THE USE OF DETERMINISTIC CODES FOR 'SEPARATING THE WHEAT FROM THE CHAFF' IN BENCHMARK MODELS AND CALCULATIONS

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An important effort in the field of nuclear criticality safety is the establishing and modeling of a set of benchmark critical (or near critical) experiments and the use of these benchmark experiment models to validate and verify computer codes and cross sections. For the most part Monte Carlo codes such as MCNP and KENO.Va have emerged as the codes of choice in the U.S. Since Monte Carlo codes generally have the capability of modeling complex geometries in great detail there is a tendency to focus attention on modeling an experiment in very great detail. Indeed, it is the author’s observation that so much effort is expended trying to exactly model unimportant details (the ‘chaff’) that many of the truly significant features and characteristics (the ‘wheat’) of the experiment can be lost in the shuffle. An obvious question now arises. How does one determine what is ‘wheat’ and what is ‘chaff’?

This presentation will focus on the use of deterministic, or, more specifically, discrete-ordinates codes for performing sensitivity calculations in determining which details are important and which are not.

The principal advantage of discrete-ordinates codes is that they can quite precisely determine the effect on $k_{ef}$ associated with distinct details of an experiment such as impurities, external structure, conflicting or missing information, etc.

Three different examples are used to demonstrate the value of using discrete-ordinates codes for separating the wheat from the chaff. It is also shown that, for all practical purposes, Monte Carlo codes are essentially unsuited for determining small effects on $k_{ef}$.

**Example 1.**

The first example uses an idealized model of the original Pu-239 Jezebel benchmark experiment, a sphere of delta-phase plutonium at a density of 15.61 g/cc. The Pu parts were all nickel plated (nominal 0.005 in. thick) for contamination control. We choose to try to determine the effect of this nickel clad on the exterior surface of a 17.020 kg sphere of plutonium metal. Using the ONEDANT discrete-ordinates code with three different multigroup cross section sets we find the results shown in Table 1. Included in the results is the incremental plutonium surface-mass-equivalent to the 58 g Ni plating on the sphere that can be readily determined with ONEDANT. The wall clock time to perform each of these calculations was less than 1 minute on a Sun SPARCstation 10.
Table 1. Effect of External Ni Plating on Jezebel: ONEDANT

<table>
<thead>
<tr>
<th>CROSS SECTION SET</th>
<th>$k_{\text{eff}}$, No Ni</th>
<th>$k_{\text{eff}}$ with Ni</th>
<th>$\Delta k_{\text{eff}}$</th>
<th>Pu Mass Equivalent</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hansen-Roach 16 Grp</td>
<td>1.00122</td>
<td>1.00227</td>
<td>0.00105</td>
<td>63 g</td>
</tr>
<tr>
<td>ENDF/B-IV 27 Grp</td>
<td>0.99776</td>
<td>0.99895</td>
<td>0.00119</td>
<td>71 g</td>
</tr>
<tr>
<td>ENDF/B-V 30 Grp</td>
<td>0.99362</td>
<td>0.99483</td>
<td>0.00121</td>
<td>72 g</td>
</tr>
</tbody>
</table>

For comparison with a Monte Carlo code, MCNP was used to make three independent estimates of the worth of the Ni plating. For each of the runs one million active histories were executed. The elapsed wall clock time for each run was about 40 minutes on a Sun SPARCstation 10. The results are shown in Table 2. These results show the difficulty in estimating the worth of the Ni plating using Monte Carlo. About all that can be said is that it doesn’t seem to be worth very much.

Table 2. Effect of External Ni Plating on Jezebel: MCNP

<table>
<thead>
<tr>
<th>Run</th>
<th>$k_{\text{eff}}$, No Ni</th>
<th>$k_{\text{eff}}$ with Ni</th>
<th>68% $\Delta k_{\text{eff}}$</th>
<th>95% $\Delta k_{\text{eff}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.99714 ± 0.00050</td>
<td>0.99914 ± 0.00060</td>
<td>0.00200 ± 0.00078</td>
<td>0.00200 ± 0.00156</td>
</tr>
<tr>
<td>2</td>
<td>0.99643 ± 0.00060</td>
<td>0.99794 ± 0.00059</td>
<td>0.00151 ± 0.00084</td>
<td>0.00151 ± 0.00168</td>
</tr>
<tr>
<td>3</td>
<td>0.99844 ± 0.00058</td>
<td>0.99936 ± 0.00064</td>
<td>0.00092 ± 0.00086</td>
<td>0.00092 ± 0.00173</td>
</tr>
</tbody>
</table>

Example 2.

For the second example we use the so-called $^{240}$Pu, or “dirty” Jezebel spherical critical assembly that was comprised of plutonium with 20.1 at. % $^{240}$Pu and 3.1 at. % $^{241}$Pu. Because $^{241}$Pu decays with a 14.4 yr half life to $^{241}$Am we will determine the reactivity effect of $^{241}$Am following five years of $^{241}$Pu decay. Results from the ONEDANT discrete-ordinates code with two different cross section sets are shown in Table 3. Each calculation required less than 1 minute wall clock time.

Table 3. Effect of $^{241}$Am Buildup in the $^{240}$Pu Jezebel Assembly

<table>
<thead>
<tr>
<th>CROSS SECTION SET</th>
<th>$k_{\text{eff}}$, No $^{241}$Am</th>
<th>$k_{\text{eff}}$ with $^{241}$Am</th>
<th>$\Delta k_{\text{eff}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>ENDF/B-IV 27 Grp</td>
<td>0.99991</td>
<td>0.99847</td>
<td>0.00144</td>
</tr>
<tr>
<td>ENDF/B-V 30 Grp</td>
<td>0.99537</td>
<td>0.99432</td>
<td>0.00105</td>
</tr>
</tbody>
</table>

For a Monte Carlo comparison, results from three independent KENO V.a pairs of calculations using ENDF/B-IV 27 group cross sections are shown in Table 4. For each of the calculations 1.8 million active histories were run and the elapsed wall clock time for each run was about 20 minutes on a Sun SPARCstation 10. Once again, Monte Carlo gives us little information other than the effect of the $^{241}$Am appears to be fairly small.

Table 4. Effect of $^{241}$Am Buildup in the $^{240}$Pu Jezebel Assembly: KENO V.a

<table>
<thead>
<tr>
<th>Run</th>
<th>$k_{\text{eff}}$, No Am</th>
<th>$k_{\text{eff}}$ with Am</th>
<th>68% $\Delta k_{\text{eff}}$</th>
<th>95% $\Delta k_{\text{eff}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.99916 ± 0.00064</td>
<td>0.99784 ± 0.00062</td>
<td>0.00132 ± 0.00089</td>
<td>0.00132 ± 0.00178</td>
</tr>
<tr>
<td>2</td>
<td>0.99935 ± 0.00063</td>
<td>0.99923 ± 0.00069</td>
<td>0.00012 ± 0.00093</td>
<td>0.00012 ± 0.00187</td>
</tr>
<tr>
<td>3</td>
<td>1.00026 ± 0.00067</td>
<td>0.99918 ± 0.00061</td>
<td>0.00108 ± 0.00091</td>
<td>0.00108 ± 0.00181</td>
</tr>
</tbody>
</table>
Example 3.

For our final example we consider a fairly common uncertainty that arises in modeling early experiments, namely an uncertainty in what kind of steel was used in an experiment. We use the SHEBA 5% enriched uranyl fluoride solution reactor as an example and determine the difference in $k_{\text{eff}}$ assuming the tank material is pure iron instead of stainless steel 304L.

Results from the TWODANT discrete-ordinates code with ENDF/B-IV 27 group cross sections give a $k_{\text{eff}}$ with SS304L of 1.00937 and a $k_{\text{eff}}$ with pure iron of 1.00982 for a $\Delta k_{\text{eff}}$ of 0.00045, a very small change in $k_{\text{eff}}$. Wall clock time for each of these calculations was about 5 minutes.

For a Monte Carlo comparison, results from two independent KENO V.a pairs of calculations using ENDF/B-IV 27 group cross sections are shown in Table 5. For each of the calculations 1.2 million active histories were run and the elapsed clock time for each run was about 3 hours on a Sun SPARCstation 10. Even with this large number of histories, the results from the Monte Carlo runs are not resolved sufficiently to give us much useful information.

Table 5. Effect of SHEBA Tank Composition on $k_{\text{eff}}$: KENO V.a

<table>
<thead>
<tr>
<th>Run</th>
<th>$k_{\text{eff}}$, SS Tank</th>
<th>$k_{\text{eff}}$, Fe Tank</th>
<th>68% $\Delta k_{\text{eff}}$</th>
<th>95% $\Delta k_{\text{eff}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.00868 ± 0.00071</td>
<td>1.00853 ± 0.00073</td>
<td>0.00015 ± 0.00102</td>
<td>0.00015 ± 0.00204</td>
</tr>
<tr>
<td>2</td>
<td>1.00706 ± 0.00067</td>
<td>1.01035 ± 0.00072</td>
<td>0.00329 ± 0.00098</td>
<td>0.00329 ± 0.00197</td>
</tr>
</tbody>
</table>

From the above examples it should be clear that discrete-ordinates codes are excellent tools for determining whether modeling details have a significant effect on the $k_{\text{eff}}$ of the basic problem being analyzed. Many modeling features or uncertainties whose effect on the basic problem is small can be simplified or omitted without diminishing the value of the basic analysis. The use of Monte Carlo codes to calculate reactivity effects of, say 0.001 in $k_{\text{eff}}$, is virtually an exercise in futility since, literally, tens of millions of histories are likely to be required to definitively resolve such small effects. Cluttering up a model with too much neutronically-insignificant detail tends to cloud over the essential features and characteristics of the system being analyzed. We must never lose sight of the fact that the Jezebel assemblies were fundamentally bare spheres of plutonium metal or that SHEBA is fundamentally a bare cylinder of uranyl fluoride solution.