A COMPARISON OF VIM AND MC²-2 -- TWO DETAILED SOLUTIONS
OF THE NEUTRON SLOWING-DOWN PROBLEM

by

R. E. Prael and H. Henryson, II

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A COMPARISON OF VIM AND MC\(^2\)-2 — TWO DETAILED SOLUTIONS* OF THE NEUTRON SLOWING-DOWN PROBLEM

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*Work supported by the U. S. Energy Research and Development Administration.
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A comparison of solutions by the Monte Carlo code VIM and by ETŒE-2/MC²-2 of a zero-dimensional slowing-down problem in the homogeneous ZPR-6 Assembly 7 core composition demonstrates the ability of either code to provide a reliable computational benchmark capability for such calculations.

(Cross section, multigroup, slowing-down, transport, Monte Carlo, resonance, reactor, eigenvalue, benchmark, stochastic)

Introduction

The generation of multigroup cross sections from point data represents one of the basic problems in reactor physics analysis. Since errors introduced into the processed data may lead to a significant uncertainty in the subsequent reactor calculations, there has been a great deal of interest in estimating the error introduced by specific methods and/or codes. In this study two distinct methods are compared for the solution of a zero-dimensional neutron slowing-down problem.¹² Both the continuous energy Monte Carlo code VIM and the multigroup code MC²-2 were designed to treat such a problem in a rigorous manner. As a consequence, a comparison of the two methods serves to evaluate both methods and codes and verify that they attain a sufficient accuracy in the representation and treatment of neutron interactions to provide a standard for future comparisons.

The problem selected for study was an infinite, homogeneous core composition representative of the benchmark ZPR-6 Assembly 7.⁴ The ENDF/B-3 data were used. The atom densities defining the problem are shown in Table I. A uniform temperature of 300°K was used.

<table>
<thead>
<tr>
<th>Isotope</th>
<th>ENDF/B Mat No.</th>
<th>Atom Density</th>
</tr>
</thead>
<tbody>
<tr>
<td>²³⁹Pu</td>
<td>1159</td>
<td>0.88672</td>
</tr>
<tr>
<td>²⁴⁰Pu</td>
<td>1105</td>
<td>0.11944</td>
</tr>
<tr>
<td>²⁴¹Pu</td>
<td>1106</td>
<td>0.0133</td>
</tr>
<tr>
<td>²³⁵U</td>
<td>1157</td>
<td>0.01259</td>
</tr>
</tbody>
</table>

Of the 12 isotopes in the problem, 8 had new cross section sets prepared as described in Ref. 1: ²³⁸U, ²³⁹Pu, ²⁴⁰Pu, Ni, Cr, Fe, ²⁴Na, and ⁵⁵Mn. A second iron cross section set was prepared, incorporating some small additional refinements, and used in a second VIM calculation.

The first VIM calculation, designated as VIM Run No. 1, consisted of 25,000 neutron histories. Absorption weighting was used to produce low variance estimates of reaction rates down to very low energies. A second VIM calculation, designated as VIM Run No. 2, consisted of 50,000 neutron histories followed with analog weighting. The iron cross section set used in the second run resulted in lower iron scattering cross sections, about 5% or less, from 320 keV to 59 keV. The results of both runs are presented below for quantities significantly affected by the change in iron scattering.

Eigenvalue estimation in VIM is made simultaneously with analog, collision, and track length estimators. Simple averaging of these estimators is used to reduce variance as is the method of combined estimators.⁵ The detailed edits of isotopic reaction rates by energy region). In an unresolved resonance region, cross sections are obtained by random sampling from probability tables corresponding to each ENDF/B specified unresolved resonance data point. Probability distributions are employed to represent anisotropy in the center of mass for both discrete level inelastic and elastic scattering. The full ENDF/B energy dependence of parameters for the determination of the energy distribution of secondary neutrons is utilized in VIM.
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TABLE I. Atom Densities (× 10^{-21} atoms/cc)

<table>
<thead>
<tr>
<th>Isotope</th>
<th>ENDF/B Mat No.</th>
<th>Atom Density</th>
</tr>
</thead>
<tbody>
<tr>
<td>^{239}Pu</td>
<td>1159</td>
<td>0.88672</td>
</tr>
<tr>
<td>^{240}Pu</td>
<td>1105</td>
<td>0.11944</td>
</tr>
<tr>
<td>^{241}Pu</td>
<td>1106</td>
<td>0.0133</td>
</tr>
<tr>
<td>^{235}U</td>
<td>1157</td>
<td>0.01259</td>
</tr>
<tr>
<td>^{238}U</td>
<td>1158</td>
<td>5.78036</td>
</tr>
<tr>
<td>Mo</td>
<td>1111</td>
<td>0.2357</td>
</tr>
<tr>
<td>^{23}Na</td>
<td>1156</td>
<td>9.2904</td>
</tr>
<tr>
<td>^{16}O</td>
<td>1134</td>
<td>13.98</td>
</tr>
<tr>
<td>Fe</td>
<td>1180</td>
<td>12.97</td>
</tr>
<tr>
<td>Ni</td>
<td>1123</td>
<td>1.240</td>
</tr>
<tr>
<td>Cr</td>
<td>1121</td>
<td>2.709</td>
</tr>
<tr>
<td>^{55}Mn</td>
<td>1019</td>
<td>0.212</td>
</tr>
</tbody>
</table>

used. Broad-group edits were produced for 24 groups
with a lethargy width of 0.5 from 10 MeV to 275.36 eV
and 1.0 from 275.36 eV to 13.71 eV. Results available
for direct comparison included broad-group edits for
flux, fission spectrum, isotopic reaction rates, and
isotopic microscopic cross sections.

Features of the VIM Calculation

As a continuous-energy Monte Carlo code, VIM pro-
vides a detailed energy and angular representation of
neutron physics data obtained from ENDF/B libraries.
Outside of the unresolved resonance region, isotopic
microscopic cross sections are obtained by linear in-
terpolation from dense cross section versus energy
tables (Doppler broadened to 300°K in the resolved

small additional refinements, and used in the second

calculation.

The first VIM calculation, designated as VIM Run
No. 1, consisted of 25,000 neutron histories. Absorp-
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consisted of 50,000 neutron histories followed with
analog weighting. The iron cross section set used in
the second run resulted in lower iron scattering cross
sections, about 5% or less, from 320 keV to 59 keV.
The results of both runs are presented below for quan-
tities significantly affected by the change in iron
scattering.

Eigenvalue estimation in VIM is made simultane-
ously with analog, collision, and track length estima-
tors. Simple averaging of these estimators is used to
reduce variance as is the method of combined estimators.5

The detailed edits of isotopic reaction rates by energy
group and group fluxes are obtained by track length
estimation.

Features of the ET0E-2/MC^2-2 Calculation

The MC^2-2 code^ solves the fundamental mode neu-
tron slowing-down equations using multigroup, con-
tinuous slowing-down, and integral transport theory algo-
rithms. The input data to MC^2-2 are prepared by the
code ET0E-2 which reformats and preprocesses data from
the ENDF/B tapes. The formats required by MC^2-2 were
specified to permit efficient access to data by a
processing code and thus are less general than the
ENDF/B formats. The reformatting done by ET0E-2 does
not, however, change the basic physics data. On the
other hand, the processing of floor cross section data
and light-element resonance data by ET0E-2 to ultra-
fine-group cross sections (Δu = 1/120) does introduce
approximations. In the initial comparisons of VIM and
MC^2-2, many of the differences were traced to an inade-
quate treatment of the light-element resonances by
ET0E-2. The numerical algorithms were refined as a con-
sequence of this testing. The MC^2-2 code uses these
data to calculate a flux and current spectrum which are
used to collapse the data to broad-group cross sections.
The rigor of the slowing-down calculation is user-specified. The comparison calculations reported in this study were performed using most of the more rigorous algorithms. In particular, isotope-dependent fission spectra, improved Goertzel-Greuling moderating parameters, detailed elastic matrix, and resonance calculations were used in the ultra-fine-group calculation and a hyperfine-group integral transport calculation was used below 4 keV to treat the resolved resonance region in detail. It has been found that one may relax the rigor of the calculation without much impact on such integral parameters as \( k_{\text{eff}} \), whereas group cross section or flux comparisons require the most rigorous methods.

**Results**

Extremely close agreement in the eigenvalue computation was obtained. The ETØE-2/MC\(^2\)-2 value of 1.2121 is well within one standard deviation of both the VIM Run No. 1 value of 1.2128 (1 \( \sigma = 0.0014 \)) and the VIM Run No. 2 value of 1.2129 (1 \( \sigma = 0.0030 \)).

A comparison of group flux calculations is shown in Table II; the VIM results are shown with uncertainties.

<table>
<thead>
<tr>
<th>Isotope</th>
<th>VIM Run No. 1</th>
<th>VIM Run No. 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>(^{24}\text{Pu})</td>
<td>0.012385</td>
<td>0.9943 ± 0.0061</td>
</tr>
<tr>
<td>(^{24}\text{Pu})</td>
<td>0.0014452</td>
<td>0.9998 ± 0.0047</td>
</tr>
<tr>
<td>(^{235}\text{U})</td>
<td>0.0017975</td>
<td>0.9925 ± 0.0042</td>
</tr>
<tr>
<td>(^{238}\text{U})</td>
<td>0.3858</td>
<td>1.0052 ± 0.0028</td>
</tr>
<tr>
<td>(^{239}\text{Pu})</td>
<td>0.11419</td>
<td>0.9947 ± 0.0050</td>
</tr>
<tr>
<td>(\text{Cr})</td>
<td>0.011056</td>
<td>0.9853 ± 0.0132</td>
</tr>
<tr>
<td>(\text{Ni})</td>
<td>0.008198</td>
<td>1.0054 ± 0.0084</td>
</tr>
<tr>
<td>(\text{Fe})</td>
<td>0.03055</td>
<td>0.9704 ± 0.0142</td>
</tr>
<tr>
<td>(^{23}\text{Na})</td>
<td>0.004485</td>
<td>0.9921 ± 0.0104</td>
</tr>
<tr>
<td>(^{16}\text{O})</td>
<td>0.0019893</td>
<td>1.0354 ± 0.0574</td>
</tr>
<tr>
<td>(55\text{Mn})</td>
<td>0.003685</td>
<td>0.9935 ± 0.0057</td>
</tr>
</tbody>
</table>

### Table II. Group Flux Comparison

<table>
<thead>
<tr>
<th>Group No.</th>
<th>MC(^2)</th>
<th>VIM Run No. 1 MC(^2)</th>
<th>VIM Run No. 2 MC(^2)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.4800</td>
<td>1.048 ± 0.106</td>
<td>0.977 ± 0.072</td>
</tr>
<tr>
<td>2</td>
<td>1.989</td>
<td>1.016 ± 0.060</td>
<td>1.048 ± 0.034</td>
</tr>
<tr>
<td>3</td>
<td>4.904</td>
<td>1.006 ± 0.034</td>
<td>1.010 ± 0.022</td>
</tr>
<tr>
<td>4</td>
<td>7.335</td>
<td>0.995 ± 0.026</td>
<td>0.993 ± 0.017</td>
</tr>
<tr>
<td>5</td>
<td>8.368</td>
<td>1.009 ± 0.022</td>
<td>1.002 ± 0.016</td>
</tr>
<tr>
<td>6</td>
<td>17.40</td>
<td>1.018 ± 0.015</td>
<td>0.997 ± 0.009</td>
</tr>
<tr>
<td>7</td>
<td>17.10</td>
<td>1.009 ± 0.011</td>
<td>1.005 ± 0.011</td>
</tr>
<tr>
<td>8</td>
<td>22.13</td>
<td>0.991 ± 0.010</td>
<td>1.002 ± 0.009</td>
</tr>
<tr>
<td>9</td>
<td>24.22</td>
<td>0.991 ± 0.008</td>
<td>1.005 ± 0.008</td>
</tr>
<tr>
<td>10</td>
<td>21.54</td>
<td>0.994 ± 0.008</td>
<td>1.000 ± 0.009</td>
</tr>
<tr>
<td>11</td>
<td>18.50</td>
<td>0.998 ± 0.008</td>
<td>0.999 ± 0.009</td>
</tr>
<tr>
<td>12</td>
<td>16.62</td>
<td>1.007 ± 0.007</td>
<td>1.005 ± 0.011</td>
</tr>
<tr>
<td>13</td>
<td>15.10</td>
<td>0.994 ± 0.008</td>
<td>1.006 ± 0.009</td>
</tr>
<tr>
<td>14</td>
<td>11.19</td>
<td>0.997 ± 0.008</td>
<td>0.999 ± 0.014</td>
</tr>
<tr>
<td>15</td>
<td>6.252</td>
<td>0.998 ± 0.006</td>
<td>1.006 ± 0.015</td>
</tr>
<tr>
<td>16</td>
<td>3.937</td>
<td>0.995 ± 0.007</td>
<td>0.992 ± 0.017</td>
</tr>
<tr>
<td>17</td>
<td>1.428</td>
<td>0.994 ± 0.010</td>
<td>0.999 ± 0.020</td>
</tr>
<tr>
<td>18</td>
<td>4.749</td>
<td>0.991 ± 0.009</td>
<td>1.000 ± 0.022</td>
</tr>
</tbody>
</table>

will be discussed below. The very significant difference in iron capture is localized in Group 19 and undoubtedly results from the difference in the treatment of self-shielding of the 1150-eV p-wave resonance. In the VIM data library, approximately 40 points are used to represent this resonance, whereas in the ETØE-2 library, its strength is almost totally confined to one ultrafine group. Apart from the exceptions noted here, however, the agreement in reaction rates is generally good.

A detailed comparison of broad-group cross sections for \(^{238}\text{U}\) capture and \(^{239}\text{Pu}\) capture and fission below 40.9 keV are given in Table V. The very close agreement in the resolved range was obtained through use of the MC\(^2\)-2 integral transport option. The VIM results are shown with ±2 uncertainties.
ties of ±2 σ. The effect of the improvement in iron scattering cross sections used in VIM Run No. 2 may be noted in the data for Groups 8, 9, and 10. Although generally good agreement is obtained over the full energy range, the VIM spectrum appears slightly harder. A slightly more rapid attenuation is apparent in the VIM-computed flux below Group 16. It should be noted that the observed agreement in low-energy flux is attainable only with the MC²-2 integral transport option.

Individual isotopic capture rates are shown in Table III and fission rates in Table IV. The MC²-2 rates shown were obtained without benefit of the integral transport option. The VIM results are again shown with ±2 σ uncertainties. The discrepancy in ²³⁹U capture rate results primarily from the difference between the VIM and the MC²-2 unresolved resonance treatment as will be discussed below. The very significant difference in iron capture is localized in Group 19 and undoubtedly results from the difference in the treatment of self-shielding of the 1150-eV p-wave resonance. In the VIM data library, approximately 40 points are used to represent this resonance, whereas in the ET0E-2 library, its strength is almost totally confined to one ultrafine group. Apart from the exceptions noted here, however, the agreement in reaction rates is generally good.

A detailed comparison of broad-group cross sections for ²³⁸U capture and ²³⁹Pu capture and fission below 40.9 keV are given in Table V. The very close agreement in the resolved range was obtained through use of the MC²-2 integral transport option. The VIM results are shown with ±2 σ uncertainties.

Although broad-group cross section agreement as shown is typically of the order of 1% and frequently better, an important difference may be noted in the ²³⁸U unresolved resonance range. The VIM code uses random linear-linear cross-section interpolation between probability tables generated for ENDF/B unresolved resonance energy points; MC²-2 uses log-log interpolation between unresolved resonance calculations at specified energies. It has been determined that the difference in interpolation schemes alone will account for the greater part of the 0.5% to 1.0% increase in the VIM estimate of ²³⁸U unresolved resonance capture over the corresponding MC²-2 results. Similar effects may be noted in ²³⁹Pu fission, particularly in Group 18 where the difference in interpolation scheme produces a 2% greater VIM result.

In Table VI, a comparison of capture cross sections for structural materials over the energy range 820.9 keV to 748.5 eV is shown. The examples shown represent what are perhaps the most difficult cases in which to attain close agreement. The VIM data presented are shown with ±2 σ uncertainties and were taken from VIM Run No. 2 for Groups 6 to 15 and from VIM Run No. 1 for Groups 16 to 19. Although the agreement is frequently very good, a number of significant exceptions
may be noted. Two major causes contribute to the differences:

(1) insufficient point densities in the VIM

...
may be noted. Two major causes contribute to the differences:

(1) insufficient point densities in the VIM library in the extreme wings of narrow resonances may cause a bias toward higher capture in the valleys between isolated narrow resonances; and

(2) the much less detailed treatment of the peaks of very narrow capture resonances in ET0E-2, causes higher ET0E-2/MC2-2 cross sections by underestimating self-shielding of the narrow resonances.

The latter effect is most noticeable in iron in Group 19, due to the 1150-eV resonance, and in chromium in Group 18, due to the 1626-eV resonance. The former difficulty probably accounts for the chromium discrepancy in Group 6 and in nickel in Group 18. A combination of these effects probably contributes to a lesser extent in other cases.

A comparison of other broad-group cross section data shows that agreement in total cross sections is generally within a few tenths of 1% and within 1% on capture throughout the resonance regions of the various isotopes. Other examples of the above difficulties with narrow capture resonances may be detected. The interpolation difficulty in the unresolved region described above appears to have little effect for 239Pu, 241Pu, or 235U. Following the preparation of an improved iron data set for the VIM library, providing improved interpolation accuracy above the resonance region, no significant disagreement is observed with respect to non-resonant cross sections.

Conclusions

In recent years several studies have been reported which compare neutron cross section processing methods and codes. Such studies have generally concentrated on comparison of k$_{eff}$ and reaction rate ratios and concluded that the methods and codes were in good agreement if k$_{eff}$ differences were less than 0.5%. The current study was designed to determine whether there was agreement on a range of parameters between an essentially exact stochastic calculation and a detailed analytic calculation for a typical fast reactor core mixture. The extremely good agreement between the two methods permits one to conclude that either code provides a reliable computational benchmark capability for such an infinite medium calculation.

References


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