VALIDATION OF WIMS-IST

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INTRODUCTION

During the past few years an exercise has been ongoing to validate Industry Standard Toolset (IST) codes used in the safety analysis of CANDU® reactors [1]. The purpose of the work reported here was to validate one of these codes, WIMS-IST, against experimental measurements. The extension of this validation against experimental conditions to reactor operating or accident conditions is the subject of additional work and is not discussed here. WIMS-IST is one of the codes of the reactor physics suite of computer codes. It performs neutron transport calculations in a representative two-dimensional cell of a CANDU reactor, in order to determine the value of k-effective for a lattice of identical cells and to provide cell-average parameters to represent the cell in a full reactor calculation. WIMS-IST is defined to be WIMS-AECL Release 2-5d, used with the ENDF/B-VI-based NDAS library Version 1a.

WIMS-IST was validated using the following five-step phenomena-based methodology:

a. Review of postulated accidents in the design basis and their associated physical phenomena,
b. Assembly of validation matrices that relate postulated accidents to physical phenomena and phenomena to data sets,
c. Preparation of a validation plan,
d. Performance of the validation exercises, and
e. Preparation of validation reports that document the results of the validation exercises.

The validation matrices identify 16 reactor physics phenomena of interest. WIMS-IST calculates 11 of these phenomena.

Thus, WIMS-IST has been validated against experimental measurements for the following 11 phenomena:

a. coolant-density-change induced reactivity,
b. coolant-temperature-change induced reactivity,
c. moderator-density-change induced reactivity,
d. moderator-temperature-change induced reactivity,

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e. moderator-poison-concentration-change induced reactivity,
f. moderator-purity-change induced reactivity,
g. fuel-temperature-change induced reactivity,
h. fuel-isotopic-composition change,
i. flux and power distribution,
j. lattice-geometry-distortion reactivity effects, and
k. coolant-purity-change induced reactivity.

The validation was accomplished by comparing the results of WIMS-IST calculations with experimental data.

EXPERIMENTAL DATA AND METHOD OF COMPARISON

Nine of the eleven phenomena involve reactivity changes. Data to validate WIMS-IST for these phenomena came from critical experiments performed in ZED-2, a zero-power reactor located at AECL Chalk River Laboratories. The appropriate calculated quantity to compare with experimental measurement is the reactivity coefficient associated with the phenomenon.

The reactivity coefficient can be quoted in either reactivity units or buckling units. It can be expressed as a change in reactivity or critical buckling associated with a given change of the relevant parameter, divided by the change in the relevant parameter.

For instance, the fuel-temperature reactivity coefficient is the rate of change of reactivity as the fuel temperature is varied. The measured reactivity coefficient must be obtained from a series of tests, each performed at a specific value of the parameter of interest. In each test the critical buckling is measured in a critical reactor. In this paper, the series of tests used to define a single reactivity coefficient for a given fuel type is referred to as an experiment.

There are two ways in which the results of the calculations can be compared with the experimental data. The two methods are actually equivalent, but provide a different outlook on the comparison.

For the first method, the measured critical bucklings are input to WIMS-IST for each test, and the WIMS-IST-predicted k-eff is obtained for each test. If both the code and the experiment are able to simulate the reactivity coefficient exactly, then the resulting calculated k-eff values will be constant as a function of the parameter of interest. Any deviation from a constant value is a measure of the bias and uncertainty between calculation and measurement.

For the second method, the experimental reactivity coefficient in buckling units can be determined from the measured critical bucklings. Then, WIMS-IST is used to calculate the critical buckling for each test. This calculation does not involve the use of any information from the experimental measurement. The calculated reactivity coefficient in buckling units can then be determined. The difference between the two determinations is the bias between calculation

and measurement. The individual uncertainties in the individual buckling measurements can be propagated through the determination of the measured reactivity coefficient, in order to provide an estimate of the uncertainty.

Although the two methods are equivalent, both of the above methods were generally used to determine the bias and uncertainty to be associated with calculations for each phenomenon with WIMS-IST; however, in the presentation here, usually only one of the methods is discussed for each phenomenon. Even though only one method is discussed per phenomenon, the quoted biases and uncertainties often come from consideration of the results of both methods.

Values for critical buckling had been determined previously in ZED-2 experiments using two different methods.

The most direct method is by flux mapping, where the flux shape is measured (and fit to cosine and Bessel functions to extract axial and radial bucklings) either in a full core or in a large region of a core containing the test fuel.

The other method is the substitution method. A substitution experiment involves a reference lattice, usually a regular, hexagonal array of vertical channels with a pitch of 31 cm. Usually, the reference lattice consists of 55 driver rods, each containing a string of five 28-element natural UO_2 fuel bundles. Sometimes, booster channels of another fuel type (depending on the particular experiment) surround these driver channels and help ensure criticality. A substitution experiment replaces the driver fuel bundles in 1, 3, 5, and then 7 of the centrally located channels with a given set of test fuel bundles. Criticality is achieved by varying the moderator height. The basic premise of this method is that the critical buckling for a full core of the test fuel can be obtained by extrapolating the results from the 1-, 3-, 5-, and 7-rod substitutions. The substitution method is less direct than the flux mapping method, and depends on an elaborate analysis of the experimental measurements; however, it can provide critical buckling values when there is insufficient test fuel to provide bucklings from flux mapping.

Two of the phenomena do not involve reactivity coefficients. For the fuel-isotopic-composition change phenomenon, the appropriate calculated quantities to compare with experimental measurement are the concentrations of various isotopes in the fuel after a given period of irradiation in a power reactor and are determined by isotopic analysis during post-irradiation examinations. For the flux and power distribution phenomenon, the appropriate calculated quantities to compare with experimental measurement are the fluxes or reaction rates in various foil materials located in the fuel elements during experiments performed in ZED-2.

WIMS-IST Input Model

The accuracy of the results generated by WIMS-IST is dependent upon the input description used and the options selected in the code. If a very detailed input description is used, then the results are more accurate. However, the greater the detail in the input model and the more sophisticated the options chosen, the greater are the resources (mainly computer time) needed to run WIMS-IST. Thus, for normal design and fuel management calculations a standard input model is chosen, which is a compromise between accuracy and required resources. The present validation is performed with this standard input model. This model calls for a combination of one- and two-dimensional collision probability methods to solve the neutron transport equation and employs 33 energy groups, shielded Zr cross-sections, end regions, and a reasonable spatial mesh.

RESULTS OF COMPARISON

Coolant-Density-Change Induced Reactivity

This phenomenon is probably the most important phenomenon in the reactor physics validation matrix, as far as safety analysis is concerned. It has been found that loss of coolant will cause a significant positive reactivity insertion. Fairly small inaccuracies in the void reactivity coefficient can cause significant uncertainties in the magnitude of the power pulse following a loss-of-coolant accident.

This phenomenon was studied by comparing the difference in k-eff values calculated by WIMS-IST using bucklings measured for a voided and a cooled critical core. If the experiment had no error and the calculation was able to model the phenomenon exactly, then there would be no difference between the two k-effectives. Thus, any difference is a measure of the bias and uncertainty in the void reactivity coefficient.

Because of the importance of the void effect in reactor safety, the effect has been studied extensively in ZED-2 over many years. Only a sampling of the available data will be discussed here, even though a larger set of experimental data was used in the actual validation. Table 1 shows the void reactivity discrepancy ($k\text{-}eff_{voided} - k\text{-}eff_{cooled}$) for the most recent fuel designs. In the table, "FNU" refers to fresh natural uranium fuel, and "MOX" refers to mixed-oxide fuel. The MOX fuel was made to simulate mid-burnup CANDU fuel. The "AECL calibration" and "OPG method" refer to different methods of determining the critical buckling from substitution measurements. The AECL calibration applies a correction, which calibrates the critical bucklings measured by substitution to those measured by flux mapping. The OPG method uses a statistical model to consider all of the flux mapping and substitution data to obtain a maximum likelihood estimate of the critical bucklings and their uncertainties.

For the fuel types presented in Table 1, WIMS-IST overpredicts the void effect. For 37-element FNU fuel this overestimate amounts to 1.9 mk, and for 37-element MOX fuel the overestimate amounts to 1.3 to 1.7 mk, depending on whether the OPG method or AECL calibration is used. The uncertainty for MOX fuel determined by the OPG method is ±0.78 mk. This error, rounded up to ±0.8 mk, was taken as a conservative estimate of the uncertainty for the calculated void reactivity for all fuel types.

Table 1. Overestimate of Void Reactivity by WIMS-IST using the Standard Input Model

Fuel 22 °C, 99.75 wt% Heavy Water, 31-cm Hexagonal Pitch	Void Reactivity Discrepancy (mk)
28-element FNU (flux mapped)	0.57 ± 0.4
28-element FNU (AECL calibration)	0.78
28-element FNU (OPG method)	0.73
37-element FNU (AECL calibration)	1.89 ± 0.64 [2]
37-element FNU (OPG method)	1.90 ±0.45
37-element MOX (AECL calibration)	1.68 ± 0.75 [2]
37-element MOX (OPG method)	1.29 ±0.78
43-element CANFLEX FNU (AECL calibration)	1.83

Coolant-Temperature-Change Induced Reactivity

From a neutronics viewpoint, a change in coolant temperature has several effects. An increase in coolant temperature will increase upscattering of neutrons into the adjacent fuel. In general, thermal neutrons of higher than average speeds are less likely to be absorbed by any fuel material, although the situation is subtle because of the existence of thermal neutron resonances in plutonium isotopes. An increase in coolant temperature will be accompanied by a decrease in coolant density, thus reducing the number of neutron scattering targets in the coolant, and thereby enhancing neutron leakage and decreasing parasitic resonance absorption in ^{238}U.

It is not possible in a measurement to separate the phenomenon of changing coolant temperature from that of changing coolant density. Also, because the fuel is contained within the coolant, the fuel temperature will change with the coolant temperature. In this validation, the coolant temperature coefficient encompasses three effects: changing coolant temperature; the associated change in coolant density; and the accompanying change in fuel temperature.

Experiments have been performed in the ZED-2 reactor, in which one to seven of the central channels were heated from 300 K to 600 K. When coolant water is present, this temperature range corresponds essentially to that for coolant found in CANDU reactors. Since only the central channels can be heated while the remainder of the reactor remains at room temperature, the critical bucklings for the heated channels must be obtained using the substitution method. For the majority of the measurements, the full 1-, 3-, 5-, and 7-rod substitutions were only performed at room temperature. For higher temperatures, only a 7-rod substitution was performed, and the extrapolation to a full core of test fuel at that temperature was based on the

extrapolation determined at room temperature. However, for one experiment, involving MOX fuel, the full 1-, 3-, 5-, and 7-rod substitutions were performed at each temperature. This experiment was analysed to extract critical bucklings both by using the room temperature extrapolation at each temperature and also by using the appropriate measured temperature-dependent extrapolation at each temperature.

ZED-2 substitution experiments with the following test fuels were performed for the coolant temperature coefficient:

- 37-element FNU fuel bundles
    - no boosters, room temperature extrapolation at all temperatures.
- 37-element simulated mid-burnup MOX fuel bundles containing dysprosium to mimic fission product absorption
    - 19-element boosters, room temperature extrapolation at all temperatures.
    - 19-element boosters, measured temperature-dependant extrapolation at all temperatures.
    - ZEEP rod boosters, room temperature extrapolation at all temperatures.
- 43-element CANFLEX® natural UO_2 fuel bundles
    - no boosters, room temperature extrapolation at all temperatures.

Figure 1 shows the k-eff values obtained with WIMS-IST when the measured critical bucklings are used as input. As expected the lines are almost horizontal. If a straight line is drawn through the points for any specific fuel type measurement, then the slope of the line gives the bias in the coolant-temperature reactivity coefficient, and the uncertainty in the slope is the uncertainty in the coefficient.

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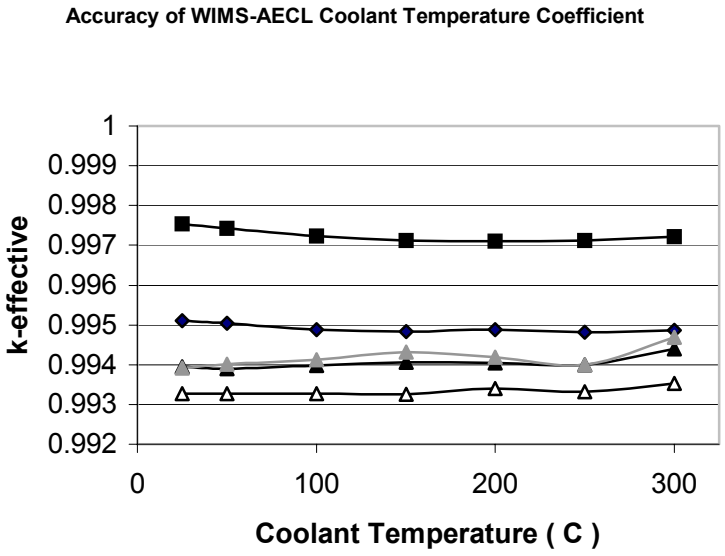

Figure 1. Accuracy of WIMS-IST Coolant-Temperature Reactivity Coefficient

Legend: square=FNU; diamond=CANFLEX; black+gray triangles=MOX(U19); white triangle=MOX(ZEEP)

Consideration of all the data lead to an assignment of zero bias to the coolant-temperature reactivity coefficient calculated by WIMS-IST, with an uncertainty of ±4%.

Moderator-Density- and Moderator-Temperature-Change Induced Reactivity

Although moderator-density-change induced reactivity and moderator-temperature-change induced reactivity were identified as separate phenomena, it is not possible to separate the two phenomena in zero-power reactor experiments, because a change in temperature will lead to a corresponding change in density. A reduced moderator density offers fewer scattering targets to neutrons, and an increased temperature alters the scattering characteristics for neutrons, such as the likelihood of upscattering. The neutron spectrum therefore changes, resulting in a change in the reactivity of the reactor. This phenomenon is commonly called the moderator-temperature reactivity coefficient.

Data for the validation came from the following three flux mapping experiments: an experiment [3] with 19-element UO_2 fuel performed in the ZEEP reactor covering the temperature range from 20 to 65 C; an experiment with 19-element UO_2 fuel performed in the ZED-2 reactor covering the temperature range from 11 to 82 C, and an experiment with 28-element UO_2 fuel performed in the ZED-2 reactor covering the temperature range from 20 to 40 C. In all cases the fuel was unirradiated natural uranium. For all cases the reactor was uniformly chilled or heated. Therefore, part of the observed effect is due to the temperature change of the fuel and coolant; this was estimated to be about 25% of the total effect.

By comparing calculated and measured buckling, it was determined that WIMS-IST accurately calculates the moderator-temperature reactivity coefficient with an uncertainty of ±2.6%.

Moderator-Poison-Concentration-Change Induced Reactivity

Neutron poison can be dissolved in the moderator of a CANDU reactor to compensate for excess reactivity or to provide emergency shutdown. Either gadolinium or boron may be used. While there are CANDU-specific experiments with boron in the moderator, none have been identified with gadolinium in the moderator.

Data from the following three experiments in ZED-2 were used in the validation: a flux mapping experiment performed with 28-element air-cooled bundles; a substitution experiment with 37-element FNU bundles that were both D_2O- and air-cooled; and a substitution experiment with 37-element MOX bundles that were both D_2O- and air-cooled. These latter bundles were meant to simulate mid-burnup CANDU fuel. The experiments covered a poison concentration range of 0 to 3.5 ppm by weight of natural boron in the moderator.

Table 2 shows the relative difference between WIMS-IST calculations and measurement for the moderator-poison buckling coefficients corresponding to the different experiments.

Table 2. Difference between Moderator-Poison (Boron) Buckling Coefficients from WIMS-IST Calculations and ZED-2 Experiments

Experiment	Bundle	Fuel Type	Coolant	Relative Difference in Coefficient
28-element air-cooled	28-element	Fresh natural UO_2	Air	-1.3%
37-element natural UO_2	37-element	Fresh natural UO_2	Air	1.7%
			D_2O	0.0%
37-element simulated mid-burnup	37-element	Simulated mid-burnup	Air	-2.6%
			D_2O	-3.0%

The uncertainty in the measured moderator-poison buckling coefficients ranges from 2 to 4%. The differences between calculation and experimental measurement in the last column of Table 2 are not significant compared to the experimental uncertainty. Thus, WIMS-IST has no bias in its calculation of the poison reactivity coefficient and an uncertainty of ±2%.

Moderator-Purity-Change Induced Reactivity

The neutron absorption cross-section of hydrogen is orders of magnitude greater than that of deuterium; thus, moderator purity (i.e., the fraction of moderator water that is D_2O) has a large impact on reactivity.

The validation exercise used data from 19 separate measurements with 28-element UO_2 fuel bundles that were arranged on a 31-cm hexagonal pitch. The experiments were performed over the period 1965 to 1999 and covered a range of moderator purity from 99.15 to 99.86 % by weight. These measurements were not made specifically to study the effect of moderator purity. They were made as part of the operational requirements for the ZED-2 reactor and as part of the characterization of reference lattices used in substitution measurements. For each of these measurements the coolant purity was the same as the moderator purity, and there were small variations in temperature from measurement to measurement. These effects were taken into account when doing the validation.

Figure 2 shows the k-eff values calculated by WIMS-IST when the experimentally measured bucklings were used as input. The line is a "least squares" fit to the data. It can be seen that the line deviates from the horizontal. It was found that the moderator-purity reactivity coefficient was overestimated by 8% with an uncertainty of ±3%.

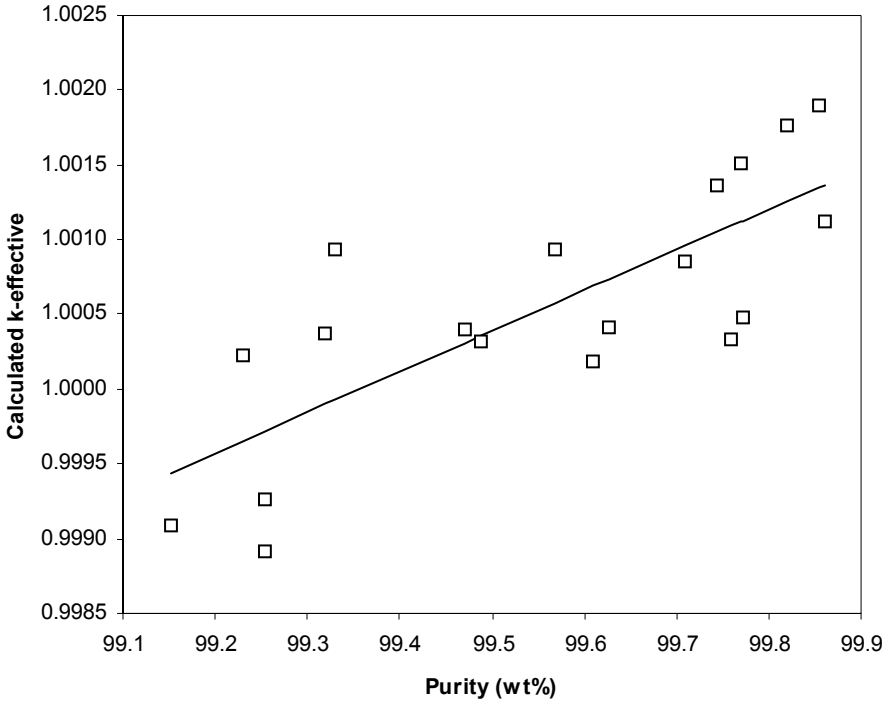

Figure 2. Calculated k-effective versus Moderator Purity

Since the experiments were performed over 35 years and were not performed specifically to measure the moderator purity coefficient, there is the possibility that minor changes in experimental conditions have gone unnoticed over this period. These changes could introduce a bias into the experimental measurements. Because of this, confidence in the measured coefficient is not sufficiently high to prove that there is a bias in WIMS-IST-calculated moderator purity coefficients.

Fuel-Temperature-Change Induced Reactivity

The reactivity induced by a fuel temperature change (also known as the fuel temperature coefficient) is the first line of defence for an unexpected power excursion in any nuclear reactor. The reason is obvious—increased fission power heats the fuel material first. In most reactors the power coefficient and the fuel temperature coefficient are negative for the whole reactor core. The main physical processes that affect the fuel temperature coefficient include Doppler broadening of resonance absorber nuclides within the fuel. In CANDU reactors this broadening primarily involves the ^{238}U isotope, along with lesser contributions from various plutonium nuclides. The rates of neutron absorption in plutonium nuclides and in the ^{235}U isotope are also affected by neutron upscattering from oxygen in the fuel as the fuel temperature changes.

Experiments were performed in the ZED-2 reactor, in which one to seven of the central channels were heated with hot CO_2 from 300 K to 600 K. This caused only the fuel to be heated and resulted in a uniform fuel temperature distribution.

The experiments suffered from a deficiency, in that an average fuel temperature of 600 K is neither a typical operating temperature nor an accident temperature for CANDU fuel. Centreline temperatures within each fuel element in a power reactor are much higher. There is also a distribution of average fuel temperatures across a bundle with different temperatures in each fuel ring. As a result, the overall validation of the lattice code WIMS-IST for the fuel temperature coefficient occurs in two parts. In the first part, discussed here, calculations made with WIMS-IST are compared with measurements in ZED-2. The second part, known informally as scale-up, uses code-to-code comparisons and other investigations to extend the conclusions on the accuracy of WIMS-IST calculations of fuel temperature coefficient to conditions of interest in operating CANDU reactors. This is the subject of further work and is not discussed here.

Experiments were performed in the ZED-2 reactor, in which one to seven of the central channels have been heated from 300 K to 600 K. Since only the central channels can be heated while the remainder of the reactor remains at room temperature, the critical bucklings for the heated channels must be obtained using the substitution method. As outlined in the section on coolant-temperature-change induced reactivity, some of the critical bucklings were obtained using an extrapolation based on room temperature measurements, while some were based on a temperature-dependent extrapolation.

ZED-2 substitution experiments with the following test fuels were performed for the fuel temperature coefficient:

- 37-element FNU fuel bundles
    - no boosters, room temperature extrapolation at all temperatures.
- 37-element simulated mid-burnup MOX fuel bundles containing dysprosium to mimic fission product absorption
    - 19-element boosters, room temperature extrapolation at all temperatures.
    - 19-element boosters, measured temperature-dependent extrapolation at all temperatures.
    - ZEEP rod boosters, room temperature extrapolation at all temperatures.
- 43-element CANFLEX natural UO_2 fuel bundles
    - no boosters, room temperature extrapolation at all temperatures.

Figure 3 shows the k-eff values obtained when the measured critical bucklings are used as input. As expected the lines are almost horizontal. If a straight line is drawn through the points for any one fuel type measurement, then the slope of the line gives the bias in the fuel-temperature reactivity coefficient and the uncertainty in the slope is the uncertainty in the coefficient.

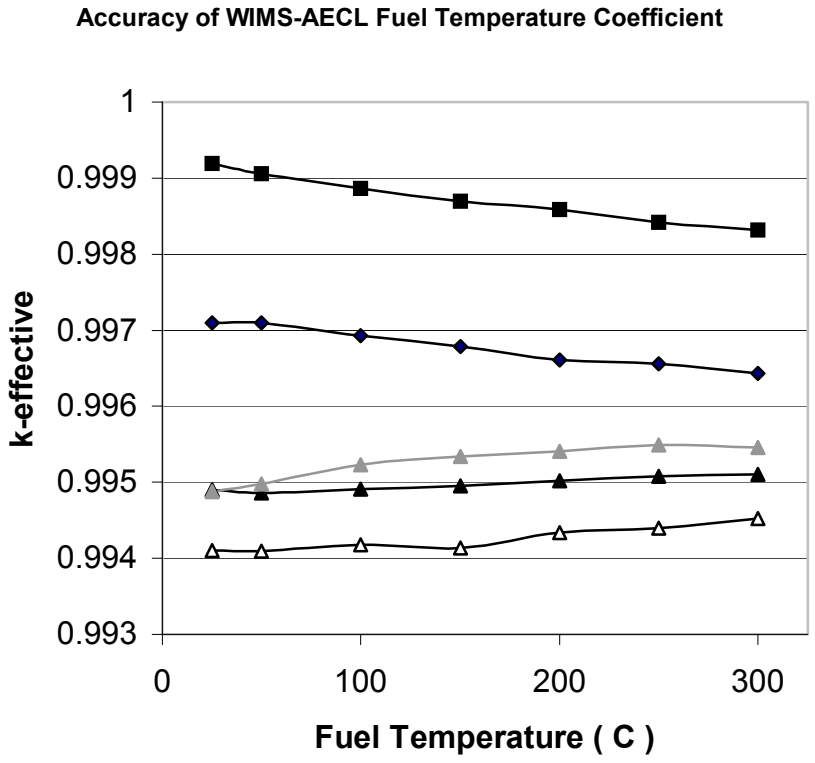

Figure 3. Accuracy of WIMS-IST Fuel Temperature Coefficient

Caption: square=FNU; diamond=CANFLEX; black+gray triangles=MOX(U19); white triangle=MOX(ZEEP)

For the temperature range from 25–300 C of the ZED-2 substitution experiments, it was found that WIMS-IST calculates the fuel temperature coefficient to lie within the 95% confidence interval of the MOX measurements. The FNU and CANFLEX comparisons are slightly better. In percentage terms, WIMS-IST calculates the fuel temperature coefficient over the measured range to within about 10%. WIMS-IST overpredicts the fuel temperature coefficient for unirradiated natural UO_2 fuel, but underpredicts the coefficient for simulated mid-burnup fuel. In a reactor core, there would be a range of fuel burnups. Thus, within this temperature range, there would be the potential for a cancellation of some error for the full-core fuel temperature coefficient. But a scale-up to higher operating temperatures must be done before any definitive statement can be made concerning the ability of WIMS-IST to predict the fuel temperature coefficient of CANDU reactors under normal operation or accident conditions.

Fuel-Isotopic-Composition Change

The phenomenon studied here is fuel-isotopic-composition change; however, fuel-isotopic-composition-change induced reactivity was the phenomenon that was listed in the validation matrix. This latter phenomenon must be calculated from a full reactor calculation, in which WIMS-IST generated data are used. Thus, it is not possible to validate WIMS-IST by itself for this phenomenon. However, it is possible to validate the WIMS-IST calculation of fuel-isotopic-composition change, which is an important component of this phenomenon. As fuel material is irradiated in a CANDU reactor, it undergoes changes in isotopic composition. The most important of these changes involve the depletion of ^{235}U, the production of Pu isotopes and the production of fission products, some of which have high absorption cross-sections and act as neutron poisons. These changes in isotopic composition affect reactivity.

Data for this validation exercise came from isotopic compositions that were measured in three bundles from CANDU power reactors. One bundle was irradiated in NPD, one in Pickering-A, and one in Bruce-A.

The 19-element NPD bundle was irradiated for 621 full-power days, followed by 182 days of decay. The Pu/U, $^{235}U/^{238}U$ and Pu isotopic ratios were measured for each fuel ring of the fuel bundle [4].

The 28-element Pickering-A bundle was irradiated to an outer element burnup of about 9208 MWd/MgU. Measurements of fissile isotope compositions and the activities of a few fission products were made on an outer element of the bundle.

The 37-element Bruce-A bundle was irradiated to a burnup of about 7800 MWd/MgU, and was then allowed to cool for 1162 days. Fuel assays were performed on 9 elements of the outer ring, 6 elements of the middle ring, and 3 elements of the inner ring. The results were averaged to give isotopic ratios for the inner, middle and outer rings of the fuel bundle.

Table 3 shows the ratio of calculated to measured (C/M) isotopic ratios for fissile isotopes. Before calculating the C/M ratio, each nuclide isotopic ratio was averaged over all of the fuel

elements from all the bundles for which that particular isotopic ratio was measured. In general the agreement is very good—within 2%, except for ^{236}U and ^{241}Pu. ^{236}U has little neutronic importance and ^{241}Pu undergoes radioactive decay; therefore, its concentration is much more dependent on the detailed power history and the length of cooling time after the fuel is removed from the reactor. In general there is no bias or only a small bias in the calculated actinide concentrations, and there is an uncertainty of ±2%.

Table 3. Bias and Uncertainty using Element Data (All Bundles)

Atom Ratio	Average C/M	Standard Deviation C/M	Bias	Uncertainty
^{235}U/U	1.005	0.016	0.5%	±2%
^{236}U/U	0.961	0.040	-4%	±4%
^{238}U/U	1.000	0.000	0	0
^{239}Pu/Pu	0.996	0.004	-0.4%	±0.4%
^{240}Pu/Pu	1.006	0.008	0.6%	±0.8%
^{241}Pu/Pu	1.037	0.023	4%	±2%
^{242}Pu/Pu	1.001	0.024	0.1%	±2%
Pu/U	1.017	0.021	2%	±2%

Table 4 shows the C/M ratios for fission-product and transuranic activities for the outer element of the Pickering-A bundle. Except for the ratios for ^{99}Tc and ^{154}Eu, all of the ratios are within one experimental standard deviation from 1. The agreement for the ^{99}Tc and ^{154}Eu ratios is significantly worse. It is not expected that this would have a significant effect on reactivity calculations, since the WIMS-IST library also includes two pseudo-fission products, which account for omitted fission products. The pseudo-fission products are determined by comparing the total absorptions in the fission products specifically represented in WIMS-IST with the total absorptions predicted in all fission products in a computer code that represents all fission products. This procedure would also compensate for inaccuracies in the represented fission products.

Table 4. Fission-Product and Transuranic Activities for Outer Element of Pickering-A Bundle

Nuclide	Measured (Bq/kgU)	Calculated (Bq/kgU)	Calculated/Measured
^{237}Np	$9.99\text{x}10^{5} \pm 20\%$	$8.60\text{x}10^{5}$	0.86
^{241}Am	$1.86\text{x}10^{10} \pm 20\%$	$1.86\text{x}10^{10}$	1.00
^{99}Tc	$1.08\text{x}10^{8} \pm 10\%$	$1.46\text{x}10^{8}$	1.36
^{129}I	$2.44\text{x}10^{5}$ †	$3.47\text{x}10^{5}$	1.42
^{134}Cs	$4.16\text{x}10^{9} \pm 7\%$	$4.00\text{x}10^{9}$	0.96
^{154}Eu	$8.14\text{x}10^{9} \pm 5\%$	$9.19\text{x}10^{9}$	1.13
^{155}Eu	$3.35\text{x}10^{9} \pm 8\%$	$3.30\text{x}10^{9}$	0.99

† Uncertainty not quantified but expected to be large due to difficulty of collecting gas.

Flux and Power Distribution

The calculation of flux and power distributions within a CANDU reactor requires the use of the entire reactor physics code suite, WIMS-IST/DRAGON-IST/RFSP-IST. WIMS-IST has been validated for one of its contributions to this phenomenon—the ability of WIMS-IST to calculate flux and power distributions within a lattice cell, and in particular, the radial flux and power distribution across a CANDU bundle.

The validation was carried out by comparing reaction rates measured by activation foils placed within demountable bundles in the ZED-2 reactor, with the reaction rates of these activated foils calculated by WIMS-IST. Calculated and measured foil activities and foil activity ratios were compared. The uncertainty in the calculated flux-power distribution in each fuel element was derived under the assumption that a bundle-average flux-power level is already known.

The data used in the validation came from eight experiments, in which foil materials, activation wires or activation wafers were irradiated in the elements of different fuel bundle types. The six experiments in which foil materials were used are

- 43-element natural UO_2 fuel in a CANFLEX bundle measured during a substitution experiment at a 31-cm hexagonal lattice pitch, cooled with heavy water at room temperature and then with the coolant removed.
- 37-element natural UO_2 fuel [5] bundle measured in a full core at a 28.575-cm-square lattice pitch, cooled with heavy water at room temperature and then with the coolant removed.
- 36-element natural UO_2 fuel [6] during a substitution experiment at a 31-cm hexagonal lattice pitch, cooled with light water and heavy water at room temperature and at elevated coolant temperatures and then with the coolant removed.

- 37-element simulated mid-burnup MOX fuel bundle measured during a substitution experiment at a 31-cm hexagonal lattice pitch, cooled with heavy water at room temperature and at elevated coolant temperatures and then with the coolant removed.
- 31-element UO_2 and $(Pu,U)O_2$ Savannah River Laboratories fuel measured during experiments at a 23.7-cm hexagonal pitch, cooled with light water and heavy water at room temperature and then with the coolant removed.
- 36-element Italian $(Pu,U)O_2$ fuel measured during experiments at 24.5-cm and 31-cm hexagonal pitches, cooled with heavy water at room temperature and an elevated temperature and then with the coolant removed.

The other two experiments were performed in the early 1960s using 28-element fuel. In one of the experiments [7], copper and manganese wires were inserted in small holes that had been drilled in some of the fuel pellets. In another related experiment [8] on the same 28-element fuel, uranium wafers were inserted.

Some of the foil materials used in the experiments were ^{63}Cu, ^{55}Mn, ^{115}In, ^{176}Lu, ^{197}Au, ^{164}Dy, ^{235}U, ^{238}U and ^{239}Pu. In a typical experiment with a 37-element bundle, reactions in specific foil materials were measured in the central pin, in two of the six pins of the inner ring of fuel, in two of the twelve pins of the middle ring, in two of the eighteen pins of the outer ring, and often along the outer surface of the calandria tube. A small correction to compensate for foil self-shielding was applied to the experimental activation data. Measured activities have unknown normalizations; hence, to make a comparison, the calculations were normalized to agree with the measured pin-weighted average over all of the fuel pins of a bundle.

The accuracy of WIMS-IST for calculating the effect of the total (primarily thermal) neutron flux and power distribution through a CANDU fuel bundle has been established by comparing calculated foil activities with the foil spatial fine structure, as measured in ZED-2. Though the number of ZED-2 experiments is small, the range of geometry, coolant material, coolant temperature and fuel composition is quite varied. The standard input model for WIMS-IST does remarkably well in calculating the flux-power distribution through the CANDU bundles. Overall, the flux-power depression through a CANDU bundle is calculated by WIMS-IST to an accuracy of about 1%. No systematic bias is detected.

Lattice-Geometry-Distortion Reactivity Effects

Lattice-geometry-distortion effects include pressure tube diametral creep, channel sag and channel elongation caused by irradiation. Of these effects, only the reactivity effect of channel sag can be modelled by WIMS-IST. Channel sag leads to a deviation of the spacing between adjacent channels from that given by the design pitch. This change in spacing between channels is equivalent to variations in lattice pitch. Thus, WIMS-IST was validated for the reactivity effect due to changes in lattice pitch.

The data for this validation come from the following two flux mapped experiments performed in ZED-2: an experiment [9] with D_2O-cooled 19-element UO_2 fuel covering hexagonal lattice

pitches from 18 to 36 cm, and an experiment [10] with D_2O-cooled 28-element UO_2 fuel covering hexagonal lattice pitches from 24 to 40 cm.

Measured and calculated reactivity spacing coefficients were compared. For the experiments with 19-element fuel, the mean difference between the calculated and measured reactivity spacing coefficients is 0.379 mk/(cm change in spacing) and the standard deviation about this mean is 0.757 mk/(cm change in spacing). For the experiments with 28-element fuel, the mean difference between the calculated and measured reactivity spacing coefficients is 0.085 mk/(cm change in spacing) and the standard deviation about this mean is 0.661 mk/(cm change in spacing). In both cases the differences are small, and less than the standard deviations, and are therefore not significant.

Coolant-Purity-Change Induced Reactivity

Coolant purity can be downgraded either by degradation of the coolant during normal operation or by the addition of light water from the emergency core cooling system during an accident. Light water in the coolant increases the absorption of neutrons, and degraded coolant is slightly more effective at slowing down neutrons than pure heavy water. An increase in the amount of light water will also affect the void coefficient.

The data used in the validation come from the following two substitution experiments performed in ZED-2: an experiment using 37-element FNU bundles, and an experiment using 37-element MOX bundles, which simulate mid-burnup CANDU fuel. Both experiments were performed with a 31-cm hexagonal lattice pitch and with three different coolant purities ranging from 99.76 to 95.1 wt% D_2O. The relative uncertainty in two individual buckling measurements at different coolant purities was taken to be equal to the uncertainty in the buckling change on voiding for the same fuel type determined from ZED-2 substitution measurements.

Measured and calculated coolant purity buckling coefficients were compared. For the experiments with FNU fuel, the difference between the calculated and measured coolant purity buckling coefficients was 8%, with an estimated uncertainty of ±11%. For the experiments with MOX fuel, the difference between the calculated and measured coolant purity buckling coefficients was -10%, with an estimated uncertainty of ±8%. WIMS-IST overpredicts the coolant-purity coefficient for unirradiated natural UO_2 fuel, but underpredicts the coefficient for simulated mid-burnup fuel. For both fuel types, calculation is within 1.5 times the uncertainty derived from the estimated uncertainties in the measured bucklings. Therefore, a bias of zero with an uncertainty of ±12% was assigned for the coolant purity reactivity coefficient.

DISCUSSION AND CONCLUSIONS

The bias and uncertainties associated with WIMS-IST predictions for the various phenomena are summarised in Table 5. It was found that WIMS-IST overpredicted the reactivity change on voiding for CANDU fuel bundle types. For fresh 37-element fuel the overprediction was

1.9±0.8 mk. The overprediction of the reactivity change on coolant voiding would lead to an overprediction of both the rate of rise of power and the peak power in the fuel during a loss-of-coolant-accident transient. The moderator-purity reactivity coefficient was overpredicted by 8±3%. For the other phenomena studied, the results of the code show little or no bias and are within the uncertainty of the experimental measurements.

Table 5. Summary of Bias and Uncertainty for Each Phenomenon

Description of Phenomenon	Bias	Uncertainty
Coolant void reactivity	Overestimate +1.9 mk (37-element FNU †)	±0.8 mk
Coolant-temperature coefficient	No bias	±4%
Moderator-density and moderator-temperature coefficient	No bias	±3%
Moderator-poison coefficient	No bias	±2%
Moderator-purity coefficient	Overestimate +8%	±3%
Fuel-temperature coefficient	Overestimate for FNU Underestimate for simulated mid-burnup fuel	±10%
Fuel isotopic change	No or small bias for actinides	±2%
Flux-power distributions	No bias in bundle flux shape	±1% in bundle flux shape
Lattice distortion reactivity	No bias in lattice cell with varying pitch	_____
Coolant-purity coefficient	No bias	±12%

† FNU fuel

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REFERENCES

1. E.O. Moeck, J.C. Luxat, L.A. Simpson, M.A. Petrilli and P.D. Thompson, "Validation of Computer Codes used in Safety Analyses of CANDU Power Plants", presented at the *IAEA Technical Committee Meeting on Advances in Heavy Water Reactors*, Bombay, 1996 January 29–February 1.

2. M.B. Zeller, A. Celli, R.S. Davis, S.R. Douglas, R.T. Jones and G.P. McPhee, "High Temperature Physics Experiments Using UO_2 and Simulated Irradiated CANDU-Type Fuel in the ZED-2 Reactor", presented at the *22nd Annual CNS Conference*, Toronto, 2001.
3. R.E. Green et al., *Temperature Coefficients for a Lattice of 19-Element UO_2 Clusters*, Atomic Energy of Canada Limited (AECL) Report, AECL-1121, 1960 October.
4. J. Griffiths, M. Lounsbury and R.W. Durham, *Uranium and Plutonium Isotopes in NPD Fuel Bundle 1016*, AECL Report, AECL-2695, 1967 March.
5. R.E. Kay, *Lattice Measurements with 37-Element Bruce Reactor Fuel in Heavy Water Moderator: Detailed Lattice Cell Parameters*, AECL Report, AECL-5307, 1976 June.
6. R.E. Kay, *Lattice Measurements with 36-Element Natural UO_2 Fuel in the ZED-2 Hot Loop Facilities: Detailed Lattice Cell Parameters*, AECL Report, AECL-5969, 1977 November.
7. K.J. Serdula and R.E. Green, *Lattice Measurements with 28-Element Natural UO_2 Fuel Assemblies. Part II: Relative Total Neutron Densities and Hyperfine Activation Distributions in a Lattice Cell*, AECL Report, AECL-2722, 1967 August.
8. P.W. de Lange, C.B. Bigham, R.E. Green, T.J. Manuel, *Experimental Initial Conversion and Fast Fission Ratios for Clusters of Natural U and UO_2 in D_2O*, AECL Report, AECL-2636, 1966 September.
9. R.E. Green et al., *Lattice Studies at Chalk River and their Interpretation*, AECL Report, AECL-2025, 1964.
10. K.J. Serdula, *Lattice Measurements with 28-element Natural UO_2 Fuel Assemblies, Part I: Bucklings for a Range of Spacings with Three Coolants*, AECL Report, AECL-2606, 1966 July.