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A MONTE CARLO METHOD FOR ANALYZING MIXED-LATTICE SUBSTITUTION EXPERIMENTS USING MCNP

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ABSTRACT – Critical experiments involving a small region of test fuel substituted into a reference lattice have traditionally been analyzed using diffusion codes to extract lattice physics parameters of the test fuel such as the critical buckling and the associated bias in the calculation of k_{eff}. A method that was first developed in 2006 uses a version of MCNP5 that was modified to allow the analyst to selectively change fission neutron production in various parts of the model. This paper describes the modification made to MCNP5, demonstrates how the substitution experiment analysis is done through several examples using data from the ZED-2 critical facility, and finally, quantifies the expected uncertainties in the method.

1. Introduction

Small critical facilities are used to investigate the behavior of assemblies of fissionable material. Typically, a single parameter, (e.g., mass, concentration, or some physical dimension) is varied until the assembly is exactly critical (k_{eff}=1.000). The experiment can be used directly to validate computer codes and data by modeling the experiment and comparing the calculated k_{eff} to unity. Many such experiments have been done to support the criticality safety discipline.

The design and licensing of nuclear reactors requires obtaining experimental benchmark data or validation data from larger and more comprehensive facilities such as the ZED-2 critical facility. A mock up of the reactor core being studied is assembled in the critical facility with fuel and other lattice parameters that are as similar as possible to those of the actual reactor. In a simplified or "clean" experiment, all of the fuel is the same, i.e., all "test" fuel. Measured results such as critical dimensions, critical buckling, and neutron flux profiles can be compared directly to calculated values.

However, for various reasons, it may be neither possible nor necessary to assemble a critical lattice using test fuel alone. In these cases a lattice of "reference" or "driver" fuel is used to produce a critical assembly. The test fuel replaces the reference fuel within some limited region, usually in the centre of the reference lattice where neutron flux and importance are the highest. These are called "substitution" experiments. Unlike clean experiments, substitution experiments require further analysis to extract the lattice parameters of interest; that is, to isolate the properties of the test fuel from those of the mixed lattice of test fuel and reference fuel. The process of analyzing substitution experiments to isolate and extract the properties of the test fuel is commonly known as *substitution analysis.*

Various substitution analysis methods have been developed and used within the international community and at the Chalk River Laboratories, going back to the 1960's [1], [2], [3]. One new

method that was developed and tested at CRL beginning in 2006 [4] involves the use of a modified version of MCNP [5]. The remainder of this paper discusses the MCNP-based substitution analysis method, along with sample results for a variety of substitution experiments performed in the ZED-2 critical facility.

Section 2 provides some examples of substitution experiments conducted in ZED-2; Section 3 presents the theory and its application to analyzing these experiments; Section 4 shows some examples of applying these analysis methods; and a discussion and the conclusions are presented in Sections 5 and 6, respectively.

2. Substitution Experiments in ZED-2

The ZED-2 critical facility contains a 3-meter by 3-meter vertical cylindrical vessel in which fuel rods or fuel channels are vertically suspended. Heavy water is introduced into the vessel to act as a moderator, and make the assembly critical; reactivity is controlled by fine adjustments of the moderator level. Fuel channels can be filled with a variety of "coolant" materials (e.g., D_2O, H_2O, air, CO_2, He, organic fluids, etc.). Neutron-flux and reaction-rate distributions are measured using various neutron activation foils. Lattice configurations can be either triangular/hexagonal or square, the lattice pitch is continuously variable, and the number of fuel rods or channels is incrementally variable.

Figure 1a shows a top view schematic of a typical ZED-2 substitution experimental setup that has a hexagonal lattice with seven test fuel sites in the centre surrounded by the reference fuel sites. The attributes that can differ between test fuel sites and reference fuel sites include fuel geometry or fissionable material, channel type or coolant, and fuel temperature, but not the moderator, or the lattice configuration or pitch. Examples of other substitution experiment layouts are shown in Figures 1b and 1c, and several of the test and reference fuels typically used in these experiments are shown in Figure 2.

Substitution experiments are used in the ZED-2 critical facility when the available number of test channels or the amount of test fuel is limited, or a lattice of pure test fuel cannot be made critical within the facility. Techniques used to extract the desired reactor physics parameters for the test fuel from these mixed-lattice experiments is the subject of the next section.

3. Analyzing Substitution Experiments

3.1 Theory

Steady state neutron behaviour in a system containing fissionable material is governed by the time-independent Boltzmann transport equation, which can be expressed in operator notation as

$$\mathrm{M}\Phi(\vec{r},E,\hat{\Omega}) = \mathrm{F}\Phi(\vec{r},E,\hat{\Omega}) + S(\vec{r},E,\hat{\Omega}) \quad (1)$$

where $\vec{r}$ is the position vector, E is energy, $\hat{\Omega}$ is the unit direction vector, M is the migration and loss operator, F is the fission neutron source operator, and S is an external neutron source that is independent of neutron flux. Integration over volume, energy, and direction is implied. These operators are defined as

$$\mathrm{M}\Phi = \hat{\Omega}\cdot\nabla\Phi(\vec{r},E,\hat{\Omega}) + \Sigma_t(\vec{r},E)\Phi(\vec{r},E,\hat{\Omega})$$
$$-\int_0^\infty dE'\int_{4\pi} d\Omega'\Sigma_s(\vec{r},E'\to E,\hat{\Omega}'\cdot\hat{\Omega})\Phi(\vec{r},E',\hat{\Omega}') \quad (2)$$

and

$$\mathrm{F}\Phi = \chi(E)\int_0^\infty dE'\nu(\vec{r},E')\Sigma_f(\vec{r},E')\int_{4\pi} d\Omega'\Phi(\vec{r},E',\hat{\Omega}') \quad (3)$$

where Σ_t is the total neutron cross section, Σ_s is the neutron scattering cross section, ν is the average number of prompt plus delayed fission neutrons produced per fission, and Σ_f is the fission cross section. Although Equation (1) does not appear anywhere in MCNP nor is the neutron flux explicitly calculated, it is in fact the time-independent Boltzmann transport equation that MCNP is solving in a fixed source (SDEF) problem. A steady state solution is not possible if neutron production exceeds neutron loss.

If S=0 in Equation (1) and the left and right sides are not equal, then the flux is not constant in time and the equation has no steady state solution except the trivial solution of Φ=0. In order to allow a steady state, nontrivial flux solution an eigenvalue is introduced and Equation (1) is rewritten as

$$\mathrm{M}\Phi = \lambda\mathrm{F}\Phi \quad (4)$$

where λ is the eigenvalue used to balance the equation and Φ is the eigenfunction, called the λ-mode flux, frequently designated by Φ_λ. If Φ_λ is positive everywhere in space then λ is the fundamental eigenvalue. There is always a solution if the system being modelled contains any fissionable material.

Since the neutron multiplication constant[1] k is defined as the ratio of fission neutron production to total neutron loss, then

$$k = \frac{\mathrm{F}\Phi}{\mathrm{M}\Phi} = \frac{1}{\lambda}, \quad (5)$$

and Equation (4) is rewritten in the more familiar form

$$\mathrm{M}\Phi = \frac{1}{k}\mathrm{F}\Phi. \quad (6)$$

This is the form of the Boltzmann transport equation that MCNP is solving in a criticality (KCODE) problem. Since λ (or k) is a constant, it could be taken inside the integrations that form the F operator in Equation (3) and interpreted as the factor that must be applied to one of the components of F throughout the system to make it critical. Traditionally the factor is viewed as being applied to ν, thus, changing the effective average number of neutrons produced per fission.

If we introduce a similar adjustment factor called the *NPCF* (Section 3.2), which is applied to all fissionable materials in the model, Equation (6) then becomes

[1] k is used here to represent k_∞ if the model is infinite or k_{eff} if the model is finite.

$$\mathrm{M}\Phi = \frac{NPCF}{k_1}\mathrm{F}\Phi \tag{7}$$

where $k_1 \neq k$ unless *NPCF*=1. It is easy to see that if

$$NPCF = \frac{1}{k}, \tag{8}$$

then $k_1 = 1$, and the adjusted model is critical. That is, the value of *NPCF* that must be applied to all fissionable materials to make the model critical is equal to the inverse of the multiplication constant *k* from a calculation *without* the *NPCF*. Thus, the *NPCF* for the reference fuel to be used in a substitution experiment can be determined in a single calculation using Equation (8) with the value of *k* determined via simulation of an experiment with a whole core of that fuel type.

Now if different *NPCF* values are applied to different fissionable materials in the model, then Equation (7) becomes

$$\mathrm{M}\Phi = \frac{1}{k_2}\left(NPCF_1 \cdot \mathrm{F}_1 + NPCF_2 \cdot \mathrm{F}_2 + \ldots\right)\Phi \tag{9}$$

where the volume integrals in F_1, F_2, … are over different regions of space, and Equation (8) is no longer valid. It is the capability of specifying a different *NPCF* for different fuel types that allows the modified version of MCNP to be used for substitution experiment analysis. However, note that the *NPCF* for the test fuel in a substitution experiment must be determined by iteration after the *NPCF* for the reference fuel has been applied.

3.2 Application of MCNP to Substitution Analysis

The use of MCNP for performing substitution analysis is somewhat similar to earlier methods of substitution analysis using approximate deterministic neutron diffusion codes such as MICRETE (1-D/2-D, source-sink, 2-group diffusion) [2] or CONIFERS (3D, 4-group diffusion) [3]. However, the use of MCNP avoids the numerous approximations inherent in neutron diffusion methods.

In an MCNP eigenvalue (KCODE) calculation, the starting weight of each neutron is approximately one; it is not *exactly* one due to small fluctuations in the source size from cycle to cycle; i.e., the normalization process that takes place when the eigenvalue *k* is determined takes proper account of these fluctuations through small adjustments to the starting particle weights. The details of this process are given in the MCNP manual [5].

The NPCF patch in MCNP simply multiplies starting particle weights in each selected region by a user-specified Neutron Production Correction Factor, or *NPCF*. The *NPCF value*s are specified by material, and effectively change the average value of ν for the affected material: decreasing ν when *NPCF*<1, and increasing ν when *NPCF*>1. *NPCF*≤0 is not allowed, and *NPCF*=1 leaves the starting weights unchanged. The capability to specify a different *NPCF* for each fissionable material allows this patch to be used to analyse substitution experiments as described below.

The following steps, illustrated in Figure 3, are used to determine geometric buckling (B^2) for test fuel from a substitution experiment in ZED-2.

1. Simulate a full core of reference fuel with MCNP, for which the critical moderator height and other data are taken from a ZED-2 experiment. The value of the $NPCF_{ref}$ needed to make the core critical is equal to $1/k$ as calculated with no *NPCF*. A comparison of the calculated flux (or buckling) with that from the experiment can be used to confirm an accurate model.
2. Simulate the substitution experiment with MCNP where the critical moderator height is again taken from the experiment, using the $NPCF_{ref}$ calculated in Step 1 for the reference fuel and using a second $NPCF_{test}$ for the substituted region.
3. Adjust $NPCF_{test}$ in the MCNP simulation of the substitution experiment (holding $NPCF_{ref}$ fixed) and iterate until $k=1.000\pm\delta k$, where δk is the desired statistical uncertainty, typically less than 0.0001. A model check can again be done by comparing calculated and measured experimental fluxes or foil activation rates.
4. Set up an MCNP simulation of an un-reflected, bare cylindrical core of test fuel using $NPCF_{test}$ applied to all of the test fuel. Adjust the radial and axial dimensions to make the core critical ($k=1.000\pm\delta k$). It is known that the critical buckling of fuel will depend somewhat on the aspect ratio (height/diameter) of the core, due to the anisotropy in the neutron leakage caused by the fuel channels. Thus, to make a consistent comparison, the aspect ratio (H/D, or B^2_z/B^2_r), or one of the buckling components (B^2_z, or B^2_r) in the substitution analysis should be as close as possible to that found in the full-core experiments.
5. Use MCNP to compute the radial and axial distributions of neutron flux (or fission energy deposition rate) in the bare critical lattice of test fuel.
6. Fit cosine and Bessel functions to the axial and radial neutron flux distributions: $\phi(z)=A_0 \cos(\alpha (z-z_{max}))$ and $\phi(r)=C_0 J_0(\lambda r)$, respectively.
7. Use the best-fit parameters for the functions to obtain the axial and radial components of buckling, and hence, the total buckling for the test fuel: $B^2=\alpha^2+\lambda^2$.
8. In the situation where the test fuel is too low in reactivity (i.e., $k_{inf} < 1$) and has a negative geometric buckling, use booster fuel surrounding the test fuel with an appropriate $NPCF_{booster}$ also derived as in Step 1. The booster fuel may be regarded as a second reference fuel type which may or may not be the same fuel used in Step 1. The size of the test fuel region must be sufficiently large to minimize edge effects, and to ensure that there is a large asymptotic region where the neutron energy spectrum is as independent of spatial position as possible, i.e., the ratio of fast to thermal neutron flux is essentially constant. Fit a modified Bessel function to the radial distribution within the asymptotic region: $\phi(r)=C_0 I_0(\beta r)$. Data near the edge or outside of the asymptotic region must be excluded from the curve fits. The total buckling for the test fuel is then: $B^2=\alpha^2-\beta^2$.
9. This total buckling for the test fuel can then be used for the direct validation of a lattice physics code, such as WIMS-AECL [6], [7]. The critical dimensions of the bare core can be used for the direct validation of a whole-core physics code, such as RFSP [6]. In both the lattice physics and core physics codes, the value of k_{eff} is computed, using either input critical buckling or input critical dimensions.

Since the ultimate goal is to isolate the bias in a physics code prediction of k_{eff} for the test fuel, it is generally not necessary to do a critical core size or critical buckling search for MCNP itself,

since $k_{eff\text{-}test} = 1/NPCF_{test}$. Once $NPCF_{test}$ is found, then the bias in k_{eff} for MCNP for the test fuel is simply the difference in calculated k_{eff} with and without $NPCF_{test}$ applied. The bare core dimensions and associated radial and axial bucklings are mainly of interest for validation of other codes (such as WIMS-AECL, RFSP, etc.).

3.3 Uncertainty in *NPCF*

Although the derivation in Section 3.1 is rigorous, the resulting value of *NPCF* is not exact due to the statistical and propagated experimental uncertainties in calculating *k* for a known critical system. If the total uncertainty in *k* is denoted by δk, then from Equation (8) the uncertainty in the *NPCF* required to make the model critical is given by

$$\delta NPCF = \frac{\delta k}{k^2}. \tag{10}$$

A substitution experiment is more complicated. Assuming there are two different fuel types in Equation (9) and that $NPCF_1$ is known from a previous full core experiment, then the uncertainty in $NPCF_2$ is given by

$$\delta NPCF_2 = \sqrt{\delta k_2^2 + \left(\frac{\partial k_2}{\partial NPCF_1}\delta NPCF_1\right)^2} \times \frac{\partial NPCF_2}{\partial k_2} \tag{11}$$

where δk_2 is the estimated statistical and experimental uncertainty in k_2, the partial derivatives are determined via sensitivity analysis using MCNP, and correlation between the full core and substitution experiments is ignored.

3.4 Validation/Benchmarking of Substitution Analysis Method

The validation (or benchmarking) of the MCNP-based substitution analysis method can be performed three ways:

1. Buckling values derived from substitution experiments can be compared against buckling values determined from full-core flux-map experiments. Bucklings should be adjusted to common values of lattice temperature and moderator purity. This approach to validation has been used traditionally in the past [3].
2. The $NPCF_{test}$ (or $k_{eff\text{-}test}=1/NPCF_{test}$) determined from the analysis of substitution experiments can be compared against the $NPCF_{test}$ or $k_{eff\text{-}test}$ determined from the analysis of full-core experiments of test fuel.
3. An indirect, or reverse method (Figure 4) is to determine $NPCF_{test}$ and $NPCF_{ref}$ from the analysis of full-core experiments of test fuel and reference fuel(s) *a priori*, and then to apply these values of *NPCF* in the subsequent MCNP analysis of a substitution experiment. If the values of *NPCF* are correct, then the MCNP calculation of k_{eff} for the substitution experiment should be unity, within expected uncertainties ($k_{eff}=1.000 \pm \delta k_{eff}$). This method is very convenient and has been used in recent studies [8].

4. Analysis Results for Sample ZED-2 Substitution Experiments

The following subsections describe sample results of using the MCNP-based substitution analysis method in the analysis of various substitution experiments performed in the ZED-2 critical facility using a variety of lattice and fuel designs. The results described involve the use of one or more of the approaches to validation/benchmarking described in Section 3.4.

4.1 Tight Pitch Experiments with 28-NU Fuel

Tight pitch critical experiments were performed in ZED-2 using 91 ZEEP uranium metal rods at room temperature conditions (Figure 1a). The hexagonal lattice pitch was varied from 20 to 22.86 cm. The test fuel consisted of fuel channels (comprising aluminum pressure and calandria tubes) filled with 28-element natural uranium dioxide (28-NU) fuel bundles (Figure 2a) with five bundles per channel. The 28-NU fuel "coolant" material was either air or H_2O. More details on the ZEEP and 28-NU fuels can be found in [2] and [9].

Values of *NPCF* were determined first for the ZEEP reference lattices, and subsequently for the test fuel in the substitution experiments. Following the procedure described in Section 3.2, MCNP models of large regions of test fuel (boosted by ZEEP rods) were created, with the *NPCF* applied to the test fuel and with model dimensions adjusted to be critical. The flux distribution was calculated, and the data were curve-fitted to obtain axial and radial components of buckling. The results are shown in Table 1, along with critical buckling values derived from the flux distribution in ZED-2 experiments with large regions of test fuel, (boosted by ZEEP rods). Also shown are earlier results obtained using the CONIFERS-based substitution analysis method [3]. The buckling data is plotted for H_2O-cooled and air-cooled 28-NU fuel in Figure 5. While the CONIFERS method provides satisfactory agreement at larger lattice pitches (e.g., 22.86 cm), it is clearly demonstrated that the MCNP-based method gives better agreement in general. The MCNP-based substitution analysis results agree with the full-core results within the experimental uncertainties.

4.2 Square Pitch Experiments with 42-LEU Fuel

Substitution experiments were performed in ZED-2 using 52 channels containing 43-SEU or 43-RU fuel bundles (5 bundles per channel) at room temperature conditions (Figure 1b). The 43-SEU and 43-RU bundles were made with 43 fuel pins containing slightly enriched (0.95 wt% $^{235}U/U$) or recovered uranium (0.96 wt% $^{235}U/U$), respectively. The square lattice pitch was 24 cm. The central 12 lattice sites were replaced with fuel channels (comprising aluminum pressure and calandria tubes) filled with 42-element low enriched uranium (~1.7 wt% $^{235}U/U$) fuel bundles (42-LEU), with 3 to 4 bundles per channel, complemented by 43-SEU bundles at the top. The 42-LEU fuel also contained a central neutron-absorbing pin made of zirconia/dysprosia/gadolinia/yttria. The 42-LEU fuel was cooled with either air or H_2O. More details on the 43-SEU, 43-RU and 42-LEU fuel types can be found in [8], [10], [11], [12].

Values of *NPCF* were determined for the 43-SEU and 43-RU reference fuels, and the *NPCF* values for the 42-LEU fuel were also isolated. Full-core experiments with 42-LEU fuel were performed and analyzed with MCNP to determine *NPCF* values. In addition, substitution analysis was used to obtain bucklings for the 42-LEU fuel (using 4-bundle, 5-bundle, and 6-

bundle-high bare cores with radii adjusted to achieve criticality) which could also be compared with the values obtained from the full-core flux-map results.

Results are shown in Table 2. Buckling results are shown in Figure 6a. The values of buckling determined from substitution analysis differ from full-core results by 0.06 m^{-2} or less, and fall within the overlap of two standard deviations in both the substitution and full-core results. The buckling results from the substitution analysis shown in Table 2 were interpolated against axial buckling, which was set to be the same as that in the full-core experiments, and differed for the H_2O-cooled and air-cooled lattices.

4.3 Hexagonal Lattice Experiments with Natural Uranium Fuel

Room-temperature full-core experiments were performed in ZED-2 using three types of test fuel in hexagonal lattices. The lattice for the substitution experiment is illustrated in Figure 1c. The test fuels included 28-NU (described in Section 4.1), 19-element natural uranium metal (19-UM), and 7-element natural uranium oxide (7-NU), which are illustrated in Figures 2b and 2c, respectively. The substitution experiment (Figure 1c) included 55 ZEEP reference fuel rods, surrounded by 30 air-cooled 28-NU channels. Thus, the reference lattice comprised two different fuel types each with its own *NPCF* value in the substitution analysis. In the substitution experiments, the central seven ZEEP rods were replaced with 28-NU, 19-UM, or 7-NU fuel bundles, cooled by either air or D_2O.

Values of *NPCF* were determined for each of the test fuels, D_2O-cooled and air- or He-cooled, with MCNP analysis of the full-core experiments. The experiments were conducted at various pitches and the results interpolated at a pitch of 31 cm (Table 3).

Then, the values of $NPCF_{test}$ determined from the full-core experiments were applied to the test fuel in the various substitution experiments (Figure 1c). Ideally, if the values of $NPCF_{test}$ are applied to the various test fuels in the MCNP analysis of the substitution experiments, then the value of k_{eff} calculated by MCNP should be unity, within uncertainties. This is an indirect validation of the substitution analysis method, as discussed previously in Section 3.4 and illustrated in Figure 4. The results of the analysis of the substitution experiments with the $NPCF_{test}$ applied are also shown in Table 3 and Figure 6b. It is found that k_{eff} differs from unity by no more than twice the ±0.5 mk estimated uncertainty. The agreement for the 28-NU fuel is particularly good, differing from unity by less than 0.1 mk.

5. Discussion

Computer capabilities have advanced to the point that whole-core Monte Carlo transport modeling for a broad range of static problems is now practical. This means that the more approximate two-step practice of using two-dimensional lattice transport calculations to produce data for three-dimensional whole-core diffusion calculations is no longer necessary for analyzing critical experiments. Historically, diffusion-based methods of analysing substitution experiments [2], [3] typically require several adjustable parameters to correct deficiencies in these methods at the interfaces between regions of different materials. Such corrections are unnecessary when using Monte Carlo transport; thus, the *NPCF* is the only test fuel parameter that must be determined from experiment.

A comment on the term *neutron production correction factor* is in order. This term was first used in the documentation describing the CONIFERS-based substitution analysis method [3]. The term was retained in the MCNP-based method for continuity since *NPCF* serves the same purpose in both codes. However, the term is somewhat misleading because it does not "correct" the neutron production – it is a constant multiplier, applied to the F operator in Equation (7), used to remove the calculation bias in *k*, regardless of where that bias arises. If a single *NPCF* is applied to the whole core, *k* changes, but everything else remains unchanged including the flux shape. The usefulness of the method is the ability to use different *NPCF* values to remove the calculation biases in *k* for different fuel types, determined experimentally. In this case, altering one of several *NPCF* values *will* change the flux shape.

6. Conclusions

A new method for analyzing substitution experiments based on the use of a modified version of MCNP has been developed and tested. The MCNP-based method is conceptually simple, only requiring a minor change to the MCNP source code in a single subroutine to allow the application of an adjustment factor (referred as a *neutron production correction factor, NPCF*) to the starting weight of neutrons born in fission in a given fuel material.

The MCNP-based substitution analysis method can be used to isolate the k_{eff} (and hence the bias in k_{eff}) of a given test fuel from the bias in k_{eff} for a substitution experiment involving one or more reference fuels, provided that the *NPCF values* for the reference fuel lattice can be determined from other critical experiments. The MCNP-based substitution analysis method can also be used to determine bare core critical dimensions and buckling for a given test fuel, which can be used for the subsequent validation of other reactor physics codes.

Testing has shown that the MCNP-based method works very well, showing good agreement (within uncertainties) between substitution analysis results and full-core experimental results, with a noticeable improvement over older, more approximate deterministic methods using few-group diffusion theory codes [3].

The use of substitution experiments and the MCNP-based substitution analysis method will provide important validation data for various types of existing and postulated fuel materials and fuel bundle designs. Such data will be relevant and important in validation of codes for future reactor designs, including the use of thorium-based [13] and alternative LEU-based [14] fuels in heavy-water reactors.

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Table 1 Substitution Analysis Results for 28-NU Test Fuel in ZEEP/D_2O Hexagonal Lattices

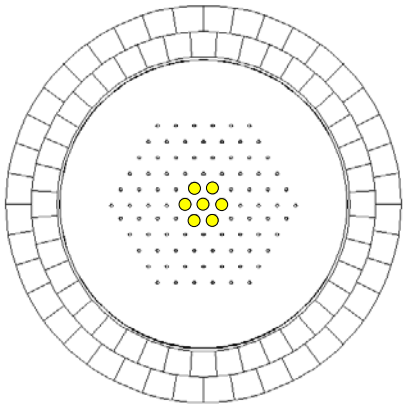
Experiment Type	Lattice Pitch (cm)	Test Fuel/ Coolant	NPCF Ref	NPCF Test	B^2 Expt (m^{-2})	B^2 MCNP (m^{-2})	B^2 CONIFERS (m^{-2})
Full Core	20.00	–	1.00265	–	6.308±0.020	6.326	6.923
Full Core	21.59	–	1.00200	–	5.590±0.012	5.592	6.235
Full Core	22.86	–	1.00284	–	5.367±0.009	5.360	5.819
Substitution	20.00	28-NU/H_2O	1.00265	1.01050	-1.380±0.127	-1.411	-1.733
Substitution	21.59	28-NU/H_2O	1.00200	1.01057	-0.502±0.163	-0.524	-0.741
Substitution	22.86	28-NU/H_2O	1.00284	1.00752	-0.047±0.047	-0.052	0.081
Substitution	20.00	28-NU/Air	1.00265	1.00708	-0.318±0.114	-0.402	-0.581
Substitution	21.59	28-NU/Air	1.00200	1.00843	1.393±0.091	1.324	1.323
Substitution	22.86	28-NU/Air	1.00284	1.00876	2.322±0.068	2.259	2.294

Table 2 Substitution Analysis Results for 42-LEU Test Fuel at a 24-cm Square Pitch

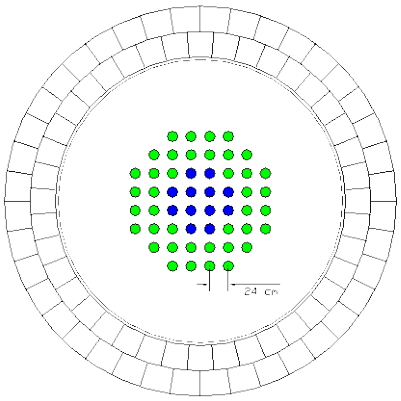
Experiment Type	Ref Fuel/ Coolant	NPCF Ref	Test Fuel/ Coolant	NPCF Test	B^2 (m^{-2})
Substitution	43-SEU/RU/H_2O	1.01897	42-LEU/H_2O	1.01089±0.00128	5.358±0.053
Substitution	43-SEU/RU/Air	1.01640	42-LEU/Air	1.00883±0.00067	3.614±0.028
Full Core	–	–	42-LEU/H_2O	1.01038±0.00007	5.374±0.025
Full Core	–	–	42-LEU/Air	1.00901±0.00007	3.669±0.026

Table 3 Substitution Analysis Results for Three Test Fuels at a 31-cm Hexagonal Pitch

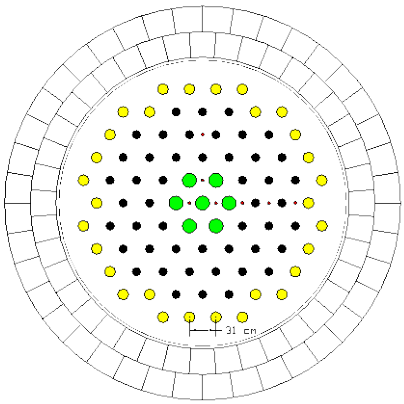
Experiment Type	Ref/Booster Fuel	Test Fuel/ Coolant	NPCF Test	k_{eff}
Full Core	–	7-NU/D_2O	1.00727±0.00067	–
Full Core	–	19-UM/D_2O	1.00772±0.00014	–
Full Core	–	28-NU/D_2O	1.00775±0.00008	–
Full Core	–	7-NU/He	1.00682±0.00058	–
Full Core	–	19-UM/He	1.00752±0.00029	–
Full Core	–	28-NU/Air	1.00791±0.00008	–
Substitution	ZEEP/28-NU	7-NU/D_2O	1.00727±0.00067	1.00084±0.00050
Substitution	ZEEP/28-NU	19-UM/D_2O	1.00772±0.00014	1.00049±0.00042
Substitution	ZEEP/28-NU	28-NU/D_2O	1.00775±0.00008	0.99996±0.00040
Substitution	ZEEP/28-NU	7-NU/Air	1.00682±0.00058	1.00100±0.00047
Substitution	ZEEP/28-NU	19-UM/Air	1.00752±0.00029	1.00062±0.00041
Substitution	ZEEP/28-NU	28-NU/Air	1.00791±0.00008	0.99990±0.00041



1a. Tight hexagonal pitch, 28-NU test fuel, ZEEP reference fuel. (Section 4.1)

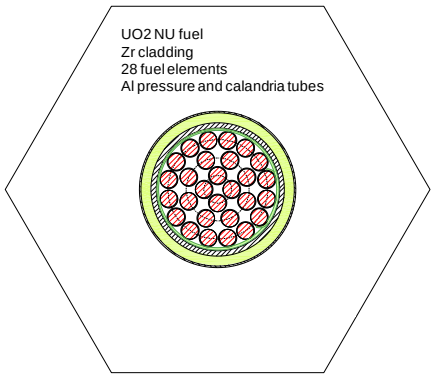


1b. 24-cm square pitch, 42-LEU test fuel, 43-SEU/RU reference fuel. (Section 4.2)

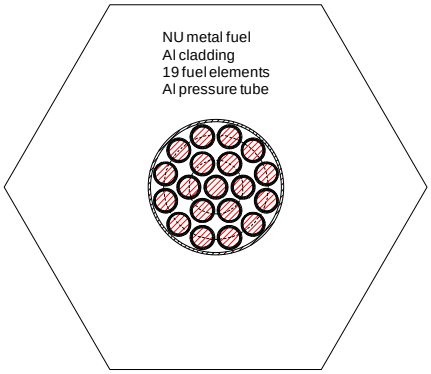


1c. 31-cm hexagonal pitch, 28-NU, 19-UM, 7-NU test fuel, ZEEP and 28-NU reference fuel. (Section 4.3)

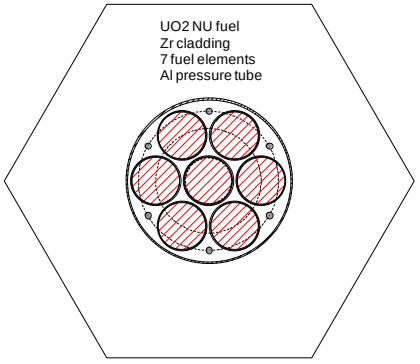
Figure 1 Mixed-Lattice Arrangements for the Sample Substitution Experiments



2a. 28-NU Test Fuel



2b. 19-UM Test Fuel



2c. 7-NU Test Fuel

Figure 2 Sample Test-Fuel Bundle and Channel Types in a Hexagonal Lattice Cell

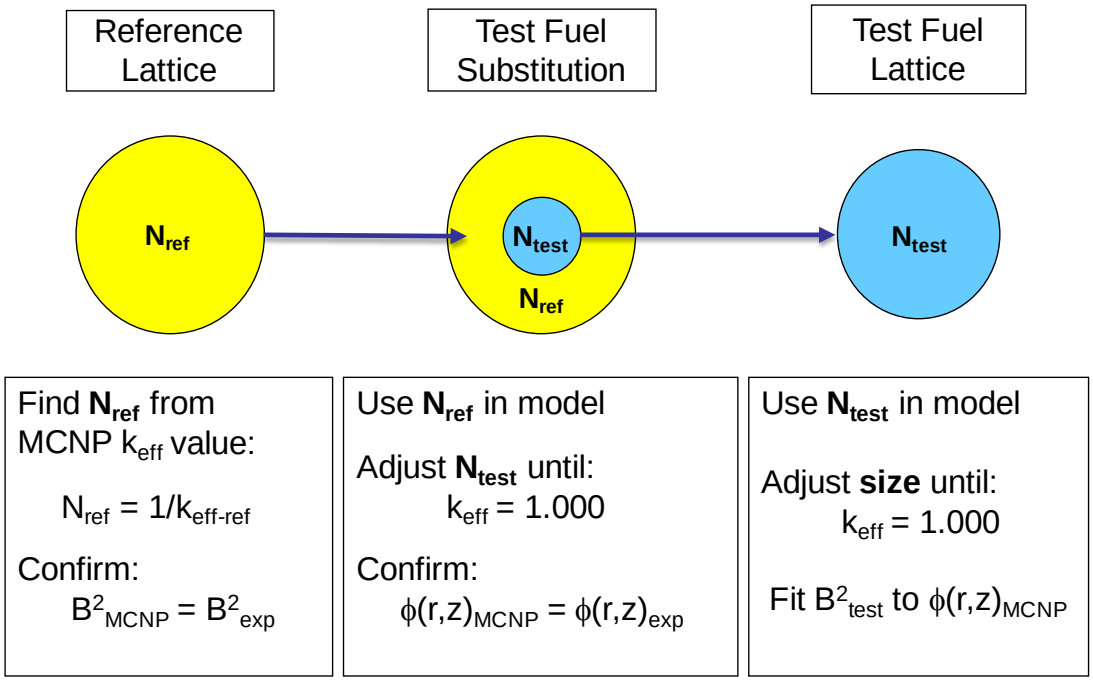


Figure 3 Schematic Representation of MCNP-Based Substitution Analysis Method (N is the neutron production correction factor, *NPCF*)

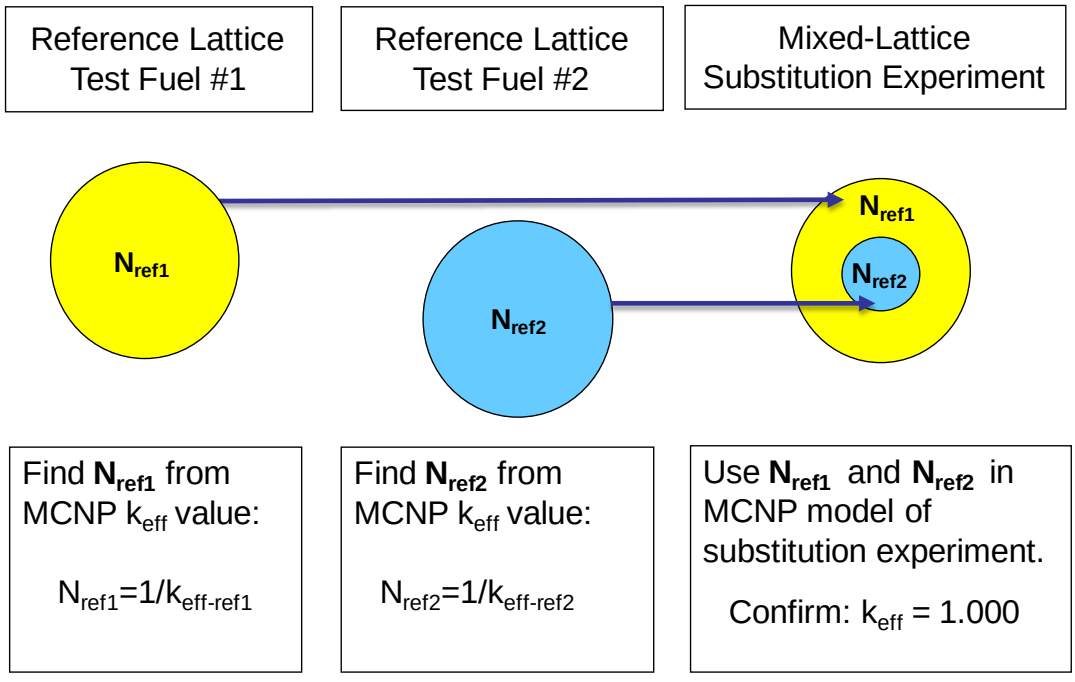


Figure 4 Indirect Validation Approach for MCNP-Based Substitution Analysis Method (N is the neutron production correction factor, *NPCF*)

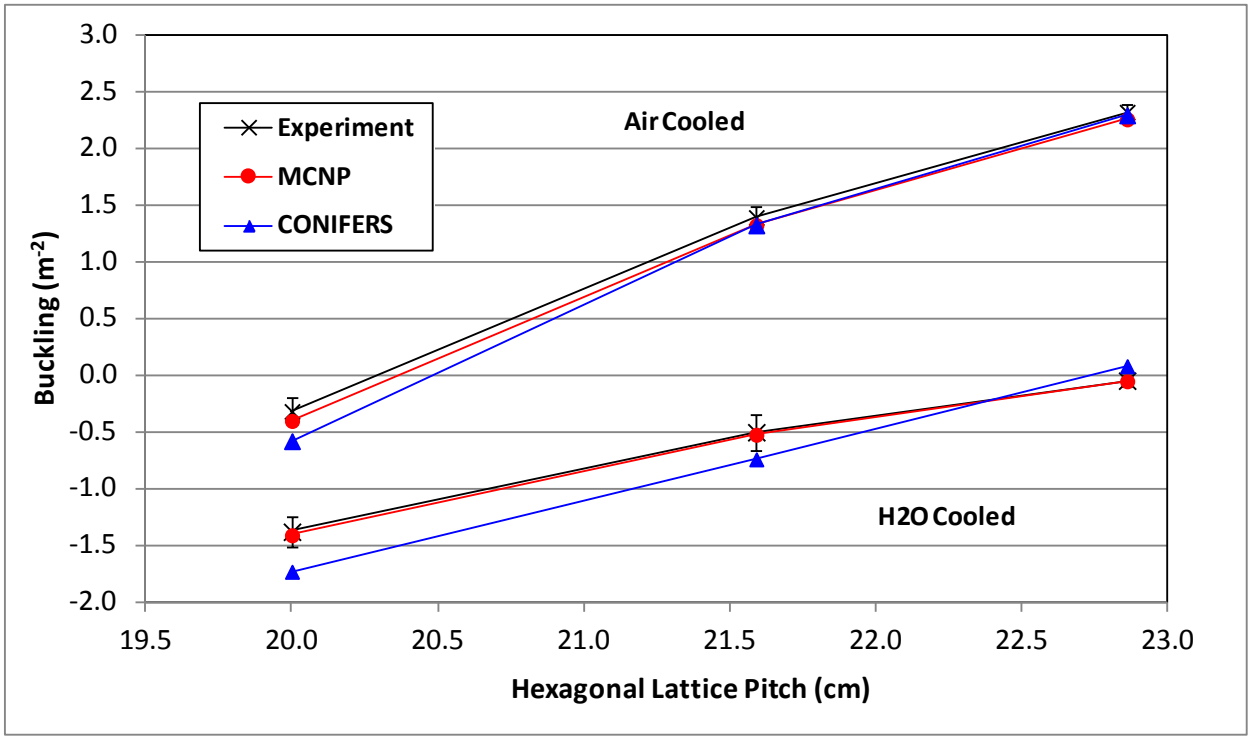
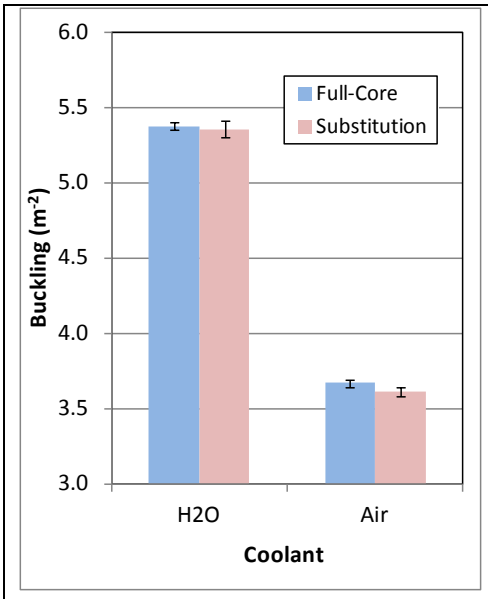
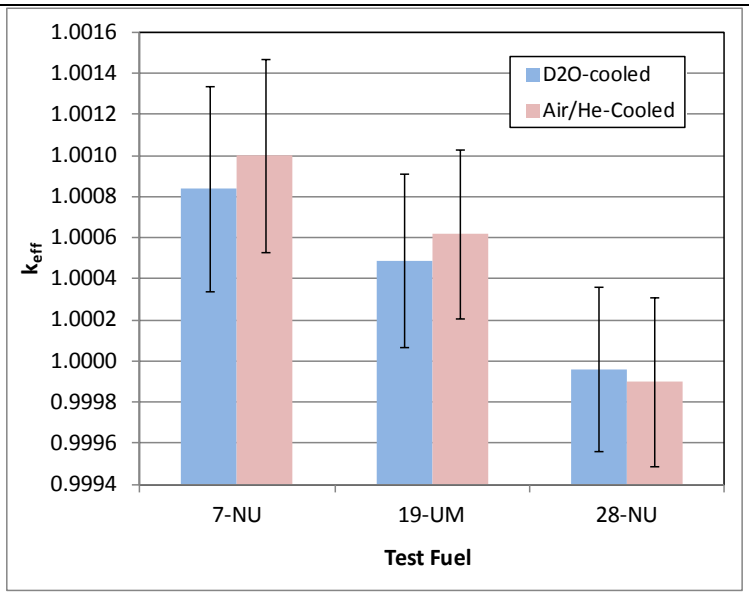


Figure 5 Comparison of Substitution Analysis Methods with Experiment for Buckling of 28-NU Test Fuel in Tight Pitch Lattices of ZEEP Reference Fuel (Section 4.1)



6a. 24-cm square pitch, 42-LEU test fuel, 43-SEU/RU reference fuel. (Section 4.2)



6b. 31-cm hexagonal pitch, 7-NU, 19-UM, 28-NU test fuel, ZEEP and 28-NU reference fuel. (Section 4.3)

Figure 6 Substitution Analysis Results for Various Test and Reference Fuels