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VALIDATION STUDIES OF THE ENDF/MC²-2/SDX
CELL HOMOGENIZATION PATH*

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ABSTRACT

An extensive validation study of the ENDF/MC²-2/SDX cell homogenization path has been made. The validation procedure has relied on the availability of rigorous Monte Carlo results obtained with the VIM code. The current study has investigated three ZPR benchmark assemblies with rather diverse characteristics. The calculations have included homogeneous zero-leakage cells, critically-buckled heterogeneous cells, and full "as-built" critical assemblies. This study has identified and eliminated several limitations and inconsistencies in these analytical methods and their application. The deterministic methods and Monte Carlo have been shown to agree very well (i.e., generally within 1σ uncertainties) for zero-buckled homogeneous and heterogeneous cell calculations. For the high-buckling cases, there was a bias on leakage-related parameters for both the homogeneous and heterogeneous cell calculations. This bias -- less leakage with MC²-2/SDX relative to VIM -- was consistent with the results observed in the full assembly calculations. MC²-2/SDX eigenvalues for the three ZPR assemblies were 0.5-0.7% δk high relative to VIM. Principal cross sections and neutron spectrum in the full assembly calculations were in good agreement between these methods. The source of these apparent differences in neutron transport or leakage between the deterministic and Monte Carlo calculations of the full assembly must be identified and eliminated.

I. INTRODUCTION

This paper summarizes the results from an extensive Monte Carlo based validation study of the unit cell homogenization prescriptions and the methods and codes used for the analysis of Zero Power Reactor (ZPR) fast breeder reactor critical experiments at Argonne National Laboratory. The present study includes a diverse set of ZPR benchmark assemblies and represents an extension in both scope and detail of earlier validation studies by Wade et al.¹⁻⁵ Results of standard analysis methods based on the ENDF/MC²-2/SDX cell homogenization path⁶⁻⁸ have been compared with results produced by the VIM continuous energy Monte Carlo code.^{9,10} The present study has intercompared these methods not only for unit cells but also for three-dimensional full reactor models. A primary goal of these efforts has been to identify and quantify the methods' biases and uncertainties in the full assembly calculations.

For each ZPR assembly, the validation effort progressed from homogenous zero-leakage tests through critically-buckled heterogeneous cells to calculations of the full "as-built" assembly. For each step in the validation study, eigenvalue, neutron spectrum, broad group cross sections, and reaction rates obtained with deterministic methods were compared to values obtained with the VIM Monte Carlo code. ENDF/B Version IV data were used for all calculations in this

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study. Sensitivities of results to many user options (e.g., P_n spectrum options in creating the intermediate SDX base library for highly buckled systems, mesh and transport corrections, use of Benoist¹¹ or Gelbard¹² methods for treating anisotropic neutron diffusion or "streaming") were also determined.

This paper is organized in the following way. Section II discusses briefly the standard ZPR analysis methods and codes employed at ANL. The validation procedure is also outlined. Section III describes the principal characteristics and unit cells of the three ZPR assemblies considered in this study. Section IV reviews the unit cell calculations, focusing primarily on the core unit cell of ZPR-9 Assembly 34, the U/Fe benchmark assembly. The full assembly calculations are presented in Section V. Section VI provides a brief summary of results and conclusions.

II. ANALYTICAL METHODS AND VALIDATION PROCEDURE

Fast reactor configurations are constructed by loading the ZPR matrix tubes with drawers which have been loaded with plates and blocks of reactor materials. These plates are approximately 2 in. (5.08 cm) high, vary in width from 1/16 to 2 in. (0.16 to 5.08 cm) and in length from approximately 2 to 12 in. (5.08 to 30.48 cm), and are loaded parallel to the drawers. Furthermore, the unit cell loading is repeated in each drawer, forming planes (interrupted by relatively thin matrix tube walls and drawer bottom) of each material in the unit cell. In the standard ZPR analysis methods, a prescription is used to convert the three-dimensional physical geometry of the plate type drawer loadings into one-dimensional calculational models for the unit cell. Details of this 3D \rightarrow 1D modeling prescription are given in Ref. 1.

The standard ZPR critical assembly analysis methods employed by ANL are diagrammed in Fig. 1. The basic nuclear data (ENDF/B) are processed by the ETOE-2/MC²-2/SDX codes. ETOE-2 reformats the ENDF/B data into libraries for MC²-2 and SDX; MC²-2 is a zero-dimensional \sim 2000 ultra-fine-energy group slowing-down code which is used to produce a \sim 200 fine group library for SDX (which excludes the contributions of selected capture and fission resonances). SDX is a one-dimensional cell homogenization code which collapses in space and energy from the \sim 200 fine group level to produce \sim 10 to 30 broad group cell-averaged cross sections. As depicted in Fig. 1, SDX produces both cell-average and plate cross sections for use in ZPR analysis. "Cell-average" cross-sections include the effects of plate spatial self-shielding and platewise resonance energy self-shielding in such a way that unit cell-average reaction rates are preserved in a calculation in which the unit cell composition is homogenized. "Plate" cross-sections are used in the generation of broad group cell anisotropic diffusion coefficients.

Anisotropic diffusion coefficients are generated using the methods of Benoist¹¹ or Gelbard¹². The resulting broad group parameters are used in multigroup diffusion and S_n transport calculations* of full reactor RZ or XYZ models which employ smeared atom densities to represent the contents of the unit cells.

The validation of these standard ZPR analysis methods was based on comparison with rigorous Monte Carlo solutions obtained with the VIM code. The VIM Monte

*All transport calculations in this study used a P_0 (transport-corrected) in-group elastic scattering cross section and σ_{tr} . No estimates of the effects of higher order scattering moments were included in this study.

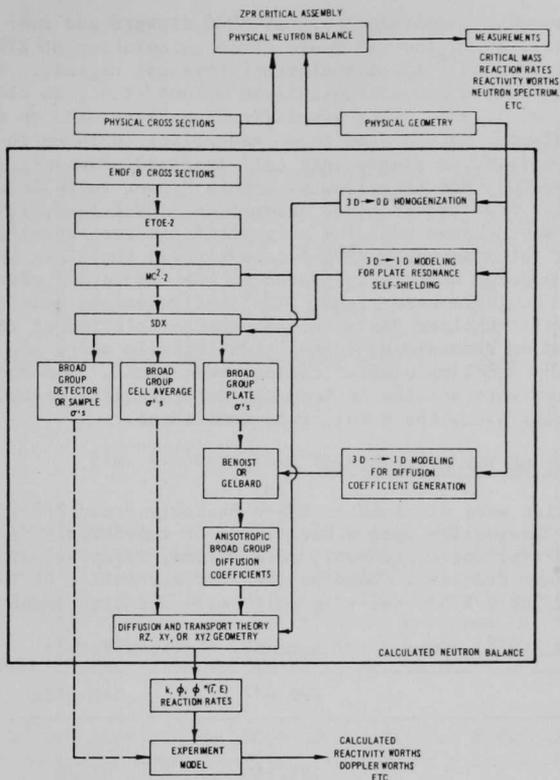


Fig. 1. Diagram of ZPR Critical Assembly Analysis Methods.

Carlo code permits an explicit three-dimensional geometrical representation of the unit cell. Neutron cross sections are derived from the ENDF/B data files and are treated as continuous functions of energy. Given the geometry and composition of the three-dimensional cells and the ENDF/B data, these Monte Carlo methods give an essentially exact solution of the Boltzmann equation and low-variance estimates of the integral parameters of interest.

As diagrammed in Figure 1, these standard methods are used with ENDF/B data to produce calculated values to compare with experimental values measured in the ZPR critical assembly. In the present study, the physical geometries of the unit cells and of the full critical assemblies have been provided in explicit three-dimensional platewise detail to the VIM code together with ENDF/B data to produce "rigorous" or "best" calculated values. That is, the physical geometry of each matrix tube and drawer, every plate loaded in the drawers, and all remaining gaps were defined explicitly. Each assembly was loaded with thousands of drawers and the entire assembly contained tens of thousands of plates. Furthermore, thirteen rectangular parallelepiped regions were required to describe each of the canned ZPR materials, such as sodium or plutonium. For

example, ZPR-6 Assembly 7 contained almost 4000 drawers and over 100,000 plates. The model used in the VIM Monte Carlo calculation of ZPR-6 Assembly 7 defined over a quarter of a million distinct physical regions. Because the goal of this study was to compare calculated values (i.e., to obtain C/C' values not C/E values), some minor simplifications were made in modeling the "as-built" assemblies. Each of the three assemblies included in this study had a single core zone (i.e., a single unit cell loading). However, limitations in the ZPR plate inventory did not allow each core drawer to be loaded with the same plate lengths. For two of these assemblies (ZPR-6 Assembly 7 and ZPR-9 Assembly 34), it was assumed that the plate loadings were identical in all drawers. For the third assembly (ZPR-9 Assembly 32) the plate loadings in each drawer were modeled exactly as loaded in the "as-built" assembly. The following points should be understood. The configurations modeled in the calculations closely retained the principal characteristics of the "as-built" assemblies, including dimensions, composition, fissile mass, and unit cell loadings, i.e., the modeling simplifications were small. And most importantly, the same assemblies were modeled in both the deterministic methods and the Monte Carlo methods, i.e., the models were consistent.

III. DESCRIPTIONS OF THE ZPR SYSTEMS

Three ZPR assemblies were examined -- ZPR-6 Assembly 7 and ZPR-9 Assemblies 32 and 34. These assemblies span a wide range of characteristics, including composition, fuel type and enrichment, core volume, spectrum, unit cell heterogeneity, and leakage fraction. Some of the characteristics of these assemblies are summarized in Table I and the core unit cells are diagrammed in Fig. 2.

TABLE I. Summary of Assembly Characteristics

	ZPR-6/7	ZPR-9/32	ZPR-9/34
Core			
Height (cm)	152.56	91.60	183.20
Diameter (cm)	161.36	88.38	125.46
Height/Diameter	0.945	1.036	1.46
Volume (liters)	3120	562	2265
No. of Enrichment Zones	1	1	1
Compositions			
Core	Pu/U/O/Na/SST	Pu/U/O/Na/SST	U/SST
Radial and Axial Blankets	U/SST	U/O/Na/SST	----
Radial and Axial Reflectors	----	U/SST	SST/U
Fuel Type	(Pu,U)oxide	(Pu,U)oxide	U metal
Fissile Enrichment (%)	13.39	22.18	93.30
Core Fe Atom Density (atoms/barn/cm)	0.0128	0.0188	0.0705
Critical Mass (kg)	1133.1	335.1	992.0
k_{∞} (for Homogeneous Core)	1.22	1.65	1.53
Core Leakage Fraction	0.22	0.39	0.36
Spectral Index, $^{28}f/^{25}f$	0.0205	0.0290	0.0202

ZPR-6 Assembly 7 was a large, uniform, dilute plutonium oxide fueled core¹³ with a single drawer unit cell. It had a relatively clean cylindrical geometry

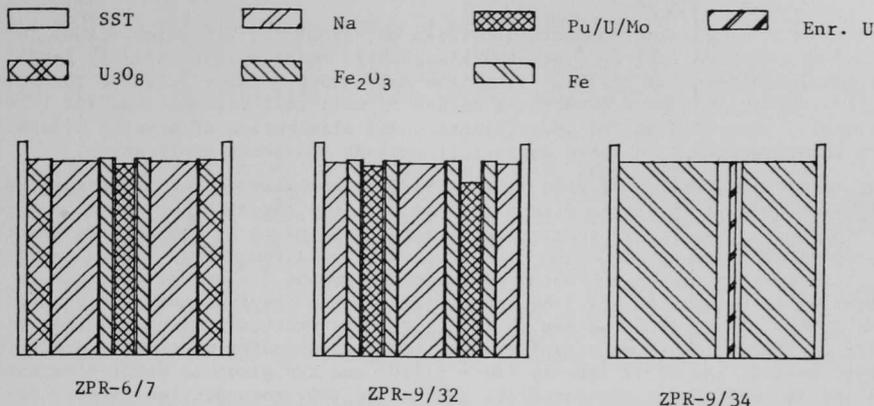


Fig. 2. Core Unit Cell Diagrams.

and a full depleted uranium blanket. It is one of the principal fast reactor data testing benchmark assemblies. The core unit cell had a symmetric loading that included a single column of Pu/U/Mo fuel and two columns of U₃O₈. In the core of Assembly 7, approximately 84% of the absorptions occurred in ²³⁹Pu (~47%) and ²³⁸U (~37%); ~82% of the core fissions occurred in ²³⁹Pu and ~12% occurred in ²³⁸U. The total core leakage fraction was ~22%. Of the three assemblies studied, Assembly 7 had the most typical LMFBR spectrum and composition.

ZPR-9 Assembly 32 was part of the LMFBR Safety-Related Critical Experiments Program.¹⁴ The reference configuration consisted of a small single-zone core with an LMFBR outer-core composition (with $k_{\infty} \approx 1.65$). The core unit cell was a single drawer cell with two columns of Pu/U/Mo fuel. These two fuel plates had substantially different enrichments (18 vs 26%) and heights (4.928 vs 4.521 cm). In the core of Assembly 32, approximately 87% of the absorptions occurred in ²³⁹Pu (~60%) and ²³⁸U (~27%); ~87% of the fissions occurred in ²³⁹Pu and ~9% occurred in ²³⁸U. Of the three assemblies included in this study, Assembly 32 had the hardest neutron spectrum and the largest core leakage fraction (~39%).

ZPR-9 Assembly 34 consisted of a single-zone core¹⁵ of enriched (93% ²³⁵U) uranium and iron with stainless steel axial and radial reflectors and an outer radial reflector of depleted uranium. The U/Fe benchmark assembly was part of a series of critical experiments to support the Safety Test Facility (STF) core design efforts. The unusual composition, ²³⁵U and iron, and the clean geometry of the core made the assembly useful as a data testing benchmark. The core had a single drawer unit cell, consisting of a single enriched uranium metal fuel plate embedded in an iron cell (with all 5.08 cm plate heights). In the core of Assembly 34, over 95% of the absorptions occurred in ²³⁵U (80%) and Fe (15%); and ~99.7% of the fissions occurred in ²³⁵U. This assembly had the simplest core unit cell in terms of heterogeneity, and virtually no "streaming" or anisotropic diffusion effects. The core leakage fraction was large (~36%) for Assembly 34 (comparable to Assembly 32).

IV. UNIT CELL STUDIES

The initial eigenvalue comparison between MC²-2/SDX and VIM calculations for ZPR-9 Assembly 34 (the U/Fe benchmark assembly) revealed unacceptably large eigenvalue biases (up to 2.1% δk) in the multigroup methods relative to Monte Carlo. Attention was focused on a series of unit cell calculations for this assembly, resulting in the identification and elimination of several limitations and inconsistencies in these analytical methods and their application.

The high concentration of iron in the ZPR-9/34 assembly caused an unexpected high-energy self-shielding effect in iron. Unlike the other principal nuclides of interest, the elastic scattering data for iron given in the ENDF/B "smooth" files exhibit strong resonance-like fluctuations in the energy region above the upper cut-off point of the resolved resonance region.* The energy range in question is between 60 keV (the upper limit of the resolved energy range for Fe) and 2 MeV. These fluctuations in the Fe elastic scattering cross section have average "half-widths" much smaller than the corresponding ultra-fine group (ufg) width used in the MC²-2 library ($\Delta u = 1/120$) and are given as point-wise data in the "smooth" cross section file. While the VIM cross section library retains the detail as given in ENDF, the data are preprocessed as infinitely dilute ultra-fine group cross sections into the MC²-2 library. Since the self-shielding effects will be significant only for a limited number of systems with high iron concentrations, special iron ufg cross sections with the appropriate self-shielding effect can be incorporated at the MC²-2 library preparation level using the narrow resonance approximation. For the present study, self-shielded iron cross sections corresponding to each assembly studied were added to the MC²-2 library. For the ZPR-9/34 assembly, the effects of the iron self-shielding were quite dramatic (changing the eigenvalue by $\sim 1.6\%$ δk). The MC²-2/SDX values were in excellent agreement with the VIM results when the iron self-shielding effects were included. This iron self-shielding effect was $\sim 0.2\%$ δk in ZPR-9/32 and $< 0.1\%$ δk in ZPR-6/7.

The unit cell validation study progressed through four stages:

- Homogeneous Tests with Zero-Leakage
- Homogeneous Tests with Critical-B²
- Heterogeneous Cell with Zero-Leakage
- Heterogeneous Cell with Critical-B².

In each step of the validation study, eigenvalue, neutron spectrum, broad group cross sections and reaction rates obtained with deterministic methods were compared to the VIM Monte Carlo results. For the non-zero leakage cases, two leakage related parameters, $\bar{\lambda}^2$ and $k_{\infty} - k(\vec{B})$, were also derived. $\bar{\lambda}^2$ is the mean-squared distance traveled from birth to fission. In the MC²-2/SDX calculations, $\bar{\lambda}^2$ has been determined from the expression

$$\bar{\lambda}^2 = - \frac{2}{k_{\infty}} \frac{\delta k}{\delta B^2},$$

for a small change in buckling, δB^2 , around the zero buckling case. In the VIM calculations of the zero-buckling infinite lattices, a site tape was generated

*The self-shielding effects in iron discussed herein refer to the self-shielding of the high energy elastic scattering cross section. All calculations in this study have included self-shielding of capture resonances of iron (and the other structural materials).

containing birth and death coordinates of each neutron and its fission weight at death. An efficient method developed by Gelbard et al.¹⁶⁻¹⁸ was used to derive Monte Carlo estimates of eigenvalue in an infinite uniform lattice as a function of buckling. (Details of these methods have been outlined by Wade in Reference 1.)

Some of the results of the unit cell studies for the core cell of ZPR-9 Assembly 34 are summarized in Table II. In the first two sections of Table II, results are presented from MC²-2 calculations obtained both with and without the high energy self-shielding of the iron elastic scattering data. In the homogeneous zero-buckled case, the effect of the Fe self-shielding on the MC²-2 eigenvalue or k_{∞} is relatively small ($\sim 0.2\% \delta k$). There were, of course, large differences in the total cross section of iron, which produced large differences in the calculated neutron spectra. In the comparison with VIM, the inclusion of the iron self-shielding in the MC²-2 calculations produced excellent agreement

TABLE II. Unit Cell Calculations for ZPR-9 Assembly 34

Homogeneous U/Fe Core Cell $B^2 = 0.0$		
	k_{∞}	Δk (Relative to VIM)
VIM $\pm 1\sigma$	1.53135 \pm 0.00127	
MC ² -2 without Self-Shielded Fe	1.52914	-0.00221
MC ² -2 with Self-Shielded Fe	1.53116	-0.00019
Homogeneous U/Fe Core Cell $B^2 \approx B_{crit}^2$		
	$\bar{\Sigma}^2$ cm ²	$k_{\infty} - k(B^2 = 0.0008)$
VIM $\pm 1\sigma$	3665.77 \pm 21.97	0.53387 \pm 0.00410
MC ² -2 without Self-Shielded Fe (B_{crit}^2)	3173.07	0.50829
MC ² -2 with Self-Shielded Fe (B_{crit}^2)	3357.84	0.53048
MC ² -2 with Self-Shielded Fe ($B^2 = 0.0$)	3582.95	0.53493
Heterogeneous U/Fe Core Cell $B^2 = 0.0$		
	k_{∞}	Δk (Relative to VIM)
VIM $\pm 1\sigma$	1.53226 \pm 0.00197	
MC ² -2(IP1)/SDX(IP1)	1.53037	-0.00189
MC ² -2(CP1)/SDX(IP1)	1.53033	-0.00193
MC ² -2(CP1)/SDX(IP1) with Fine Mesh	1.52959	-0.00267
Heterogeneous U/Fe Core Cell $B^2 \approx B_{crit}^2$		
	$\bar{\Sigma}^2$ cm ²	$k_{\infty} - k(B^2 = 0.0008)$
VIM $\pm 1\sigma$	3713.78 \pm 23.19	0.53582 \pm 0.00411
MC ² -2(CP1)/SDX(IP1) - B_{crit}^2	3568.82	0.52977
MC ² -2(IP1)/SDX(IP1) - B_{crit}^2	3453.89	0.51774
MC ² -2(CP1)/SDX(IP1) - $B^2 = 0.0$	3605.44	0.52823

IP1 and CP1 refer to inconsistent and consistent P1 options in MC²-2/SDX.

(i.e., generally within 1σ uncertainties). The eigenvalue bias ($<0.02\% \delta k$) is much less than the Monte Carlo estimated 1σ ($0.127\% \delta k$); the neutron spectrum agrees well; and the principal cross sections agree within 0.1 - 0.2% over most of the energy range.

The effects of the iron self-shielding on leakage parameters are very dramatic in the high buckling case. Note the MC²-2 calculation which did not include the self-shielding of iron underestimates $\bar{\lambda}^2$ by almost 15% (relative to VIM) and underestimates the decrease in k_{eff} due to the imposed buckling ($B^2 = B_{\text{crit}}^2$) by almost 5% of its value, i.e., the MC²-2 $k_{\text{eff}}(B^2 = 0.0008)$ is $\sim 2.2\% \delta k$ higher than the VIM estimate. The MC²-2 calculation which did include the self-shielding of iron yields a zero-buckling estimate of $\bar{\lambda}^2$ which is $\sim 2.3\%$ low relative to VIM ($1\sigma \pm 0.6\%$); MC²-2 underestimates the change in the k due to leakage by $\sim 0.6\%$ of its value relative to VIM ($1\sigma \pm 0.8\%$). Alternately, MC²-2 overpredicts $k_{\text{eff}}(B^2 = 0.0008)$ by $\sim 0.34\% \delta k$. Although the agreement of MC²-2 with VIM is much better in this case, the underprediction of $\bar{\lambda}^2$ in these homogeneous cell calculations is symptomatic of difficulties in predicting leakage. As will be discussed in the following section, the MC²-2/SDX calculation of the full ZPR-9 Assembly 34 overpredicted the eigenvalue by about this same amount ($\sim 0.47\% \delta k$). Furthermore, a similar bias was observed in the earlier validation study by Wade.¹ In that study, estimates of $\bar{\lambda}^2$ for a homogeneous GCFR composition ($k_{\infty} = 1.43$) obtained from various options of MC²-2/SDX were all low relative to VIM.

In the final two sections of Table II which pertain to the heterogeneous core unit cell, all MC²-2/SDX calculations utilized the self-shielded iron data. For the zero-buckling case, three options in the MC²-2 and SDX cross section collapse codes were compared with the VIM results. Specifically, in the first stage of the cross section collapse, the P1 option of MC²-2 was used in both its consistent and inconsistent (energy loss upon P1 scattering is neglected) forms. In the second stage of this process, SDX collapses σ_{tr} using an inconsistent P1 (ϕ/Σ_{tr}) weighting. The values in Table II indicate these options do not impact the MC²-2/SDX eigenvalue (k_{∞}) calculations, which agree well with the three-dimensional VIM Monte Carlo calculation of the infinite array of core unit cells. The multigroup neutron spectra agree well with the VIM spectrum over the entire energy range, except for the iron window group (21-31 keV) which is $\sim 4\%$ higher. All the principal broad group cross sections agree well over most of the range of interest. There is, however, a consistent bias in the MC²-2/SDX cross sections (which are 0 - 15% larger than VIM) in the MeV range. Two principal sources of this bias are differences in the treatment of the fission source spectrum and (more importantly) differences in the calculated flux peaking in the fuel plate -- a single $1/16$ in. (0.16 cm) enriched ($93\% \text{ }^{235}\text{U}$) uranium plate. With regard to the fission spectrum, VIM handles the fission chi matrix as specified in the ENDF/B files. The secondary energy distributions are a function of the incident neutron energies. The MC²-2/SDX codes handle only a chi vector for each isotope which is based on an average fission temperature (derived for a typical fast reactor spectrum). Adjunct calculations indicate the sensitivity of the eigenvalues to the differences between the MC²-2/SDX and VIM fission spectra are negligible ($<0.01\% \delta k$). However, replacement of the multigroup chi with the VIM chi did improve agreement in the neutron spectra in the top two energy groups (6-14 MeV) and the threshold reaction rates. With regard to the calculated flux peaking in the fuel plate, the peaking factors are large (typically 1.2 - 1.4 in the higher energy groups). The initial SDX calculations specified only one mesh per material region. This

was refined by subdividing the fuel region (with 5 mesh/plate) and the adjacent stainless steel regions (with 4 mesh/plate). This change had a negligible effect on the eigenvalue ($-0.00074 \delta k$). There was a significant (up to 7%) improvement in the agreement of MC^2 -2/SDX versus VIM in the broad group cross sections in the top 6 or 7 groups.

For the non-zero buckling tests of the heterogeneous core cell, the MC^2 -2/SDX values of leakage-related parameters exhibit a bias relative to the VIM values as was observed in the homogeneous tests. Additionally, these values are significantly affected by the collapsing spectrum option of MC^2 -2. With the consistent P1 option of MC^2 -2, the change in eigenvalue due to leakage is under-predicted by $\sim 0.6\% \delta k$ (relative to VIM). With the inconsistent P1 option of MC^2 -2, this change in k_{eff} is underpredicted by $\sim 1.8\% \delta k$. Using the consistent P1 spectrum calculation in MC^2 -2, the SDX zero-buckling estimate of $\bar{\lambda}^2$ is $\sim 3\%$ low (3605.44 cm^2 compared to the VIM estimate of $3713.78 \pm 23.19 \text{ cm}^2$).

One additional observation from the unit cell studies will be made. The unit cell of ZPR-9 Assembly 32 provided the most difficult analytical test for the one-dimensional modeling used with the SDX code. The core unit cell of ZPR-9/32 (which is illustrated in Figure 1) included two metal fuel plates with substantially different heights ($\sim 9\%$) and enrichments (18% vs 26%). The one-dimensional modeling in the MC^2 -2/SDX treatment was found to mispredict the multi-dimensional effect of the ZPR-9/32 core cell (due to differing heights of the fuel plates). This was reflected in errors in the flux peaking factors in the fuel plates and principally impacted the cross sections in the top 6 or 8 broad energy groups (above $\sim 500 \text{ keV}$). A simple correction* was implemented in SDX which produced cell averaged broad group cross sections in excellent agreement with VIM.

V. FULL ASSEMBLY CALCULATIONS

One of the principal goals of the current work was to extend the validation study to full reactor calculations -- to intercompare the results of standard analysis methods based on the ENDF/ MC^2 -2/SDX cell homogenization path with the results of detailed VIM Monte Carlo calculations for the full critical assembly. As outlined in Section II, the standard ZPR analysis methods employ two- and three-dimensional diffusion theory with RZ and XYZ models of the critical assembly. Additional calculations, e.g., with S_n transport theory, anisotropic diffusion theory, or finer spatial mesh, are used to obtain corrections or refinements. In the present study the reference MC^2 -2/SDX calculations for the full assemblies utilized two-dimensional S_4 transport theory in 29 broad energy groups ($E_{top} = 14.19 \text{ MeV}$) with RZ models having $\sim 2.5 \text{ cm}$ mesh. Adjunct calculations, utilizing diffusion theory with isotropic diffusion coefficients and with Benoist and/or Gelbard anisotropic diffusion coefficients, various mesh spacings, alternative broad group energy structures, three dimensional diffusion theory, and S_n transport theory with various higher orders of angular quadrature, were performed for each assembly to refine the reference calculations. Some of the details of various eigenvalue calculations for ZPR-6 Assembly 7 based on MC^2 -2/SDX are displayed in Figure 3.

*The modeling in SDX is one-dimensional. In calculating the flux self-shielding factors or "flux-peaking" factors, SDX takes the volume of each plate (or the entire cell) to be proportional to its thickness. A simple modification to the code allowed the user to input the height of each plate, and the volume of each plate was taken to be proportional to the product of the thickness and height of the plate.

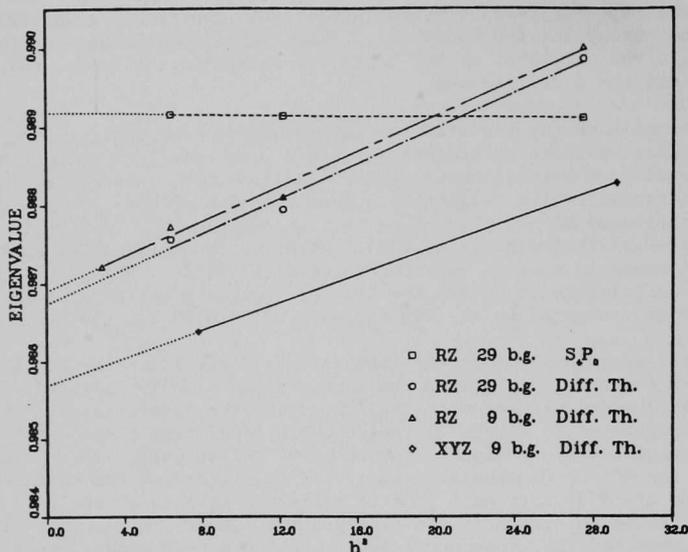


Fig. 3. Extrapolation of ZPR-6/7 Calculated Eigenvalue vs Square of Average Mesh Spacing (k_{eff} vs h^2).

- There is a significant difference in the extrapolations of the eigenvalue to zero mesh spacing between diffusion and transport theory solutions. Consequently, any transport correction (i.e., diffusion theory to transport theory correction) to the eigenvalue must be made consistently with the appropriate mesh correction.
- The eigenvalue differences between the 9 and 29 broad group energy structures were consistent and small ($<0.0002 \delta k$). Further extrapolation of eigenvalue to finer energy group structures was neglected.

The MC²-2/SDX results for ZPR-6 Assembly 7 eigenvalue calculations are summarized in Table III. The mesh correction is almost negligible (because the fine mesh transport theory solution has been used as the reference). For Assembly 7, the largest eigenvalue corrections account for streaming and 2D-to-3D modeling effects.* The streaming correction is obtained as the difference in eigenvalue between diffusion theory solutions with isotropic diffusion coefficients and Benoist anisotropic diffusion coefficients. In the XYZ calculations, the X direction is perpendicular to the plates in the unit cell and the Y and Z directions are parallel to the plates. In XYZ calculations, the Benoist D_{\perp} is used for D_x and the Benoist D_{\parallel} is used for D_y and D_z . In RZ calculations, D_R is set equal to $(D_{\perp} + D_{\parallel})/2$. The close agreement for $\delta k_{\text{streaming}}$ obtained by RZ and XYZ calculations confirms the adequacy of this definition of D_T for these relatively clean, simple configurations. Applying all of the corrections summarized in Table III, the MC²-2/SDX eigenvalue for ZPR-6 Assembly 7 is 0.983679.

*All of these corrections can vary significantly depending on the assembly. For example, in Assembly 34, the $\delta k_{\text{streaming}}$ correction is very small; in Assembly 32, the $\delta k_{S_4 + S_{\infty}}$ is significant.

TABLE III. Summary of MC²-2/SDX k_{eff}
Calculations of ZPR-6 Assembly 7

1. Reference Calculation.
ENDF/B Version IV data; MC²-2/SDX; 29 broad energy groups
RZ Model with ~2.5 cm mesh spacing
Two-Dimensional Transport Theory (S₄P₀)
k₁ = 0.989162
2. Mesh Correction.
Two-Dimensional Transport Theory (S₄P₀) with various mesh spacings

Mesh Spacing, cm	k
5.2396	0.989098
3.4931	0.989142
2.5310	0.989162

These values extrapolate to a value with zero mesh spacing

$$k_2 = 0.989180$$

$$\delta k_{\text{Mesh}} = k_2 - k_1 = 0.000018$$

3. Angular Quadrature Correction.
Two-Dimensional Transport Theory; 29 broad energy groups
RZ Model with ~2.5 cm mesh spacing

Quadrature	k
S ₄	0.989162
S ₈	0.988591
S ₁₆	0.988511

$$\delta k_{S_4+S_\infty} = \delta k_{S_4+S_{16}} = k_{S_{16}} - k_{S_4} = -0.000651$$

4. Streaming Correction.
RZ Model with ~2.5 cm mesh spacing; 29 broad energy groups
Two-Dimensional Diffusion Theory
with Isotropic Diffusion Coefficients

$$k_{\text{RZ,Iso}} = 0.987563$$

with Benoist Anisotropic Diffusion Coefficients

$$k_{\text{RZ,Ben}} = 0.984572$$

$$\delta k_{\text{RZ,Streaming}} = k_{\text{RZ,Ben}} - k_{\text{RZ,Iso}} = -0.002991$$

XYZ Model with ~5.4 cm mesh spacing; 29 broad energy groups
Three-Dimensional Diffusion Theory
with Isotropic Diffusion Coefficients

$$k_{\text{XYZ,Iso}} = 0.988120$$

with Benoist Anisotropic Diffusion Coefficients

$$k_{\text{XYZ,Ben}} = 0.985149$$

$$\delta k_{\text{XYZ,Streaming}} = k_{\text{XYZ,Ben}} - k_{\text{XYZ,Iso}} = -0.002971$$

5. 2D + 3D Correction.
Three-Dimensional Diffusion Theory with ~5.4 cm mesh spacing
29 broad energy groups
k_{XYZ} = 0.988120

Two-Dimensional Diffusion Theory extrapolated to ~5.4 cm
mesh spacing; 29 broad energy groups

$$k_{\text{RZ}} = 0.989999$$

$$\delta k_{2\text{D}+3\text{D}} = k_{\text{XYZ}} - k_{\text{RZ}} = -0.001879$$

Applying all of the above corrections, i.e.,

$$k_1 + \delta k_{\text{Mesh}} + \delta k_{S_4+S_\infty} + \delta k_{\text{XYZ,Streaming}} + \delta k_{2\text{D}+3\text{D}}$$

yields: k = 0.983679

This value is to be compared with the VIM Monte Carlo calculated eigenvalue for Assembly 7 of 0.977517 ± 0.002081 ($k_{\text{eff}} \pm 1\sigma$ based on 100,000 neutron histories). The MC²-2/SDX eigenvalue is $0.006162 \delta k$ (or 3.0 standard deviations) higher than the VIM calculation.

The calculations for the other two assemblies exhibit a similar bias. The MC²-2/SDX eigenvalues, including all the corrections discussed previously for the Assembly 7 calculations, are $0.007239 \delta k$ (or 4.7 standard deviations) and $0.004728 \delta k$ (or 1.8 standard deviations) higher than the VIM calculations for Assemblies 32 and 34, respectively. These results are summarized in Table IV. The source of this eigenvalue bias has been investigated by comparing MC²-2/SDX and VIM group- and region-wise edits of cross sections, reaction rates and fluxes. Similar trends were observed in the comparisons for each of these assemblies. Some of these details will be provided for the comparison of MC²-2/SDX versus VIM calculations of ZPR-6 Assembly 7. These Assembly 7 results and conclusions may be considered to apply to all three assemblies; exceptions from the calculations for ZPR-9 Assemblies 32 and 34 will be noted.

TABLE IV. Summary of MC²-2/SDX vs VIM Eigenvalues

	$k_{\text{eff}} \pm 1\sigma$ (VIM) ^a	k_{eff} (MC ² -2/SDX) ^b	$\frac{k_{\text{eff}} \text{ (MC2-2/SDX)}}{k_{\text{eff}} \text{ (VIM)}}$
ZPR-6 Assembly 7	0.977517 ± 0.002081	0.983679	1.0063 ± 0.0021
ZPR-9 Assembly 32	0.995190 ± 0.001552	1.002429	1.0073 ± 0.0016
ZPR-9 Assembly 34	0.981748 ± 0.002600	0.986476	1.0048 ± 0.0026

^aVIM Monte Carlo calculations for three-dimensional detailed platewise models of the full assemblies. Calculations for ZPR-6/7 and ZPR-9/34 are based on 100,000 neutron histories; calculation for ZPR-9/32 is based on 200,000 neutron histories.

^bThese MC²-2/SDX eigenvalues are based on fine mesh two-dimensional S₄ transport theory calculations and include corrections for δk_{Mesh} , $\delta k_{S_4+S_\infty}$, $\delta k_{\text{Streaming}}$ and δk_{2D+3D} .

Overall neutron balances calculated for Assembly 7 are summarized in Table V. These neutron balances have been normalized such that total production in the assembly equals unity, i.e.,

$$(\text{Fission Production}/k_{\text{eff}}) + \text{Net } (n,2n) \text{ Source} = \text{Absorption} + \text{Leakage} = 1.0$$

for the assembly. The VIM neutron balance was obtained from the track length estimates of the isotopic reaction rates. The track length estimate of the eigenvalue (0.977361 ± 0.002984) is $0.000156 \delta k$ lower than the estimate quoted above (which was based on an average of three VIM estimators). However, the track length k_{eff} is inherently consistent with these reaction rate edits. The neutron balance labelled MC²-2/SDX represents a composite of the results for the RZ model calculated with the 29 broad group MC²-2/SDX generated cross sections.

TABLE V. Neutron Balance Summary for Assembly 7^a

	VIM $\pm 1\sigma^b$	MC ² -2/SDX ^c	$\frac{\text{MC}^2\text{-2/SDX}^b}{\text{VIM}}$
<u>Fission Production</u>			
Core	0.92257 \pm 0.00361	0.93136	1.00953 \pm 0.00391
Axial Blanket	0.01591 \pm 0.00036	0.01634	1.02729 \pm 0.02240
Radial Blanket	0.03605 \pm 0.00063	0.03587	0.99503 \pm 0.01760
Matrix	---	---	---
Total	0.97452 \pm 0.00328	0.98357	1.00929 \pm 0.00337
<u>Net (n,2n) Source</u>			
Core	0.00217 \pm 0.00008	0.00203	0.93479 \pm 0.03620
Axial Blanket	0.00018 \pm 0.00003	0.00025	1.37855 \pm 0.18600
Radial Blanket	0.00055 \pm 0.00006	0.00055	1.00100 \pm 0.11000
Matrix	---	---	---
Total	0.00290 \pm 0.00010	0.00284	0.97847 \pm 0.03550
<u>Capture</u>			
Core	0.39843 \pm 0.00220	0.40199	1.00894 \pm 0.00553
Axial Blanket	0.07549 \pm 0.00118	0.07488	0.99187 \pm 0.01560
Radial Blanket	0.17241 \pm 0.00200	0.16862	0.97802 \pm 0.01160
Matrix	0.00006 \pm 0.00000	0.00006	0.99646 \pm 0.04540
Total	0.64640 \pm 0.00260	0.64555	0.99869 \pm 0.00403
<u>Fission</u>			
Core	0.31643 \pm 0.00124	0.31954	1.00983 \pm 0.00392
Axial Blanket	0.00592 \pm 0.00013	0.00604	1.02074 \pm 0.02170
Radial Blanket	0.01336 \pm 0.00022	0.01327	0.99356 \pm 0.01670
Matrix	---	---	---
Total	0.33571 \pm 0.00112	0.33885	1.00935 \pm 0.00335
Eigenvalue	0.97736 \pm 0.00298	0.98637	1.00922 \pm 0.00305
<u>Leakage</u>			
from Core	0.23125 \pm 0.00532	0.22473	0.97181 \pm 0.02301
from Reactor	0.01789 \pm 0.00284	0.01560	0.87180 \pm 0.15860

^aThis neutron balance is normalized such that total production in the assembly is unity, i.e., (Fission Production/ k_{eff}) + Net (n,2n) Source = Absorption + Leakage = 1.0 for the entire assembly.

^bThe VIM neutron balance was obtained from the track length estimates of the isotopic reaction rates based on 100,000 neutron histories. All uncertainties represent 1- σ intervals and include only the VIM Monte Carlo uncertainties.

^cThe MC²-2/SDX neutron balance was obtained by adjusting the S₄P₀ transport theory values by the ratio of values obtained with anisotropic and isotropic diffusion theory.

To account for both streaming and transport effects, the MC^2-2/SDX values in these tables were obtained by multiplying the S_4P_0 transport theory values by the ratio of the values obtained with anisotropic and isotropic diffusion theory, or

$$[MC^2-2/SDX] \equiv S_4P_0 * \frac{\text{Anisotropic}}{\text{Isotropic}} .$$

The MC^2-2/SDX calculations (relative to VIM) produce more absorptions in the core -- more capture and more fission (and therefore more net production and larger eigenvalue). Alternately, the increased absorptions in the core result in less leakage from the core (MC^2-2/SDX 22.5% vs VIM 23.1%).

The MC^2-2/SDX and VIM broad group capture and fission cross sections for ^{239}Pu and ^{238}U (which account for ~84% of the absorptions in the core of Assembly 7) are in good agreement. A comparison of the broad group ^{238}U capture cross section is provided in Table VI. Above group 18 (3.35 keV) agreement is generally within the VIM estimated 1σ values. The MC^2-2/SDX values are generally lower in the resolved range.* The MC^2-2/SDX calculated value of c^{28}/f^{49}

TABLE VI. Comparison of VIM Monte Carlo and MC^2-2/SDX Values of σ_c^{28}

Group	VIM Monte Carlo	MC^2-2/SDX	$\frac{MC^2-2/SDX}{VIM}$
1	0.0017616 ± 0.0000583	0.0017641	1.0014 ± 0.0331
2	0.0044323 ± 0.0000429	0.0044394	1.0016 ± 0.0097
3	0.011556 ± 0.0000566	0.011510	0.9960 ± 0.0049
4	0.030535 ± 0.000103	0.030645	1.0036 ± 0.0034
5	0.068772 ± 0.000173	0.068680	0.9987 ± 0.0025
6	0.11570 ± 0.00019	0.11608	1.0033 ± 0.0017
7	0.11577 ± 0.00014	0.11578	1.0001 ± 0.0012
8	0.11022 ± 0.00014	0.11008	0.9987 ± 0.0013
9	0.12954 ± 0.00017	0.12979	1.0019 ± 0.0014
10	0.16188 ± 0.00018	0.16194	1.0004 ± 0.0011
11	0.20927 ± 0.00027	0.20894	0.9984 ± 0.0013
12	0.32658 ± 0.00043	0.32689	1.0009 ± 0.0013
13	0.41144 ± 0.00078	0.41041	0.9975 ± 0.0019
14	0.49685 ± 0.00091	0.49600	0.9983 ± 0.0018
15	0.59424 ± 0.00164	0.59496	1.0012 ± 0.0028
16	0.70024 ± 0.00256	0.69420	0.9914 ± 0.0037
17	0.79923 ± 0.00560	0.79432	0.9939 ± 0.0070
18	0.94978 ± 0.01140	0.90018	0.9478 ± 0.0120
19	0.88196 ± 0.01032	0.86654	0.9825 ± 0.0117
20	1.1041 ± 0.01358	1.0726	0.9715 ± 0.0123
21	1.1519 ± 0.02592	1.1090	0.9628 ± 0.0225
22	1.0320 ± 0.04324	0.96954	0.9395 ± 0.0419
23	1.6302 ± 0.06260	1.4358	0.8808 ± 0.0384
24	1.6600 ± 0.15919	1.7016	1.0251 ± 0.0959
25	5.0663 ± 1.68201	4.7218	0.9320 ± 0.3320
26	27.963 ± 0.00011	2.4757	0.0885 ± 4.0×10 ⁻⁶
27	---	0.25955	---
28	---	0.058418	---
29	---	0.54549	---

Note: All uncertainties represent 1- σ intervals and include only the VIM Monte Carlo uncertainties.

* The results are expected to be in better agreement with Monte Carlo in the resolved range if calculated with RABANL,⁷ the hyper-fine-group integral transport theory module of MC^2-2 . This was demonstrated in calculations for the ZPR-9 Assembly 32 core unit cell.

(the ratio of capture rate per atom in ^{238}U to the fission rate per atom in ^{239}Pu) agrees well with the VIM value. Core-averaged values in Assembly 7 were:

	<u>VIM $\pm 1\sigma$</u>	<u>MC²-2/SDX</u>	<u>$\frac{\text{MC}^2\text{-2/SDX}}{\text{VIM}}$</u>
c^{28}/f^{49}	0.1549 ± 0.0010	0.1542	0.9954 ± 0.0065

The core-averaged real flux spectra from the MC²-2/SDX anisotropic diffusion theory and S_4P_0 transport theory calculations are displayed in Fig. 4 for comparison with the VIM calculated spectrum ($\pm 1\sigma$ error bands). The differences between the Benoist diffusion theory and S_4P_0 transport theory spectra are very small with the S_n spectra slightly harder. There is general agreement between these spectra and the VIM spectrum (i.e., within $\pm 1\sigma$ error bands); however, the VIM spectrum is somewhat harder.

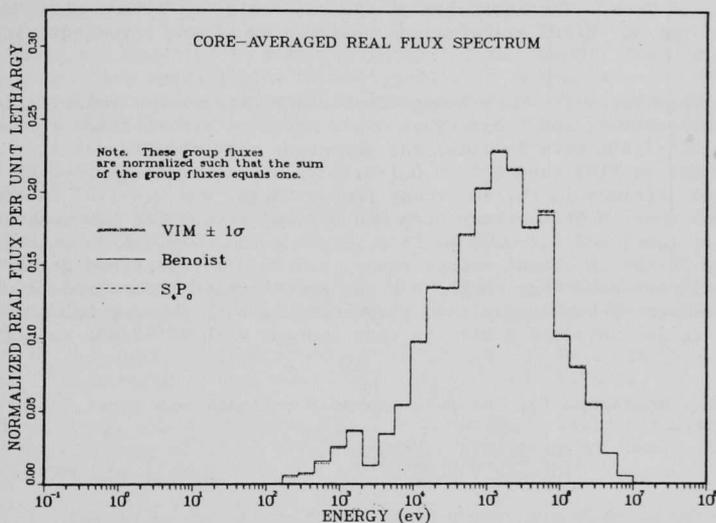


Fig. 4. Core-Averaged Flux Spectrum for ZPR-6 Assembly 7.

The larger core absorption fractions in the MC²-2/SDX calculations relative to VIM do not result from the differences in the capture and fission cross sections (which are in fact slightly smaller in the MC²-2/SDX case) or from the differences in the energy spectra of the core neutron flux. The increase in the MC²-2/SDX absorption rate in the core is the result of larger total flux in the core. That is, there are significant differences between the MC²-2/SDX and VIM calculations of the spatial distribution of the neutron flux. The treatment of the neutron transport in the MC²-2/SDX calculations (both S_n and diffusion theory) produces a higher flux in the core relative to the external regions than produced by the VIM Monte Carlo calculations. Therefore, the major

source of the eigenvalue bias observed for each of these three ZPR assemblies appears to be global effects of neutron transport through the assemblies. This conclusion is consistent with the results discussed in the preceding section. That is, the unit cell studies, both homogeneous and heterogeneous, indicated a similar bias on leakage, namely, less leakage with MC²-2/SDX relative to VIM or equivalently a shorter mean flight to fission, $\bar{\lambda}^2$, in MC²-2/SDX than in VIM.

VI. SUMMARY

The present benchmark calculations of three ZPR assemblies with significantly different characteristics have provided an excellent opportunity to study the ENDF/MC²-2/SDX cell homogenization codes. With the inclusion of appropriate modifications discussed above, the agreement between the deterministic methods and Monte Carlo was very good (i.e., generally within 1σ uncertainties).

Initial results revealed a large eigenvalue bias (~2.1% δk) for ZPR-9 Assembly 34 in the multigroup methods relative to Monte Carlo. This error was the result of an unexpected high energy self-shielding effect in the elastic scattering cross sections of iron. The inclusion of the self-shielded iron elastic scattering data in the MC²-2/SDX calculations produced excellent agreement with the VIM results.

In the non-leakage tests for both homogeneous and heterogeneous cells, eigenvalue, neutron spectrum, and broad group cross sections and reaction rates obtained with MC²-2/SDX were in excellent agreement with the VIM results. The biases (MC²-2/SDX vs VIM) ranged from 0.1-0.2% δk in eigenvalue, 0.1-0.2% in principal cross sections in the important energy range, and 0.5-1.0% in broad group cross sections in unimportant (top and bottom) groups for homogeneous zero-buckled systems; and 0.1-0.2% δk in eigenvalue and 0.2-0.5% in principal cross sections in the important energy range, and 1-4% in the broad group cross sections in unimportant energy ranges for the zero-buckled heterogeneous cell. However, comparison of leakage-related parameters in both homogeneous and heterogeneous cells indicated a bias -- less leakage with MC²-2/SDX relative to VIM.

The eigenvalue comparisons for the full assembly calculations were:

	$\frac{k(\text{MC}^2\text{-2/SDX}) - k(\text{VIM})}{\pm \text{uncertainty}}$
ZPR-6/7	+0.0062 ± 0.0021
ZPR-9/32	+0.0072 ± 0.0016
ZPR-9/34	+0.0047 ± 0.0026

These calculations show a consistent bias -- the MC²-2/SDX eigenvalues being 0.5-0.7% δk high relative to VIM. The apparent source of the bias is also consistent. For each assembly, the MC²-2/SDX calculations (relative to VIM) produce more absorptions in the core and less leakage from the core.

These δk biases are much larger (by an order of magnitude) than the uncertainties in the integral experiments. However, they are comparable to the combined uncertainties in the analysis methods. A full discussion of methods uncertainties is beyond the scope or intent of the present summary. However, a point of reference on these uncertainties would be useful in assessing the impact of

these δk biases. The methods uncertainty in calculated eigenvalue depends on the nature of the system (i.e., critical assembly). For a well-studied system, that is, one which requires little or no extrapolation from a system for which the analytical methods have been validated and for which methods biases have been determined and/or eliminated, the uncertainties will be comparable to the uncertainties in the validation method. In the present study, this would be the precision of the Monte Carlo methods ($\sim 0.2\% \delta k$). For systems with unique characteristics which require extrapolation of the methods beyond the range of their validation, the estimated uncertainties must be increased. The initial MC²-2/SDX calculations for ZPR-9/34 (the U/Fe benchmark assembly), which produced a bias of over 2% δk , illustrate that point.

For the present case, the consistency of the results indicate the potential of an eigenvalue bias of $\sim 0.5\% \delta k$ between these methods. Further studies are planned to investigate these apparent differences in neutron transport or leakage between the MC²-2/SDX codes and Monte Carlo.

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