Examination of Validation Outlier Cases Using the Sensitivity and Uncertainty Analysis Tools of SCALE 6.1*

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INTRODUCTION

In the course of criticality code validation, outlier cases are frequently encountered. Historically, the causes of these unexpected results could be diagnosed only through comparison with other similar cases or through the known presence of a unique component of the critical experiment. The sensitivity and uncertainty (S/U) analysis tools available in the SCALE 6.1 [1] code system provide a much broader range of options to examine underlying causes of outlier cases. This paper presents some case studies performed as a part of the recent validation of the KENO codes in SCALE 6.1 using S/U tools to examine potential causes of biases.[2]

CODE DESCRIPTIONS

The S/U tools in SCALE can quantify the predicted change in system responses—such as k_{eff}, reactivity differences, or ratios of fluxes or reaction rates—due to changes in the energy-dependent, nuclide-reaction-specific cross-section data. Where uncertainties in the neutron cross-section data are available, the sensitivity of the system to the cross-section data can be applied to obtain the uncertainty in the system response. Uncertainty quantification is useful for identifying potential sources of computational biases and highlighting parameters important to code validation.[3]

SELECTION OF OUTLIERS

An overview of the recent KENO validation, presented in Ref. 4, identifies the largest single outlier in each category of experiments examined. A review of the calculated-to-experiment (C/E) ratio for each experiment is also performed to identify potential trends that may merit further examination. Several cases and/or trends are examined in some detail in the full validation report [2], but a subset of those cases is also presented here. These cases are presented to provide examples of how the S/U tools can be used to diagnose, or eliminate, potential sources of error relating to outlier cases identified during validation. The three cases presented here relate to PU-MET-FAST-005-001 (PMF-005-001), IEU-MET-FAST-005-001 (IMF-005-001), and the HEU-SOL-THERM-014 (HST-014) and HEU-SOL-THERM-016 (HST-016) series in *International Handbook of Evaluated Criticality Safety Benchmark Experiments* (IHECSBE) [5].

RESULTS

PU-MET-FAST-005

The first case examined is PMF-005-001, which produces C/E ratios of 1.006 and 1.009 for multigroup and continuous energy calculations, respectively. Other PMF cases examined produce C/E ratios near or below unity that are consistent between multigroup and continuous energy. An examination of the IHECSBE description of the experiment reveals that this case involves a tungsten reflector and is in fact the only experiment examined in the validation suite with a significant quantity of tungsten. Traditional validation techniques would allow for the identification of tungsten as the probable cause of the aberrant behavior, but other tungsten cases would be needed to add confidence to this hypothesis. The SCALE S/U tools were used to calculate the total cross-section uncertainty for a system and to tabulate the individual contributions by isotope and reaction. Of the 11 individual reactions that contribute the most to the overall cross-section uncertainty for this system, 7 involve tungsten, as presented in Fig. 1. This fact alone is not proof that the presence of a significant quantity of tungsten is causing the poor results, but it is additional independent evidence that it may be a key contributor.

Covariance Matrix		Unc. in % dk/k
Nuclide-Reaction	Nuclide-Reaction	Due to this Matrix
^{239}Pu nubar	^{239}Pu nubar	1.1953E+00 ± 1.2703E-05
^{184}W n,n'	^{184}W n,n'	7.8394E-01 ± 5.4380E-04
^{186}W n,n'	^{186}W n,n'	7.2679E-01 ± 4.7947E-04
^{182}W n,n'	^{182}W n,n'	6.7679E-01 ± 3.8972E-04
^{239}Pu n,n'	^{239}Pu n,n'	5.5915E-01 ± 3.3604E-04
^{183}W n,n'	^{183}W n,n'	5.5555E-01 ± 2.3994E-04
^{239}Pu elastic	^{239}Pu n,n'	-5.2229E-01 ± 1.6806E-04
^{184}W elastic	^{184}W elastic	3.2915E-01 ± 4.8450E-05
^{186}W elastic	^{186}W elastic	3.2714E-01 ± 4.5977E-05
^{239}Pu fission	^{239}Pu fission	3.2659E-01 ± 7.9042E-06
^{182}W elastic	^{182}W elastic	2.5963E-01 ± 3.1905E-05

Fig. 1. Contributors to uncertainty in k_{eff} for PMF-005-001.

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To further examine why the tungsten contributions to cross-section uncertainty are so high, plots of energy-dependent sensitivity data and the cross-section uncertainty data from the SCALE covariance library are examined. The sensitivities of the system k_{eff} to the elastic scattering of four tungsten isotopes are presented in Fig. 2. This figure demonstrates that the k_{eff} is very sensitive to the tungsten elastic scattering cross sections in the 500 keV to 2 MeV range. This is not surprising because the model describes a fast system with a tungsten reflector that provides a significant increase in k_{eff}. The uncertainty for the same tungsten elastic scattering cross sections is shown in Fig. 3. The cross-section uncertainties are in the 5–7% range in the 500 keV to 1 MeV range, but they rise to 20% or more in the range just above 1 MeV, where significant sensitivity still exists. The contribution to system total cross-section uncertainty is related to the product of individual sensitivity and data uncertainty, so these figures demonstrate the combination of large sensitivity and significant uncertainty, which leads to the large contribution to total cross-section uncertainty. Neither the large tungsten contribution to system uncertainty nor the underlying cause could have been identified without the sensitivity/uncertainty analysis.

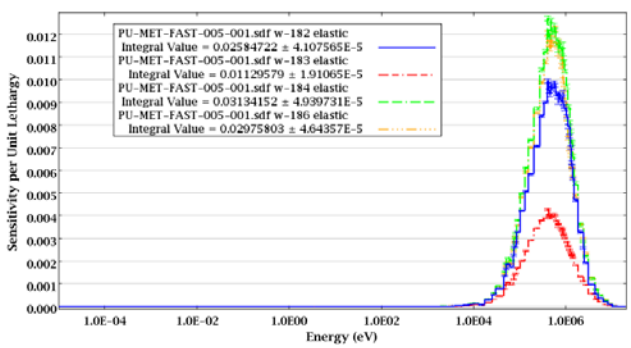

Fig. 2. Sensitivity of k_{eff} to tungsten elastic scattering cross sections for PMF-005-001.

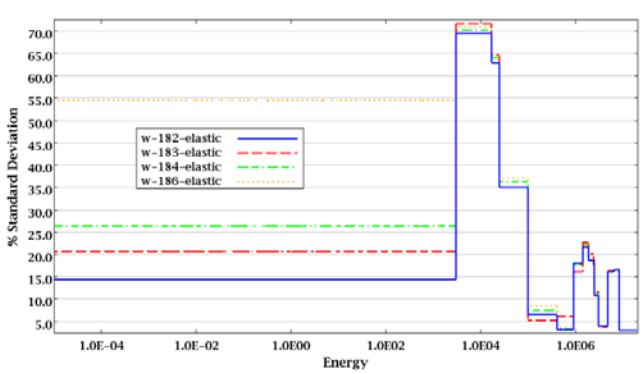

Fig. 3. Uncertainty in tungsten elastic scattering cross sections.

HEU-SOL-THERM-014 and HEU-SOL-THERM-016

The HST-014 and HST-016 series both consist of three experiments and focus on the reactivity effect of gadolinium in solution. In each series, the first experiment has no gadolinium, the second experiment has a moderate gadolinium concentration, and the third experiment has a high gadolinium concentration. The C/E values in each series are low (~0.99) for the first experiment, high (~1.01) for the second experiment, and very high (~1.025) for the third experiment. Traditional validation techniques would indicate that the gadolinium cross section is probably too small, as the calculated results are not reduced enough by the presence of the gadolinium in solution. Sample results provided in the IHECSBE [5] using other codes and cross-section sets indicate the same trends in calculated k_{eff} though, so this might indicate a problem with the description of the experiment. The S/U tools can be used to further investigate the likelihood that the gadolinium cross section is the culprit in these poorly calculated results.

Fig. 4 shows the sensitivity of k_{eff} to the absorption cross section of ^{157}Gd for both experiments containing gadolinium in both HST-014 and HST-016. The sensitivity profiles are very similar, with experiment 3 in each series showing a larger negative sensitivity than experiment 2, and HST-016 having a larger negative sensitivity in both cases than HST-014. Most of the sensitivity is also in the range between 0.001 and 0.1 eV, which is expected given the energy behavior of the gadolinium cross section and the fact that these are thermal systems. Because the sensitivity is measured in units of reactivity change per cross section change, $(\Delta k/k)/(\Delta\sigma/\sigma)$, it is possible to estimate the magnitude of the cross-section error in gadolinium that would cause the observed biases of the cases containing gadolinium. For HST-016 case 3, for instance, the bias is approximately 2.5% Δk, and the integral sensitivity is -0.156 $(\Delta k/k)/(\Delta\sigma/\sigma)$. This indicates that the gadolinium cross section would have to be in error by a factor of 16 to explain the observed bias in HST-016 case 3. The uncertainty in the ^{157}Gd cross section as a function of energy is shown in Fig. 5. The figure shows that the uncertainty in the cross section is less than 5% in the energy range where the vast majority of the ^{157}Gd sensitivity lies. It is therefore extremely unlikely that the gadolinium absorption cross section is the cause of the bias in the results for these cases. This calculation provides quantitative support for the qualitative indications provided by other codes and cross-section sets provided in Ref. [5]. The indications are that there probably is a problem with the description of the critical experiment, although this conclusion could be established with confidence only if the experiments in question were reviewed further.

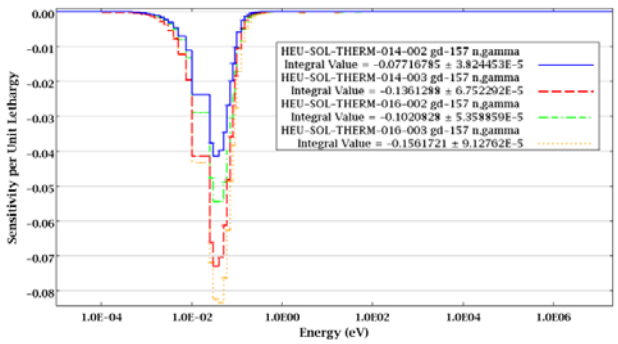

Fig. 4. Sensitivity of k_{eff} to ^{157}Gd for HST-014 and HST-016.

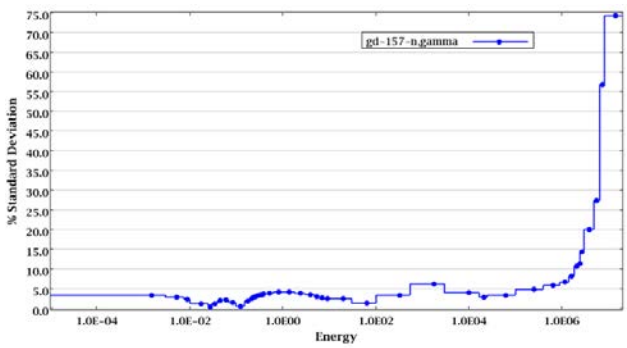

Fig. 5. Uncertainty in ^{157}Gd (n, gamma) cross section.

IEU-MET-FAST-005

The review of the C/E values for the IMF experiments shows that IMF-005 [2], for which there is only one case, is a significant outlier in terms of the difference between continuous energy and multigroup predictions. For the specific case of IMF-005, the C/E value for the continuous energy library is around 1.001, but the multigroup C/E is nearly 1.014. This difference of 1.3% in the C/E value is significantly greater than for the similar experiment IMF-003. A comparison of these two cases can be used to investigate potential causes of the aberrant results from IMF-005. At this point, there is no tool available for continuous-energy S/U analysis, so sensitivity data are available only for the multigroup calculations.

The overall cross-section uncertainties for both IMF-003 and IMF-005 are shown in Fig. 6 and Fig. 7, respectively. As expected, the cross-section uncertainties are related to ^{235}U and ^{238}U. The sensitivities to ^{235}U fission and capture are shown for both systems in Fig. 8. The sensitivity for IMF-003 and IMF-005 is nearly identical for both reactions, indicating that the difference in calculated k_{eff} is not caused by ^{235}U. The system sensitivities to elastic and inelastic scattering in ^{238}U are shown in Fig. 9. IMF-005 has a significantly lower sensitivity to ^{238}U scattering, which indicates that this is the likely difference between the two systems. The lower ^{238}U sensitivity is the most likely cause of the higher C/E value for IMF-005. This may indicate a problem in the multigroup cross-section processing performed in the multigroup calculation or with the multigroup energy structure for this calculation. Additional investigation would be needed to determine which, if either, of these areas could be improved to yield more accurate results.

Covariance Matrix		Unc. in % dk/k
Nuclide-Reaction	Nuclide-Reaction	Due to this Matrix
^{235}U n,gamma	^{235}U n,gamma	1.1151E+00 ± 1.1516E-04
^{238}U elastic	^{238}U n,n'	-4.5765E-01 ± 1.5852E-04
^{238}U elastic	^{238}U elastic	3.6909E-01 ± 1.8811E-05
^{238}U n,n'	^{238}U n,n'	3.5513E-01 ± 3.0403E-04
^{235}U elastic	^{235}U n,gamma	3.0515E-01 ± 1.1863E-05
^{235}U chi	^{235}U chi	2.7049E-01 ± 4.5186E-07
^{235}U n,n'	^{235}U n,n'	2.6154E-01 ± 5.6635E-05
^{235}U elastic	^{235}U n,n'	-2.4297E-01 ± 2.0807E-05
^{235}U fission	^{235}U fission	2.2699E-01 ± 1.7859E-06
^{238}U nubar	^{238}U nubar	1.6996E-01 ± 2.0705E-07

Fig. 6. Contributors to uncertainty in k_{eff} for IMF-003.

Covariance Matrix		Unc. in % dk/k
Nuclide-Reaction	Nuclide-Reaction	Due to this Matrix
^{235}U n,gamma	^{235}U n,gamma	1.2077E+00 ± 1.1803E-04
^{235}U chi	^{235}U chi	2.6004E-01 ± 4.1739E-07
^{235}U elastic	^{235}U n,gamma	2.4774E-01 ± 1.0598E-05
^{238}U elastic	^{238}U elastic	2.4699E-01 ± 1.0719E-05
^{235}U fission	^{235}U fission	2.2369E-01 ± 1.6854E-06
^{238}U elastic	^{238}U n,n'	-2.0925E-01 ± 9.7319E-05
^{56}Fe elastic	^{56}Fe elastic	2.0083E-01 ± 9.0655E-06
^{235}U n,n'	^{235}U n,n'	1.9520E-01 ± 4.3250E-05
^{238}U n,n'	^{238}U n,n'	1.8882E-01 ± 2.1825E-04
^{235}U elastic	^{235}U n,n'	-1.6855E-01 ± 1.2801E-05

Fig. 7. Contributors to uncertainty in k_{eff} for IMF-005.

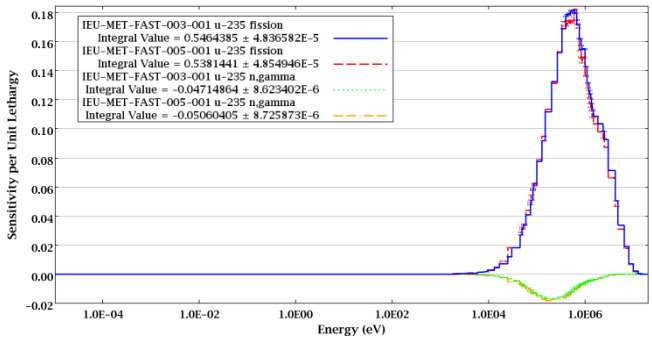

Fig. 8. ^{235}U sensitivities for IMF-003 and IMF-005.

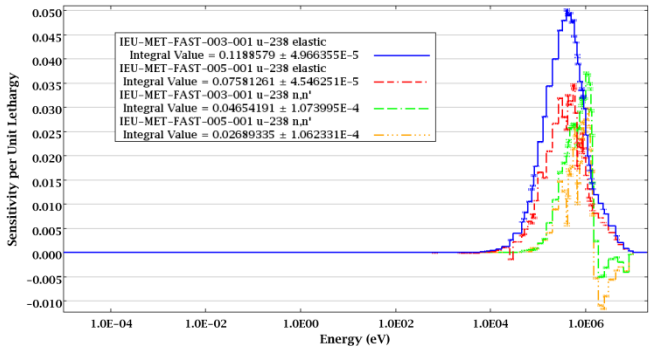

Fig. 9. ^{238}U sensitivities for IMF-003 and IMF-005.

CONCLUSIONS

The purpose of this paper is to provide three case studies for how the S/U tools of SCALE can be used to examine unexpected results from validation calculations. The case of PMF-005 is used to demonstrate that S/U analysis can provide quantitative support for the qualitative supposition that the presence of a unique nuclide in a calculation, in this case tungsten, is responsible for poor results. The tools can also be used to support the elimination of potential causes, as demonstrated with the HST-014 and HST-016 series involving gadolinium. Finally, TSUNAMI tools can also isolate areas of further investigation to explain poor results, as in IMF-005. In all three cases, the use of the S/U tools allowed more information to be gleaned from the cases already available in the validation suite. Use of these advanced tools can eliminate the need to select and model additional experiments to investigate outliers within a validation suite and can provide more confidence in the causes of unexpected results than could otherwise be demonstrated.

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