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# Automatic Coarse Energy Group Structure Optimization by Minimizing Reaction Rate Differences for the SCALE and CASL Code Systems

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**Abstract** - *A new algorithm has been developed to automatically optimize the coarse energy group structure for the SCALE multigroup procedures based on either a pointwise slowing down calculation or intermediate resonance approximation for resonance self-shielding. A coarse group structure will be determined to minimize reactivity differences between the fine and coarse group calculations for several variations of states. A new 56-group structure has been developed for the pressurized water reactor and boiling water reactor fuels by using the algorithm with the SCALE 252-group structure, which could be used in the regular SCALE and intermediate resonance approaches. The computational results for benchmark problems show that the new 56-group structure developed by using coarse group optimization is reasonable.*

## I. INTRODUCTION

The SCALE 6.2 code system [1] includes two types of multigroup (MG) cross section processing procedures. The conventional procedure computes problem-dependent cross sections through a combination of the conventional Bondarenko shielding-factor method and a deterministic pointwise (PW) slowing down calculation of the fine-structure spectra in the resolved resonance and thermal energy ranges. CENTRM is used to calculate problem-specific fluxes on a fine energy mesh (30,000–70,000 points), which can be used to generate self-shielded MG cross sections for subsequent criticality or shielding analysis. A new approach is based on the embedded self-shielding method (ESSM) [2] developed at Oak Ridge National Laboratory (ORNL), as well as the subgroup method. Both methods are branches of the Bondarenko method. The processed 252-group cross sections through these procedures will be used in the following MG transport calculations by using XSDRN, NEWT, KENO or Polaris in SCALE.

A new 252-group structure has been developed for the SCALE 6.2 AMPX MG library to resolve the large reactivity bias issue in the SCALE 6.1 AMPX 238-group library. The reactivity bias can be significantly improved by developing a better group structure, method of characteristics (MOC)-based slowing down capability, new PW weighting functions, and other changes. The new 252-group library has been very successful for resolving small problems, including those involving single pins, single and multiple fuel assemblies, and reflectors, and will work well for large problems, including addressing a whole reactor core. However, both the standard SCALE and Bondarenko procedures with the AMPX 252-group library are extremely expensive to use when simulating a large problem in computing time. These procedures require significant memory overhead for cross sections. A neutronic reactor core simulator in the Virtual Environment for Reactor Applications (VERA) [3] is under development by the Consortium for Advanced Simulation of Light Water Reactors (CASL) project [4]. This simulator will use the two different SCALE procedures with the 252-group AMPX library to generate macroscopic cross sections. However, the computing capacity is still not practical. Therefore, a coarse group library must be developed to achieve better computational efficiency while minimizing an accuracy loss.

A coarse group library with a Bondarenko approach is commonly considered the best approach to a whole core neutronic simulation with temperature feedback for resonance self-shielding calculation. Therefore, a new cross section library is being developed with a coarse group structure using about 50 groups for the conventional procedure and the Bondarenko approach, such as the ESSM and subgroup methods with temperature feedback. The objectives of this study are (1) to develop an automatic procedure and program to optimize a coarse group structure so that computational accuracy of fine group calculations would be maintained as much as possible, and (2) to develop a new coarse group structure from the 252-group structure.

## II. OPTIMIZATION ALGORITHM

The Coarse Group Optimization (CGOP) program was developed to optimize coarse energy group structure by using fine group reference calculations. The fundamental concept for this program is to optimize coarse group structure so that coarse group boundaries are determined to minimize reaction rate differences between the reference fine and coarse group calculations for various variations of stated parameters. Currently the SCALE code package

includes the 252-group AMPX master library, which can be a starting point for a reference solution in optimizing coarse energy group structure. Figure 1 provides an overall algorithm of CGOP. This program includes three major functions, which are (1) to read the AMPX working libraries and the XSDRN input files, (2) to perform eigenvalue calculations, and (3) to perform reaction rate and reactivity analyses. The transport eigenvalue solver is using the method of characteristics (MOC) with the coarse mesh finite difference (CMFD) acceleration scheme. Currently the scattering source term is approximated by $P_1$ transport correction and will be extended to consider high**er** order scattering moments.

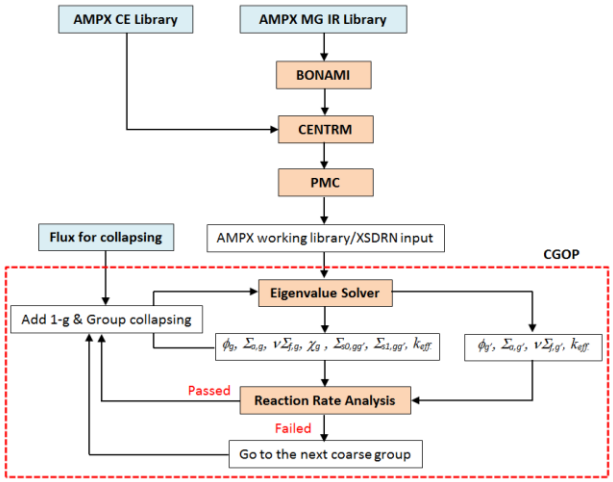


Fig. 1. Flow chart of the CGOP algorithm.

Since neutron spectra are highly dependent upon reactor types, coarse energy group structure optimization should be performed for each type of reactor. The overall optimization procedure is as follows:

a. A representative single pin cell (or basic unit model) is selected for the specified reactor type (e.g., pressurized water reactor [PWR], boiling water reactor [BWR], or high-temperature gas-cooled reactor [HTGR]).
b. Possible variations for composition, geometry, and state are considered for single pins as in the following example:
   - Temperatures: cold, hot zero, and hot full powers
   - $^{235}$U enrichments: 1.0 ~ 5.0 wt%
   - Burnups: 0.0 ~ 50.0 MWD/kgU
   - Soluble boron concentration: 0.0 ~ 1000.0 PPM
   - Geometry configurations: 17 × 17 WH type
   - Void fractions: 0.0 ~ 90.0 %
   - Gadolinia rods: $UO_2$+$Gd_2O_3$
c. The SCALE-CENTRM calculations with the AMPX 252-group library are performed for all variations. The AMPX MG working libraries for each variation are saved to be used in CGOP as input data.
d. CGOP reads the user input file, the AMPX working libraries, and the composition and geometry data. Then fine-group macroscopic cross sections ($\Sigma_{t,g,i}$, $\Sigma_{a,g,i}$, $\nu\Sigma_{f,g,i}$, $\nu\Sigma_{t,g,i,j}$, $\chi_{g,i,j}$) and scattering matrices ($\Sigma_{s0,g,g',i}$, $\Sigma_{s1,g,g',i}$) are obtained and saved in memory. The subscripts *t*, *a*, *f* and *s* denote total, absorption, fission and scattering cross sections, respectively. The subscript $\nu$ is the number of neutrons released per fission. The subscript *g* is the energy group, and *i* and *j* denote the zone number and nuclide, respectively.
e. CGOP performs reference eigenvalue transport calculations by using the AMPX working libraries for each variation. Neutron fluxes ($\phi_{g,i}$), absorption ($R_{a,g,i}$) and $\nu$*fission ($R_{\nu f,g,i}$) reaction rates for each group and total absorption ($R_{a,i}$), and $\nu$*fission reaction rates ($R_{\nu f,i}$) for each zone are saved to be reference solutions:

$$R^{ref}_{a,g,i} = \Sigma^{ref}_{a,g,i}\phi^{ref}_{g,i}\,, \tag{1}$$

$$R^{ref}_{\nu f,g,i} = \nu\Sigma^{ref}_{f,g,i}\phi^{ref}_{g,i}\,, \tag{2}$$

$$R^{ref}_{a,i} = \sum_{g=1}^{G}\Sigma^{ref}_{a,g,i}\phi^{ref}_{g,i}\,, \text{ and} \tag{3}$$

$$R^{ref}_{\nu f,i} = \sum_{g=1}^{G}\nu\Sigma^{ref}_{f,g,i}\phi^{ref}_{g,i}\,, \tag{4}$$

f. Energy group collapsing begins such that group-2 (*g+1*) is collapsed into group-1 (*g*) and the number of groups will be G-1, in which new collapsed macroscopic cross sections and scattering matrices are obtained by using user specified weighting functions. Three options are available in CGOP, including reference CENTRM and user-provided scalar fluxes:

$$\Sigma^{col}_{a,G_k,i} = \frac{\sum_{g'\in G_k}\Sigma^{ref}_{a,g',i}\phi^{inp}_{g',i}}{\sum_{g'\in G_k}\phi^{inp}_{g',i}}, \quad \{g, g+1\}\in G_k\,, \tag{5}$$

$$\nu\Sigma^{col}_{f,G_k,i,(j)} = \frac{\sum_{g'\in G_k}\nu\Sigma^{ref}_{f,g',i,(j)}\phi^{inp}_{g',i}}{\sum_{g'\in G_k}\phi^{inp}_{g',i}}, \tag{6}$$

$$\chi^{col}_{G_k,i,j} = \sum_{g'\in G_k}\chi^{ref}_{g',i,j}\,, \text{ and} \tag{7}$$

$$\Sigma^{col}_{s,G_k\to G'_k,i} = \frac{\sum_{g''\in G'_k}\sum_{g'\in G_k}\Sigma^{ref}_{s,g'\to g'',i}\phi^{inp}_{g',i}}{\sum_{g'\in G_k}\phi^{inp}_{g',i}}\,. \tag{8}$$

g. The eigenvalue calculations are performed by using the collapsed cross sections for all variations. Eigenvalues and neutron fluxes are saved for the reaction rate analysis.
h. Reaction rate analyses are performed for all variations. Absorption and nu-fission reaction rates for the reference and the collapsed with new coarse energy group structure are obtained by using the following equations:

$$R^{ref}_{a,G_k,i} = \sum_{g'\in G_k}\Sigma^{ref}_{a,g',i}\phi^{ref}_{g',i}\,, \tag{9}$$

$$R^{ref}_{\nu f,G_k,i} = \sum_{g'\in G_k}\nu\Sigma^{ref}_{f,g',i}\phi^{ref}_{g',i} \tag{10}$$

$$R^{col}_{a,G_k,i} = \Sigma^{col}_{a,G_k,i}\phi^{col}_{G_k,i}\,, \text{ and} \tag{11}$$

$$R^{col}_{\nu f,G_k,i} = \nu\Sigma^{col}_{f,G_k,i}\phi^{col}_{G_k,i}\,. \tag{12}$$

Reaction rate differences are obtained by using Eqs. (13) and (14):

$$\Delta R_{a,G_k,i} = R^{ref}_{a,G_k,i} - R^{col}_{a,G_k,i}, \text{ and} \quad (13)$$

$$\Delta R_{\nu f,G_k,i} = R^{ref}_{\nu f,G_k,i} - R^{col}_{\nu f,G_k,i}. \quad (14)$$

The reaction rate differences can be converted into reactivity differences, as follows:

$$\Delta\rho_{a,G_k,i} = \left[\frac{1}{k_\infty} - \frac{R^{ref}_{a,i} - \Delta R_{a,G_k,i}}{R^{ref}_{\nu f,i}}\right]\cdot 10^5, \quad (15)$$

$$\Delta\rho_{\nu f,G_k,i} = \left[\frac{1}{k_\infty} - \frac{R^{ref}_{a,i}}{R^{ref}_{\nu f,i} - \Delta R_{\nu f,G_k,i}}\right]\cdot 10^5, \quad (16)$$

$$\Delta\rho_{G_k,i} = \Delta\rho_{a,G_k,i} + \Delta\rho_{\nu f,G_k,i}, \quad (17)$$

$$\Delta\rho_0 = \sum_{k=1}^{K}(\Delta\rho_{a,G_k} + \Delta\rho_{\nu f,G_k}), \text{ and} \quad (18)$$

$$k_\infty = \frac{R^{ref}_{\nu f,i}}{R^{ref}_{a,i}}. \quad (19)$$

i. Total reactivity differences are obtained independently by comparing eigenvalues between the reference and the collapsed one.

$$\Delta\rho_1 = \left[\frac{1}{k^{ref}_{eff}} - \frac{1}{k^{col}_{eff}}\right]\cdot 10^5. \quad (20)$$

In addition, reactivity change by adding one group also can be obtained by using eigenvalues from the previous and new coarse energy group structures, which will correspond to $\Delta\rho_{G_k,i}$.

$$\Delta\hat{\rho}_{G_k,i} = \left[\frac{1}{k^{col(pre)}_{eff}} - \frac{1}{k^{col(new)}_{eff}}\right]\cdot 10^5. \quad (21)$$

j. If the reactivity change in Eq. (21) is less than the user entered criterion, the current group can be involved in the coarse group to form a new coarse group boundary. If it is larger, then the current group will be a new starting coarse group. The calculation would then move to the next group (step f) until it reaches the final energy group.

## III. CALCULATION AND RESULTS

### 1. Coarse Group Structure Optimization

A typical Westinghouse type fuel pin has been selected for the geometrical and compositional configurations. This includes five variations for moderator and fuel temperatures, as shown in Table I. Table II describes other variations, including three for $^{235}U$ enrichment, three for burnup, two for soluble boron concentration, one for $Gd_2O_3$ enrichment, and three for void fraction. The total number of variations is 160. The CGOP program has optimized a new 56-group structure for PWR and BWR to keep consistency in the reactivity contributions of each coarse group to the total reactivity between the 252- and 56-group calculations. Figures 2–4 provide comparisons of group structures and neutron spectra between 252- and 56-groups for typical fresh PWR fuel pins with various void fractions. Table III shows the number of energy groups at each group category in the 252- and 56-group structures.

Figure 3 shows the reactivity differences between the 252- and 56-group calculations obtained from CGOP, where red squares represent the ESSM reactivity differences. After selecting the 56-group structure, another CGOP calculation was performed to determine whether the new coarse group structure is effective to the conventional SCALE procedure. The green rhombus in Figure 5 denotes the reactivity differences for the conventional SCALE procedure. The new 56-group structure was determined for both the conventional and Bondarenko SCALE procedures.

Table I. Temperature Variations

| Case | Moderator (K) | Cladding (K) | Fuel (K) |
|---|---|---|---|
| 1 | 300 | 300 | 300 |
| 2 | 600 | 600 | 600 |
| 3 | 600 | 600 | 900 |
| 4 | 600 | 600 | 1,200 |
| 5 | 600 | 600 | 2,000 |

Table II. Composition and State Variations

| Case | $^{235}U$ w/o | $Gd_2O_3$ w/o | PPM | Void Fraction (%) | Burnup (MWD/kgU) |
|---|---|---|---|---|---|
| 1 | 1.5 | | 0 | 0 | 0 |
| 2 | 1.5 | | 1,000 | 0 | 0 |
| 3 | 1.5 | | 0 | 50 | 0 |
| 4 | 1.5 | | 1,000 | 50 | 0 |
| 5 | 3.0 | | 0 | 0 | 0 |
| 6 | 3.0 | | 1,000 | 0 | 0 |
| 7 | 3.0 | | 0 | 50 | 0 |
| 8 | 3.0 | | 1,000 | 50 | 0 |
| 9 | 3.0 | | 0 | 90 | 0 |
| 10 | 3.0 | | 1,000 | 90 | 0 |
| 11 | 5.0 | | 0 | 0 | 0 |
| 12 | 5.0 | | 1,000 | 0 | 0 |
| 13 | 5.0 | | 0 | 50 | 0 |
| 14 | 5.0 | | 1,000 | 50 | 0 |
| 15 | 5.0 | | 0 | 90 | 0 |
| 16 | 5.0 | | 1,000 | 90 | 0 |
| 17 | 5.0 | | 0 | 0 | 25 |
| 18 | 5.0 | | 1,000 | 0 | 25 |
| 19 | 5.0 | | 0 | 50 | 25 |
| 20 | 5.0 | | 1,000 | 50 | 25 |
| 21 | 5.0 | | 0 | 90 | 25 |
| 22 | 5.0 | | 1,000 | 90 | 25 |
| 23 | 5.0 | | 0 | 0 | 50 |
| 24 | 5.0 | | 1,000 | 0 | 50 |
| 25 | 5.0 | | 0 | 50 | 50 |
| 26 | 5.0 | | 1,000 | 50 | 50 |
| 27 | 5.0 | | 0 | 90 | 50 |
| 28 | 5.0 | | 1,000 | 90 | 50 |
| 29 | 2.6 | 6.0 | 0 | 0 | 0 |
| 30 | 2.6 | 6.0 | 1000 | 0 | 0 |
| 31 | 2.6 | 6.0 | 0 | 0 | 17.5 |
| 32 | 2.6 | 6.0 | 1000 | 0 | 17.5 |

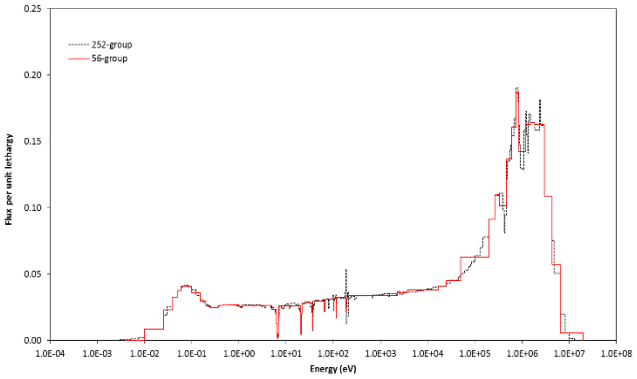


Fig. 2. Comparison of neutron spectra (5.0 w/o, 300 K, 1,000 ppm, 0% void).

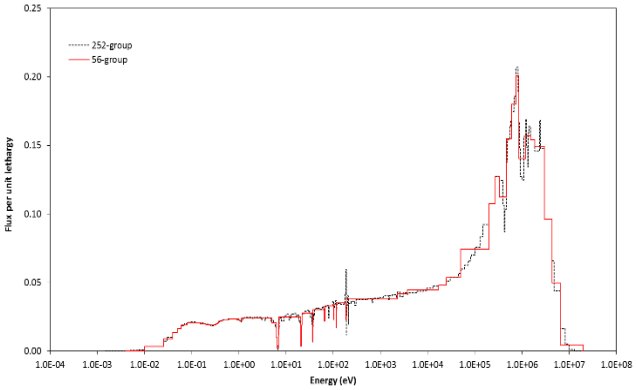


Fig. 3. Comparison of neutron spectra (5.0 w/o, 300 K, 1,000 ppm, 50% void).

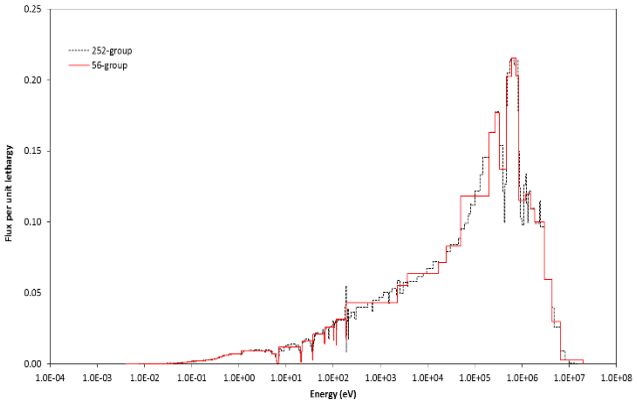


Fig. 4. Comparison of neutron spectra (5.0 w/o, 300 K, 1,000 ppm, 90% void).

Table III. Comparison of the Number of Energy Groups

| Group Category | Energy Boundary | # of Energy Groups | |
|---|---|---|---|
| | | 252-g | 56-g |
| Unresolved/fast | 17 KeV – 20 MeV | 55 | 16 |
| Resolved | 0.625 eV – 17 KeV | 158 | 24 |
| Thermal | 0.0 eV – 0.625 eV | 39 | 16 |
| Upscattering | 0.0 eV – 5.0 eV | 97 | 20 |

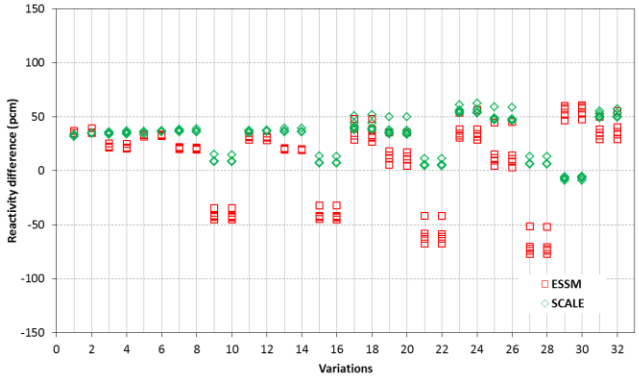


Fig. 5. CGOP reactivity differences (252-g vs. 56-g).

## 2. Benchmark Calculations

As shown in Table IV, the VERA progression benchmark problems [5] were selected to see if the new AMPX 56-group library works reasonably when using the conventional SCALE and Bondarenko approaches.

Table IV. VERA Progression Benchmark Problems

| Case | Description | $^{235}U$ | Mod/Fuel | g/cm$^3$ |
|---|---|---|---|---|
| 1A | pin | 3.1 | 565/565 | 0.743 |
| 1B | pin | 3.1 | 600/600 | 0.661 |
| 1C | pin | 3.1 | 600/900 | 0.661 |
| 1D | pin | 3.1 | 600/1200 | 0.661 |
| 1E | pin + IFBA | 3.1 | 600/600 | 0.743 |
| 2A | FA, no BP | 3.1 | 565/565 | 0.743 |
| 2B | FA, no BP | 3.1 | 600/600 | 0.661 |
| 2C | FA, no BP | 3.1 | 600/900 | 0.661 |
| 2D | FA, no BP | 3.1 | 600/1200 | 0.661 |
| 2E | FA + 12 Pyrex | 3.1 | 600/600 | 0.743 |
| 2F | FA + 24 Pyrex | 3.1 | 600/600 | 0.743 |
| 2G | FA + 24 AIC CR | 3.1 | 600/600 | 0.743 |
| 2H | FA + 24 B4C CR | 3.1 | 600/600 | 0.743 |
| 2I | FA + instrument thimble | 3.1 | 600/600 | 0.743 |
| 2J | FA + instrument thimble + 24 Pyrex | 3.1 | 600/600 | 0.743 |
| 2K | FA + zoned enrichment + 24 Pyrex | 3.1/3.6 | 600/600 | 0.743 |

Table V compares the multiplication factors between the conventional SCALE results with the ENDF/B-VII.1 252- and 56-group libraries. The $k_{eff}$ differences in SCALE are very consistent with the predicted $k_{eff}$ differences by CGOP shown in Figure 5. The SCALE 56-group calculations overestimate the multiplication factors for most cases. The cases 2g and 2h are single fuel assemblies with AIC and $B_4C$ control rod insertions, which are not included in the variations for CGOP. The reactivity differences between 252- and 56-group results come from a buffer fuel model for control rod cell in CENTRM. A more representative control rod model would improve the result significantly.

Table VI provides the computational results for the VERA benchmark problems by using the SCALE-Polaris transport lattice code with ESSM. Even though the trend is opposite of the conventional SCALE results, there is very good agreement between the 252- and 56-group results.

Since ESSM is solving fixed source transport equations for the whole domain, there is not a significant reactivity difference for the control rod insertion cases.

Table V. Comparison of $k_{eff}$ (MG-KENO 252-g vs. 56-g)

| No. | Description | CE-KENO | KENO MG-CE Δk(pcm) | | |
|---|---|---|---|---|---|
| | | | 252g[a] | 56g[b] | [a–b] |
| 1A | 565 K @ 0.743 g/cc | 1.18740 | 74 | 107 | -33 |
| 1B | 600 K @ 0.661 g/cc | 1.18240 | 61 | 89 | -28 |
| 1C | 900 K @ 0.661 g/cc | 1.17173 | 74 | 135 | -61 |
| 1D | 1,200 K @ 0.661 g/cc | 1.16273 | 102 | 157 | -55 |
| 1E | IFBA | 0.77198 | 53 | 119 | -66 |
| 2A | 565 K @ 0.743 g/cc | 1.18297 | -12 | 38 | -50 |
| 2B | 600 K @ 0.661 g/cc | 1.18419 | 0 | 36 | -36 |
| 2C | 900 K @ 0.661 g/cc | 1.17463 | 55 | 8 | 47 |
| 2D | 1,200 K @ 0.661 g/cc | 1.16646 | 33 | 65 | -31 |
| 2E | 12 Pyrex poison rods | 1.07039 | 1 | 63 | -62 |
| 2F | 24 Pyrex poison rods | 0.97684 | -1 | 68 | -69 |
| 2G | 24 AIC control rods | 0.84917 | 86 | 306 | -220 |
| 2H | 24 B4C control rods | 0.78942 | -2 | 243 | -244 |
| 2I | Instrument thimble (IT) | 1.18004 | -143 | -103 | -40 |
| 2J | IT + 24 Pyrex | 0.97531 | 63 | 146 | -82 |
| 2K | Zoned $^{235}$U w/o+24 Pyrex | 1.02022 | 59 | 155 | -96 |

Table VI. Comparison of $k_{eff}$ (Polaris 252-g vs. 56-g)

| No. | Description | CE-KENO | Polaris-KENO, Δk(pcm) | | |
|---|---|---|---|---|---|
| | | | 252g[a] | 56g[b] | [a–b] |
| 1A | 565 K @ 0.743 g/cc | 1.18740 | -36 | -74 | 38 |
| 1B | 600 K @ 0.661 g/cc | 1.18240 | -36 | -76 | 41 |
| 1C | 900 K @ 0.661 g/cc | 1.17173 | -20 | -60 | 40 |
| 1D | 1,200 K @ 0.661 g/cc | 1.16273 | -18 | -58 | 40 |
| 2A | 565 K @ 0.743 g/cc | 1.18297 | 16 | -36 | 52 |
| 2B | 600 K @ 0.661 g/cc | 1.18419 | 13 | -43 | 57 |
| 2C | 900 K @ 0.661 g/cc | 1.17463 | 21 | -51 | 72 |
| 2D | 1,200 K @ 0.661 g/cc | 1.16646 | 26 | -56 | 82 |
| 2E | 12 Pyrex poison rods | 1.07039 | 14 | -11 | 25 |
| 2F | 24 Pyrex poison rods | 0.97684 | 11 | 6 | 5 |
| 2G | 24 AIC control rods | 0.84917 | 33 | -38 | 71 |
| 2H | 24 B4C control rods | 0.78942 | -14 | -60 | 47 |

## IV. CONCLUSIONS

A new program, CGOP, was successfully developed to automatically optimize coarse energy group structure from fine energy group structure for the conventional SCALE MG procedures. CGOP is based on a pointwise slowing down calculation and a Bondarenko approach for resonance self-shielding calculation. A coarse group structure will be determined to minimize reactivity differences between the fine and coarse group calculations for variations of stated parameters. A new 56-group structure was developed for PWR and BWR fuels using CGOP with the SCALE 252-group structure. Benchmark results show that the multiplication factors and pin power distributions between the 252- and 56-group calculations are very consistent with each other, and the newly developed 56-group structure has been determined to be reasonable.

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