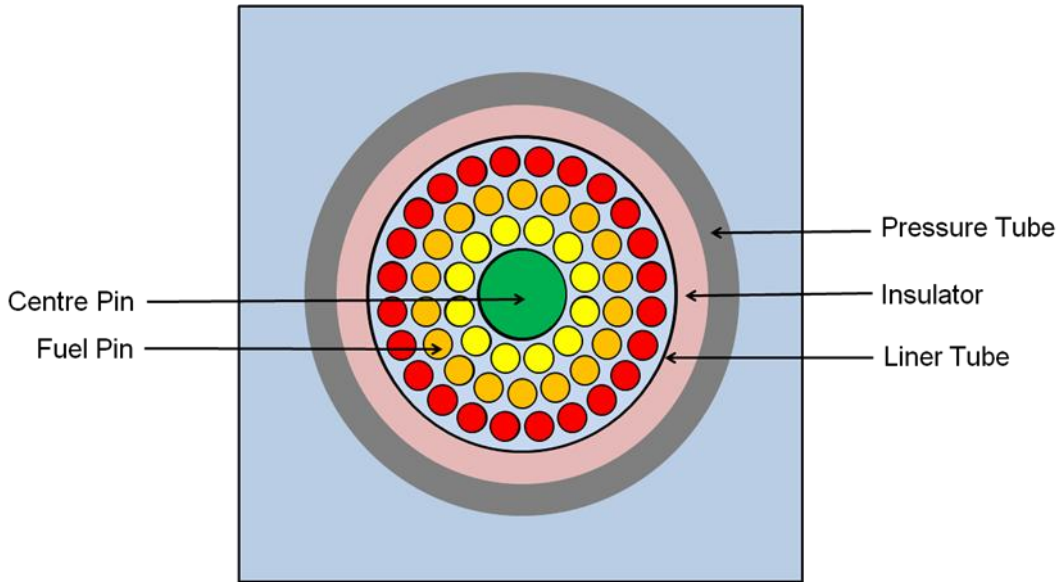

Figure 1 The SCWR Channel Cross section

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
Coolant	H_2O
Moderator	0.09% by weight H_2O in D_2O
Reactor Grade Pu Isotopic Composition	2.5wt% ^{238}Pu; 54.3wt% ^{239}Pu; 23.8wt% ^{240}Pu; 12.6wt% ^{241}Pu; 6.8wt% ^{242}Pu

Estimated values of temperatures for the materials at each nominal axial location are also taken from (Magill et al., 2011) and are shown in Table 3. While these temperatures are expected to qualitatively reflect trends within the fuel channel, more detailed and accurate temperature values will require coupled and self-consistent physics and thermalhydraulics calculations, which have not yet been performed.

Table 3
Material Temperatures

Axial dist. from Top (mm)	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)
500	592.54	632.35	960.15	796.35	632.35	554.88	477.55	342.16
1500	382.46	656.30	960.15	808.30	656.30	570.83	485.51	342.16
2500	160.92	675.27	960.15	817.76	675.27	583.46	491.82	342.16
3500	89.49	774.05	960.15	867.04	774.05	649.25	524.65	342.16
4500	69.63	881.45	960.15	920.63	881.45	720.78	560.35	342.16

The model contains a single fuel assembly and coolant within a fuel channel, surrounded by moderator. The moderator is bounded in the x-y plane by reflecting boundary conditions, which define a 25 cm x 25 cm square lattice cell (one square lattice pitch). In the axial direction, the cell has a 30 cm layer of coolant at both axial ends. The coolant region at the ends is of the same density as 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 sub-assemblies 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), for 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.

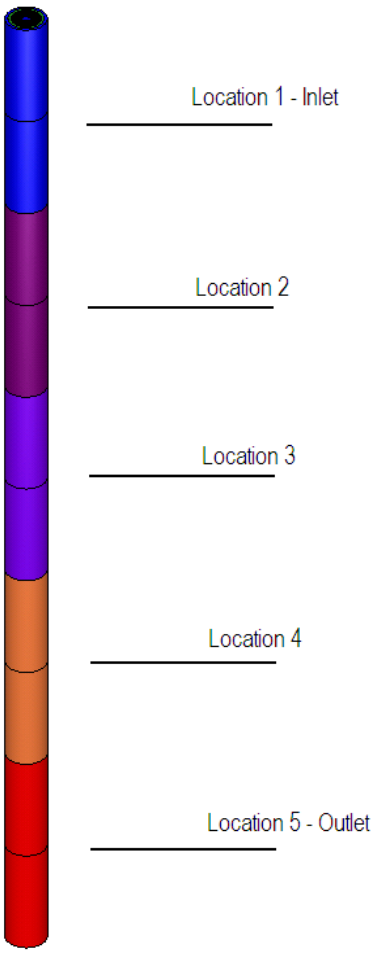

Figure 2 Axial Partitioning of Model

Each ring of fuel pins used different material designation numbers, although the material compositions 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 differences 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

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
Coolant Hot	Coolant temperature increased by 50 K	1.2303 ± 0.0001
Coolant Cool	Coolant temperature decreased by 50 K	1.2274 ± 0.0001
Moderator Hot	Moderator temperature increased by 20 K	1.2295 ± 0.0001
Moderator Cool	Moderator temperature decreased by 20 K	1.2304 ± 0.0001

4. Results and Discussion

4.1 Reference Case

The value of *k* 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 direction opposite to 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 are for plutonium isotopes which are in the fuel material in the outer ring of fuel pins. The ^{239}Pu $\overline{\nu}$, 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 fairly uniform along the channel, with neither the inlet nor outlet materials contributing much to the sensitivities. It is important to note that although the ten most sensitive materials are listed here, this is an arbitrary cut-off.

Table 5
Top 10 Sensitivities by Reaction and Nuclide

Distance from Inlet (m)	Nuclide	Reaction	Sensitivity
2.5	^{239}Pu	$\bar{\nu}$	2.12E-01
3.5	^{239}Pu	$\bar{\nu}$	1.60E-01
1.5	^{239}Pu	$\bar{\nu}$	1.22E-01
2.5	^{239}Pu	fission	9.44E-02
3.5	^{239}Pu	fission	7.06E-02
2.5	^{241}Pu	$\bar{\nu}$	7.03E-02
2.5	^{239}Pu	n,γ	-5.91E-02
1.5	^{239}Pu	fission	5.40E-02
3.5	^{241}Pu	$\bar{\nu}$	5.34E-02
3.5	^{239}Pu	(n,γ)	4.47E-02

The ten nuclides to which *k* has the highest sensitivity are shown in Table 6, along with the component breakdown for each nuclide. Here, ^{239}Pu, ^{232}Th and ^{2}H are the dominant nuclides.

Table 6
Top 10 Nuclide Sensitivities and their Components

Nuclide	Fission	Elastic	Inelastic	Capture	Total
^{239}Pu	3.30E-01	-3.50E-04	-1.59E-04	-1.95E-01	1.34E-01
^{232}Th	4.68E-03	8.69E-03	-2.97E-03	-1.21E-01	-1.10E-01
^{2}H		1.02E-01	7.40E-04	-7.44E-04	1.03E-01
^{241}Pu	1.23E-01	-1.24E-04	-8.17E-02	-4.13E-02	8.16E-02
^{240}Pu	7.16E-03	1.29E-03	-6.97E-05	-7.94E-02	-7.11E-02
^{91}Zr		9.03E-04	-1.62E-04	-2.60E-02	-2.52E-02
^{56}Fe		-1.07E-03	-4.16E-04	-1.65E-02	-1.80E-02
^{1}H		2.45E-02		-1.11E-02	1.34E-02
^{93}Nb		3.67E-04	-3.34E-05	-1.11E-02	-1.08E-02
^{58}Ni		-6.45E-04	-9.37E-05	-9.20E-03	-9.94E-03

The sensitivity of *k* to nuclear data can be combined with a nuclear data covariance matrix to find the uncertainty in *k* due to uncertainties in nuclear data. Thus, the total uncertainty due to

nuclear data is found to be ±11.20 mk[1]. The nuclides that make contributions to the uncertainty above 0.5 mk and the values of those contributions are shown in Table 7. The uncertainty contributors are elements of the covariance matrix, where covariance terms are between energies and in some cases reactions. Hence, there are two columns and the uncertainty contribution cannot be simplified in the same way as the sensitivity terms in Table 6, although 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.

Table 7
Contributions to Nuclear Data Uncertainty in the Reference Case

Covariance Matrix		**Contributions to Uncertainty (mk) Due to this Matrix**
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 (χ)	^{239}Pu (χ)	0.66
^{53}Cr (n,γ)	^{53}Cr (n,γ)	0.62
Total of contributions above		11.15
Total from all contributions		11.20

[1] A unit of reactivity. 1 mk = 1000×Δk or 1000×Δρ. 1 mk = 100 pcm.

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 that of ^{239}Pu(n, γ), yet the sensitivity of *k* to this reaction does not appear in the top sensitivities shown in Table 5. The greater uncertainty associated with (n,γ) reactions on Zr is likely the result of greater uncertainty in the cross section for this reaction compared to that for Pu, and demonstrates the importance of this reaction for SCWR modeling, despite the comparatively low sensitivity.

4.2 Coolant Void Reactivity

The code module TSAR was used with sensitivity input from both cooled and voided cases. The coolant void reactivity (CVR) calculations were performed assuming that the voided condition corresponded to the replacement of coolant in the channels by air (represented in the models by 1.0 wt% light water in dry air under a pressure of 1 atm). There were no other changes made to these models.

The value of the CVR worth according to the cooled and voided *k* calculations is -2.2 mk. The TSAR calculated sensitivities are shown in Table 8. The primary contributors to uncertainty are shown in Table 9, with the total uncertainty due to nuclear data assessed to be ±1.12 mk. As was the case with the evaluation of *k*, absorption in zirconium is a high contributor to the total uncertainty but is not high on the list of sensitivities seen in Table 8. A comparison between Table 8 and Table 9 demonstrates that the determining factor for the relative contribution of isotopes to the uncertainty in CVR is the high nuclear data uncertainty of them, rather than the corresponding sensitivity.

Table 8
Top Ten CVR Nuclear Data Sensitivities Calculated by TSAR

Nuclide	Fission	Scatter	Capture	Total
^{2}H		44.12	0.08	44.20
^{232}Th	0.25	2.24	-13.16	-10.67
^{1}H		-18.65	8.54	-10.10
^{239}Pu	-0.34	-0.13	7.85	7.38
^{240}Pu	0.66	0	1.92	2.58
^{91}Zr		0.52	1.70	2.22
^{241}Pu	2.90	-0.04	-0.66	2.21
^{90}Zr		-0.31	0.87	0.56
^{56}Fe		-0.77	0.39	-0.38
^{58}Ni		-0.43	0.13	-0.30

Table 9
Top Ten CVR Nuclear Data Uncertainties Calculated by TSAR

Covariance Matrix		Contributions to Uncertainty (mk) Due to this Matrix
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
Total of contributions above		1.10
Total from all contributions		1.12

4.3 Fuel Temperature Reactivity

The TSAR code module was also used to examine the effect of fuel temperature reactivity. For these calculations, in addition to perturbations to the fuel temperature, the fuel cladding temperature was also changed, but the coolant temperature remained the same as the reference case. The TSAR calculation determined 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 reactivity change 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 coefficient gives information relating to fuel temperature feedback effects during normal operation.

4.3.1 Fuel Temperature Reactivity under Cooled-Channel Conditions

The reactivity worth of the 200 K increase in fuel temperature in the cooled case is -3.61 mk, corresponding to a fuel temperature reactivity coefficient (FTC) of -0.02 mk/K. The highest contributors to nuclear data sensitivity are shown in Table 10. The highest sensitivities of the fuel temperature reactivity to nuclear data are to deuterium, plutonium and thorium reactions. The total uncertainty in fuel temperature reactivity due to nuclear data is assessed to be ±0.07 mk, corresponding to an uncertainty in FTC of $\pm 3.5\times10^{-4}$ mk/K, with the ten most important components listed in Table 11. In this case, deuterium scattering and absorption in ^{232}Th and ^{239}Pu are the most important.

Table 10
Cooled Fuel Temperature Reactivity Nuclear Data Sensitivities Calculated by TSAR

Nuclide	Fission	Scatter	Capture	Total
^{2}H		2.67	0	2.67
^{239}Pu	2.19	-0.01	-0.51	1.68
^{232}Th	0.06	0.19	-1.89	-1.64
^{241}Pu	0.77	0	-0.07	0.70
^{1}H		-1.13	0.69	-0.44
^{16}O		-0.18	-0.01	-0.19
^{242}Pu	0.02	-0.01	-0.09	-0.08
^{90}Zr		0.04	0.02	0.06
^{91}Zr		0.01	0.04	0.05
^{238}Pu	0.03	0	0.01	0.04

Table 11
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
Total of contributions above		3.08E-4
Total from all contributions		3.5E-4

4.3.2 Fuel Temperature Reactivity under Voided-Channel Conditions

The reactivity worth of the 200 K increase in fuel temperature in the voided case is -4.0 mk, corresponding to an FTC of -0.02 mk/K. The highest sensitivity nuclides are listed in Table 12. Increasing the scattering cross section in the moderator has a positive effect on FTC, whereas capture in the fuel has a negative effect. The main differences observed from the cooled FTC sensitivities are the relative increase in the importance of deuterium scattering and the relative decrease in the importance of plutonium fission.

The uncertainty in fuel temperature reactivity due to nuclear data is assessed to be ±0.10 mk, corresponding to an uncertainty in FTC of $\pm 5.0 \times 10^{-4}$ mk/K, with the ten most important components listed in Table 13. As with the sensitivities, deuterium scattering and thorium absorption are high contributors to the uncertainty.

Table 12
Voided Fuel Temperature Reactivity Nuclear Data Sensitivities Calculated by TSAR

Nuclide	Fission	Scatter	Capture	Total
^{2}H		4.20	0	4.20
^{232}Th	0.06	0.07	-1.94	-1.82
^{239}Pu	0.92	-0.01	-1.53	-0.62
^{240}Pu	0.09	-0.06	-0.54	-0.50
^{56}Fe		-0.06	-0.07	-0.13
^{241}Pu	0.13	0	-0.26	-0.12
^{242}Pu	0.02	-0.01	-0.09	-0.08
^{91}Zr		0	-0.07	-0.07
^{58}Ni		-0.03	-0.04	-0.07
^{1}H		0.04	0.02	0.06

Table 13
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 (χ)	^{239}Pu (χ)	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
Total of contributions above		4.6E-4
Total from all contributionsall contributions		5.0E-4

4.4 Coolant Temperature Reactivity

The reactivity effect of changes in coolant temperature was examined using the TSAR code module. For these perturbations, as well as perturbations to coolant temperature, the temperatures of adjacent materials, e.g., the bundle liner and insulator, were also changed. The densities of these materials were also changed corresponding to the temperature changes. The TSAR calculation was used to examine the reactivity difference between a state with the coolant temperature 50 K above the nominal conditions and one at 50 K below the nominal conditions.

The reactivity worth of the 100 K temperature increase in the coolant is +1.9 mk, corresponding to a coolant temperature reactivity coefficient (CTC) of +0.02 mk/K. The highest contributors to nuclear data sensitivity are shown in Table 14. The sensitivities are almost as high as for the CVR calculation. The CTC is most sensitive to scattering from hydrogen and absorption in thorium.

The uncertainty in coolant temperature reactivity due to nuclear data is assessed to be ±0.71 mk, corresponding to an uncertainty in CTC of ±0.007 mk/K. The highest contributors to the nuclear data uncertainty are shown in Table 15. Deuterium scattering and zirconium absorption are the most important, followed by reactions in ^{239}Pu.

Table 14
Coolant Temperature Coefficient Sensitivities Calculated by TSAR

Nuclide	Fission	Scatter	Capture	Total
^{232}Th	0	0.11	0.72	0.83
^{1}H		1.61	-0.84	0.76
^{239}Pu	1.66	0	-0.92	0.74
^{241}Pu	0.31	0	0.20	0.51
^{91}Zr		0.07	0.26	0.33
^{56}Fe		0.07	0.18	0.26
^{2}H		-0.22	0.04	-0.18
^{238}Pu	-0.01	0	0.14	0.13
^{16}O		0.12	0	0.12
^{58}Ni		0.03	0.09	0.12

Table 15
Coolant Temperature Coefficient Nuclear Data 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)	5.2E-3
^{92}Zr (n, γ)	^{92}Zr (n, γ)	3.2E-3
^{91}Zr (n, γ)	^{91}Zr (n, γ)	2.3E-3
^{90}Zr (n, γ)	^{90}Zr (n, γ)	2.0E-3
^{2}H (n,2n)	^{2}H (elastic)	-1.7E-3
^{239}Pu (n, γ)	^{239}Pu (n, γ)	1.2E-3
^{239}Pu ($\bar{\nu}$)	^{239}Pu ($\bar{\nu}$)	1.1E-3
^{239}Pu (fission)	^{239}Pu (n, γ)	0.90E-3
^{239}Pu (fission)	^{239}Pu (fission)	0.90E-3
^{232}Th (n, γ)	^{232}Th (n, γ)	0.90E-3
Total of contributions above		7.0E-3
Total from all contributions all contributions		7.1E-3

4.5 Moderator Temperature Coefficient

The TSAR code module was used to investigate the effect of changing the moderator temperature. The TSAR calculation examined the reactivity difference between a state with the moderator temperature 20 K above the nominal operating conditions and one at 20 K below the nominal operating conditions. No other changes were made to the models.

The reactivity worth of the 40 K temperature increase in the moderator is -0.6 mk, corresponding to a moderator temperature reactivity coefficient (MTC) of -0.01 mk/K. The highest contributors to nuclear data sensitivity of the MTC are shown in Table 16. Again, deuterium, plutonium and thorium reactions have high sensitivity. In general, the sensitivities are on the same order as those for the fuel temperature reactivity.

The uncertainty in moderator temperature reactivity due to nuclear data is assessed to be ±0.08 mk corresponding to an uncertainty in MTC of ±0.002 mk/K, with the ten most important contributors listed in Table 17. This uncertainty is small enough that it is unlikely that the nuclear data uncertainty will be a limiting factor in calculating the MTC.

Table 16
Moderator Temperature Reactivity Sensitivities Calculated by TSAR

Nuclide	Fission	Scatter	Capture	Total
^{2}H		25.37	0.06	25.42
^{232}Th	0.13	0.21	-8.99	-8.65
^{1}H		-12.42	8.14	-4.29
^{239}Pu	-1.41	-0.05	4.16	2.70
^{240}Pu	0.37	0.06	1.20	1.63
^{241}Pu	1.72	-0.02	-0.16	1.53
^{91}Zr		0.02	1.22	1.24
^{92}Zr		-0.03	0.57	0.54
^{90}Zr		-0.19	0.70	0.51
^{16}O		0.31	0.02	0.33

Table 17
Moderator Temperature Reactivity Nuclear Data Uncertainties Calculated by TSAR

Covariance Matrix		Contributions to Uncertainty Due to this Matrix (mk/K)
Nuclide-Reaction	**Nuclide-Reaction**	
^{239}Pu (n,γ)	^{239}Pu (n,γ)	7.5E-4
^{239}Pu (fission)	^{239}Pu (fission)	7.5E-4
^{239}Pu (fission)	^{239}Pu (n,γ)	7.5E-4
^{92}Zr (n,γ)	^{92}Zr (n,γ)	7.5E-4
^{91}Zr (n,γ)	^{91}Zr (n,γ)	5.0E-4
^{90}Zr (n,γ)	^{90}Zr (n,γ)	5.0E-4
^{2}H (elastic)	^{2}H (elastic)	2.5E-4
^{56}Fe (n,γ)	^{56}Fe (n,γ)	2.5E-4
^{239}Pu ($\bar{\nu}$)	^{239}Pu ($\bar{\nu}$)	2.5E-4
^{239}Pu (χ)	^{239}Pu (χ)	2.5E-4
Total of contributions above		1.73E-3
Total from all contributions all contributions		2.00E-3

5. Conclusions

The *k* calculations show that, in the fresh fuel case, the nuclides to which *k* has the highest sensitivity are ^{239}Pu, ^{232}Th and ^{2}H. Interestingly, the reactions contributing the greatest uncertainties to *k* are ^{239}Pu($\bar{\nu}$), ^{239}Pu(fission) and ^{92}Zr(n,γ). The most sensitive individual reactions are on plutonium in the outer fuel ring.

For CVR calculations, the calculations are most sensitive to ^{2}H, ^{232}Th and ^{1}H. The nuclear data contributing the most to uncertainty are scattering in ^{2}H, (n,γ) in isotopes of zirconium and various reactions in isotopes of plutonium.

The results are very similar for FTC calculations. Here, the system is highly sensitive to ^{2}H ^{232}Th and ^{239}Pu. The highest contributors to the nuclear data induced uncertainty are scattering in ^{2}H and absorption in isotopes of plutonium and thorium. The fuel temperature coefficient sensitivities and uncertainties do not change significantly between the SCW and air cooled models.

The nuclides for which the CTC calculations are highly sensitive include ^{232}Th, ^{1}H and ^{239}Pu. These contribute to the uncertainty in the calculation, along with the largest contributors to uncertainty which are scattering in ^{2}H and absorption in isotopes of zirconium.

For MTC calculations, the reactions with high sensitivity are in ^{2}H, ^{232}Th and ^{1}H, and the reactions that make the largest contributions to uncertainty are in ^{239}Pu and isotopes of zirconium. As was discussed above, it is unlikely that the nuclear data uncertainty will be a limiting factor in calculating the MTC.

In all of the cases above, the reactions making the highest contributions to the uncertainties in *k* and various reactivity coefficients are not the same as those to which the reactivities show the highest sensitivities. This reflects the good quality of data for many of these reactions, which are of general interest. The reactions that impact SCWR modeling the most are those for which both sensitivity and uncertainty are high, as indicated by the uncertainty results. The sources for these large uncertainties could be large uncertainties in the original experiments performed to obtain the nuclear data, gaps in the nuclear data or assumptions made in the construction of the covariance data for these reactions. Now that the highest sensitivity and highest uncertainty reactions have been identified for the Canadian SCWR, the next phase of this study will include an evaluation of the source data and assumptions made in assembling the cross section and covariance data for these reactions.

Upcoming related studies will also include examination of partly irradiated fuel (e.g., mid- and end-of-cycle burnups) in order to assess and compare the relative contributions to sensitivity and uncertainty of important nuclides in the irradiated fuel such as ^{233}U, ^{233}Pa and various fission products.

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7. References

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