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# USE OF METAL/URANIUM MIXTURES TO EXPLORE DATA UNCERTAINTIES



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A table of $k_\infty$ values for three homogenized metal/$^{235}$U systems calculated using both MCNP[1] and the SCALE code system[2] was presented in Ref. 3. The homogenized metal/$^{235}$U ratios were selected such that the MCNP analyses for each mixture provided $k_\infty \approx 1.0$. The metals considered were aluminum, zirconium, and iron. These simplified systems were created in an effort to ease an investigation of discrepant results obtained using MCNP and SCALE to analyze large, dry systems of metal-clad, highly enriched fuel assemblies. The simplified systems are all dominated by scattering and fission in the intermediate energy range of 10 eV to 1 MeV and, as such, provide a severe test of the cross-section data and processing methodologies in this energy range. Unfortunately, no experiments adequately represent the characteristics of these metal/$^{235}$U systems, thus the ability of the codes to predict the "correct" critical metal/$^{235}$U ratios is not known. In the absence of experimental data, Ref. 3 states that the continuous-energy cross sections, in combination with MCNP, are "most likely to give the correct results." However, the results in this paper illustrate the potential dangers embedded in drawing such a conclusion in the absence of applicable experimental data.

Reference 3 has received considerable attention at Oak Ridge National Laboratory (ORNL) and elsewhere because the reported $k_\infty$ values varied by as much as 38% between the MCNP results and those of SCALE. The ORNL approach was to analyze the systems using a broad range of codes

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and data (multigroup and continuous-energy) and to seek an understanding of the discrepancies by studying differences in the basic data and processing methods. The continuous-energy codes and data applied in the ORNL study were (1) MCNP, using ENDF/B-V, ENDF/B-VI, and Los Alamos National Laboratory (LANL) data evaluations, (2) VIM,[4] using ENDF/B-V data (results provided by Roger Blomquist, Argonne National Laboratory), and (3) MONK,[5] using a 8200-point library based on UKNDL evaluations and a preliminary JEF library (results provided by Nigel Smith, AEA Technology). The VIM code provides treatment of unresolved resonances; MCNP does not. The MONK analyses provided a result using both an independent code and independent data evaluations. Although accessing continuous-energy data typically requires the use of Monte Carlo codes, one-dimensional (1-D) deterministic codes can be used to accurately calculate $k_\infty$ values using a variety of multigroup data libraries and processing methods. The multigroup codes used in the study were $MC^2$ (Ref. 6) and the CSAS1X (i.e., BONAMI/NITAWL/XSDRNPM) sequence of the SCALE system.[2] Both systems provide problem-dependent resonance processing of cross-section data and available fine-group libraries were used for the analyses. Broad-group libraries were not studied in any depth because there were none readily available for intermediate-energy systems.

The results obtained using the variety of codes and cross-section libraries discussed above are provided in Table I. A study of the aluminum-capture cross section revealed that the ENDF point representation of the cross section does not appear to adequately represent the resonances in the energy range of interest (see, for example, the region from 1 to 500 keV, as shown in Ref. 7). A reevaluation of the data to provide a more physical representation of the capture cross-section data was performed at ORNL, and the subsequent analysis yielded a value of $k_\infty$ that was 14% higher. This increase shows the high sensitivity of $k_\infty$ to the aluminum evaluation in this energy region and casts doubt on whether this Al/$^{235}$U mixture actually represents a critical system. Further indication of the

need for a new ENDF evaluation is provided by the MONK results, which are 6 to 14% higher than the MCNP and VIM results.

The results in Table I for the Fe/$^{235}$U mixture provide an indication that this system $k_\infty$ may also be far from critical. One fact that is very clear from the ORNL study is that proper representation of all the iron resonances, including the *p*-wave and *d*-wave resonances, is important for this mixture. Failure to properly shield the *p*-wave iron resonance at 1.15 keV results in a $k_\infty$ value that is 20% lower. The fact that only *s*-wave resonances are available in the SCALE 218-group library is the major reason for the very low $k_\infty$ value that it predicts. The result with the SCALE 238-group is high for two reasons:

1. The group structure is too broad in the region of some iron resonances that are important to this system.
2. The NITAWL procedure for resolved resonance processing calculates a background cross section using the scattering radius from ENDF. This assumption is inadequate for iron in the energy range of importance to this system.

These two reasons also contribute to the poor result with the 218-group library. Most of the remaining results are bunched between approximately 1.075 and 1.115. It is unclear as to what causes the MCNP result with the LANL iron evaluation to be 9% lower than the ENDF/B-V evaluation. The LANL iron evaluation is the default used by MCNP, but it does not appear to be consistent with ENDF/B-V or ENDF/B-VI. However, the LANL iron evaluation provides results consistent with the results obtained by MONK using a preliminary JEF library.

Like the Fe/$^{235}$U mixture above, the consensus of results for the Zr/$^{235}$U mixture is far above critical. The SCALE 218-group result is low because zirconium is a nonresonance material in ENDF/B-IV and was processed as an essentially infinite dilute material. The infinite dilute treatment

overestimates capture and leads to a low value of $k_\infty$. The other result that is significantly lower than the consensus values is the MCNP result using ENDF/B-V data. A review by LANL confirmed that the zirconium data in the MCNP ENDF/B-V library had an error that has been corrected in the MCNP ENDF/B-VI library.

As indicated at the beginning of this paper, these metal/uranium mixtures are very sensitive to the metal cross-section data in the intermediate-energy range and the processing methods that are used. Even after discarding results having known inadequacies, a significant amount of uncertainty remains in the actual $k_\infty$ values of these mixtures. These investigations highlight the need for code developers and data evaluators to work together to ensure that the processed data accurately represent the structure of the cross sections over the entire energy range. In addition, independent data evaluations and code methodologies should be considered when analyzing systems with little or no relevant experimental data. However, the problem is more fundamental than whether continuous-energy cross sections are "more likely to give the correct answer" or which data evaluation is the "best." Any code or data set can contain an error or be inadequate for specific situations. The real problem is that the calculational bias of codes and data cannot be accurately assessed in the absence of relevant critical experiments.

The criticality safety community must continue to encourage nuclear data development and the understanding of the physics of neutron interactions in light of new and ever-changing applications that are being presented. Improvements in the physics modeling and the basic data will surely enable greater confidence in calculated results. *One must remember, however, that unless adequate validation of the methodology can be performed against applicable experimental data, there will always be a risk of establishing an inadequate margin of subcriticality.*

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TABLE I

Additional $k_\infty$ Values for Mixtures of Al, Fe, and Zr with $^{235}U$[a]

| Code and cross-section data | Al/$^{235}$U = 2470 | Fe/$^{235}$U = 320 | Zr/$^{235}$U = 103 |
|---|---|---|---|
| SCALE | | | |
| 218-group ENDF/B-IV | 1.0009 | 0.8198 | 0.9602 |
| 238-group ENDF/B-V | 0.9802<br>(1.1176)[b] | 1.1446 | 1.1070 |
| VITAMIN-E<br>174-group ENDF/B-V | 1.003 | 1.081 | 1.0679 |
| VITAMIN-B6<br>199-group ENDF/B-VI | 1.0071 | 1.1085 | 1.1077 |
| VIM[c]<br>Continuous ENDF/B-V | 0.9983 ± 0.0006 | 1.0877 ± 0.0007 | 1.1068 ± 0.0009 |
| MC$^{2c}$<br>2040-group ENDF/B-V | 0.9738 | 1.0965 | 1.0972 |
| Point energy MONK[d] | | | |
| UKNDL | 1.0627 ± 0.0008 | 1.0762 ± 0.0012 | 1.1205 ± 0.0010 |
| Preliminary JEF library | 1.1318 ± 0.0004 | 0.9884 ± 0.0008 | 1.0703 ± 0.0006 |
| MCNP continuous: | | | |
| ENDF/B-V | 0.9983 ± 0.0016 | 1.0895 ± 0.0017[e]<br>0.9901 ± 0.0021[f] | 1.0048 ± 0.0025 |
| ENDF/B-VI | 1.0061 ± 0.0008 | 1.1135 ± 0.0008 | 1.1142 ± 0.0008 |

[a]Calculations performed by ORNL, except as noted.
[b]ORNL aluminum evaluation by R. Q. Wright.
[c]Results provided by R. Blomquist, Argonne National Laboratory.
[d]Results provided by Nigel Smith, Atomic Energy Authority Technology, Winfrith, UK.
[e]Iron cross section 26000.50c from file endf5p.
[f]Default iron cross section 26000.55c from file rmccs.