SCALE USER NOTICE
SCALE h1-poly incoherent elastic scattering can cause k-eff underprediction approaching 1% in criticality problems with polyethylene as the primary moderator
Feb 26, 2021

In SCALE 6.1.0-6.1.3 and 6.2.0-6.2.4 [1], h1-poly incoherent elastic scattering can cause k-eff underprediction approaching 1% in criticality problems with polyethylene as the primary moderator. **Note that there is no discrepancy for hydrogen-1 in h2o.**

Per the requirements of the Quality Assurance Plan for the SCALE Code System [2] and specifically the SCALE Procedure for Discrepancy Reports [3], this defect is being categorized as a Significant Software Error and is reported in this User Notice.

Director, SCALE Code Suite	Feb 26, 2021 Date

1. Summary

A defect has been found in SCALE's h1-poly incoherent elastic scattering which can cause k-eff underprediction approaching 1% in criticality problems with polyethylene as the primary moderator.

Code-to-code comparisons between MCNP and KENO-VI for the PU-MET-MIXED-002 (Pu metal mixed spectrum) benchmark in the ICSBEP Handbook uncovered a k-eff difference between the two codes that is increasing with increasing the amount of the polyethylene moderator. A discrepancy in the processing of h1-poly incoherent elastic scattering cross section was discovered between NJOY (used to generate ACE libraries for MCNP) and AMPX (used to create the SCALE libraries). The integrated cross sections for Incoherent Elastic Scattering differ by the number of scattering atoms in the chemical formula. The ENDF format manual does not state the need to divide the ENDF data by the number of scattering atoms and the number of scattering atoms is not present in the relevant thermal scattering section of the evaluation but in another section. **Note that there is no discrepancy for hydrogen-1 in h2o.**

2. Recommended Actions

Users should review their problems for the use of h1-poly as a significant moderator and understand the bias that is introduced. **Note that there is no discrepancy for hydrogen-1 in h2o.**

3. Details

This defect was originally reported by an internal user where the user was evaluating cases within the PU-MET-MIXED-002 ICSBEP benchmark. A simplified CSAS5 input (using the KENO V.a Monte Carlo transport code) that demonstrates the discrepancy is shown below. An MCNP input for the same model is also provided for comparison; the difference between calculated k-eff values for this model is approximately 500 ± 150 pcm.

```
=csas5 parm=()
hpoly test bed
ce_v7.1
read comp
 u 1  1  293 92235 26 92238 74 end
'
' polyethylene number densities input
' to highlight h-poly
'
 c      2  0  3.949960e-2 293 end
 h-poly 2  0  7.899920e-2 293 end
end comp
read parm
  htm=no
end parm
read geom
unit 1
  cylinder 2 1  22 2p2.54
  cuboid 0 1  4p22 2p2.54
unit 2
  cylinder 1 1  20 2p0.15
  cylinder 2 1  22 2p0.15
  cuboid 0 1  4p22 2p0.15
unit 3
  cylinder 2 1  22 2p0.9
  cuboid 0 1  4p22 2p0.9
global unit 4
  array 1 0 0 0
end geom
read array
 ara=1 nuz=11
  fill 1 2 3 2 3 2 3 2 3 2 1 end fill
end array
end data
end
```

```
988_hpoly
c cells
10   2   -0.91937  -2  -4             imp:n=1   $ layer 1
11   1   -19.05    -1   4  -5         imp:n=1   $ layer 2
12   2   -0.91937  -2   1   4   -5    imp:n=1
13   2   -0.91937  -2   5  -6         imp:n=1   $ layer 3
14   1   -19.05    -1   6  -7         imp:n=1   $ layer 4
15   2   -0.91937  -2   1   6   -7    imp:n=1
16   2   -0.91937  -2   7  -8         imp:n=1   $ layer 5
17   1   -19.05    -1   8  -9         imp:n=1   $ layer 6
18   2   -0.91937  -2   1   8   -9    imp:n=1
19   2   -0.91937  -2   9  -10        imp:n=1   $ layer 7
20   1   -19.05    -1   10 -11        imp:n=1   $ layer 8
21   2   -0.91937  -2   1   10  -11   imp:n=1
22   2   -0.91937  -2   11 -12        imp:n=1   $ layer 9
23   1   -19.05    -1   12 -13        imp:n=1   $ layer 10
24   2   -0.91937  -2   1   12  -13   imp:n=1
25   2   -0.91937  -2   13 -14        imp:n=1   $ layer 11
26   0              2  -15            imp:n=0
27   0              15                imp:n=0

c surfaces
1    rcc   0 0 0    0 0 18.86   20
2    rcc   0 0 0    0 0 18.86   22
4    pz   5.08  $ top layer 1
5    pz   5.38  $ top layer 2
6    pz   7.18  $ top layer 3
7    pz   7.48  $ top layer 4
8    pz   9.28  $ top layer 5
9    pz   9.58  $ top layer 6
10   pz   11.38 $ top layer 7
11   pz   11.68 $ top layer 8
12   pz   13.48 $ top layer 9
13   pz   13.78 $ top layer 10
14   pz   18.86 $ top layer 11
15   rpp  -22 22  -22 22  0 18.86

c data
m1   92235.80c   1.26903e-02
     92238.80c   3.56622e-02
m2   1001.80c    7.89992e-02
     6000.80c    3.94996e-02
mt2  poly.20t
kcode   5000   1   25   175


ksrc    0 0 9.43
```

Figure 1. A CSAS5 (Left) and MCNP (Right) H-POLY test input

Our investigations indicated that an unexpected difference occurs between KENO-VI and MCNP at higher polyethylene content. For example, PU-MET-MIXED-002 contains 5 cases, with case 1 having no polyethylene between plutonium plates and case 5 having one inch of polyethylene between the plates. The k-eff values calculated with the two codes are consistent for cases 1-3 but begin to deviate in cases 4 and 5, as illustrated in Figure 2, which shows the relative comparison of calculations (C) with MCNP and KENO to measurement (E). The energy average lethargy of fission (EALF) decreases by case, starting at 60 keV for case 1, 5 keV for case 2, 200 eV for case 3, 10 eV for case 4, and 2 eV for case 5.

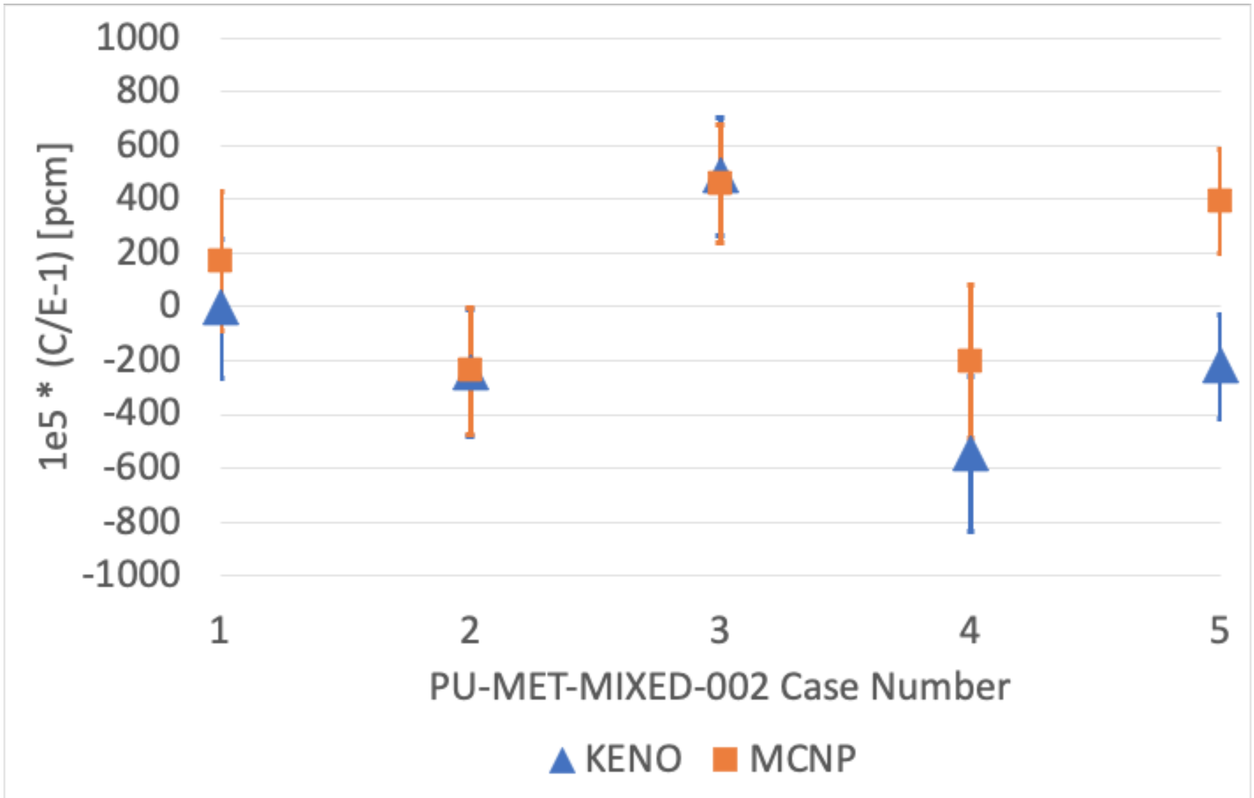

Figure 2. MCNP vs KENO PU-MET-MIXED-002 case comparison (uncertainty bars show evaluation uncertainty)

These inconsistencies between the MCNP and SCALE k-eff results originate from the differences between NJOY and AMPX in their polyethylene scattering cross sections, as illustrated in Figure 3. The AMPX incoherent elastic cross section (right) is a factor of two higher than the corresponding NJOY value, which combined with the consistent incoherent inelastic component (center) results in the inconsistent scattering cross section (left) between AMPX and NJOY.

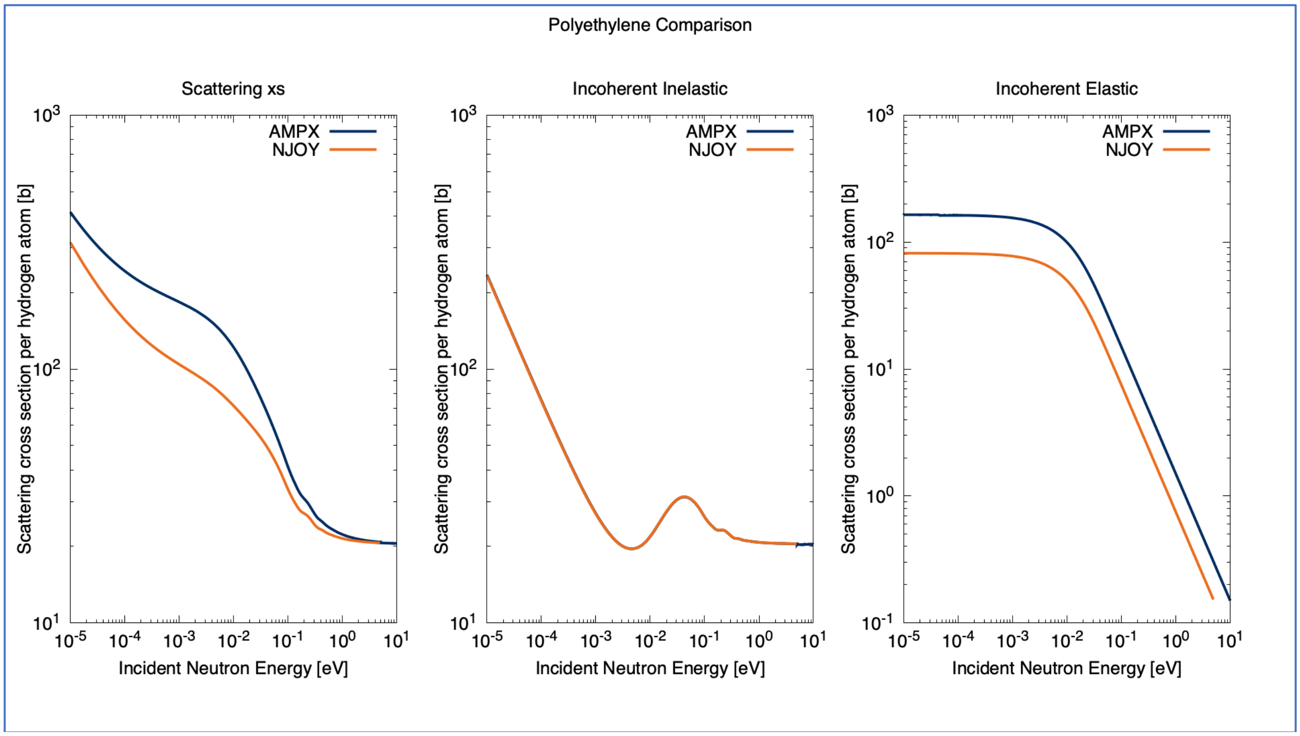

Figure 3. Polyethylene Scattering Cross Section comparison between AMPX and NJOY

Checklist for Significant Software Error Notification	
Item	**Description**
Software identification	- Code name: XSProc and all codes which rely on it (CSAS, MAVRIC, TRITON, TSUNAMI, and STARBUCS) - Version impacted: SCALE 6.2 (CCC-834) and subsequent updates 6.2.1, 6.2.2, 6.2.3, 6.2.4 - SCALE 6.1 and subsequent updates (6.1.1, 6.1.2, and 6.1.3)
Data library	ENDF/B-VI.8, ENDF/B-VII.0, ENDF/B-VII.1
Computing platform (Unix, Windows, Linux, etc.)	All
Description of the error	**SCALE h1-poly incoherent elastic scattering can cause k-eff underprediction approaching 1% in criticality problems with polyethylene as the primary moderator. Note that there is no discrepancy for hydrogen-1 in h2o.**
How was the error identified?	An ORNL internal user reported unexpected behavior related to code-to-code comparison between KENO and MCNP. Further investigation uncovered the underlying defect.
When does this error occur?	Any use of H-POLY incoherent elastic scattering cross section data from libraries based on ENDF/B-VI.8, ENDF/B-VII.0, and/or ENDF/B-VII.1.

Checklist for Significant Software Error Notification	
Item	**Description**
Potential impact of this error	The magnitude of the error is problem dependent. In terms of reactivity and impact on k_{eff}, the amount of H-POLY used will drive the k_{eff} underestimation. Larger dependence on H-POLY will increase the magnitude of the misprediction.
Frequency / likelihood of this error occurring	All systems that involve polyethylene (modeled as h-poly) will exhibit this error. The magnitude of the error depends on the system sensitivity to the 1H thermal scattering data. Generally, the effect should be small except for in thermal systems in which the polyethylene is providing the primary source of moderation.
How can users determine if this error affects their calculations?	The primary indication is the use of the h-poly thermal scattering law (TSL). This is nuclide ID 9001001 in SCALE 6.2 and 1901 in prior versions. The magnitude of the error is more difficult to determine as corrected data are not available. Test the sensitivity to h1-poly by replacing with the h1-freegas cross section.
What action should users take if this error affects them?	Assume underprediction in these systems based on running with the h1-poly CE library. For critical benchmark PU-MET-MIXED-002 case 5, 800 pcm was found. Users can evaluate the magnitude of the underprediction for their cases using a corrected CE h1-poly data file provided to users.
Is correction to code/data available?	SCALE 6.3.0 will include data processing corrections. A corrected CE h1-poly data file will be provided to users.
How to obtain/install correction	SCALE 6.3.0 will be announced to the user distribution list in 2021 when it is released. A corrected CE h1-poly data file will be provided to users through a future email to the SCALE user community. This data file could be used with any SCALE version within the 6.2 series and will be included in SCALE 6.3.0.

4. SCALE Quality Assurance Program

After the 2011 release of SCALE 6.1 [4], the SCALE Quality Assurance Program, associated procedures, and supporting infrastructure were substantially upgraded in 2013 as an essential starting point to SCALE modernization activities. As part of the ongoing modernization initiative, the SCALE team is continually seeking means of self-improvement.

5. References

1. W. A. Wieselquist, R. A. Lefebvre, and M. A. Jessee, Eds., SCALE Code System, ORNL/TM-2005/39, Version 6.2.4, UT-Battelle, LLC, Oak Ridge National Laboratory (2020).

2. B. T. Rearden, M. T. Sieger, S. M. Bowman, and J. P. Lefebvre, Quality Assurance Plan for the SCALE Code System, SCALE-QAP-005, Rev. 4, Oak Ridge National Laboratory (2013).

3. B. T. Rearden, J. P. Lefebvre, and S. M. Bowman, SCALE Procedure for Discrepancy Reports, SCALE-CMP-004, Rev. 5, Oak Ridge National Laboratory (2013).

4. SCALE: A Comprehensive Modeling and Simulation Suite for Nuclear Safety Analysis and Design, ORNL/TM-2005/39, Version 6.1, UT-Battelle, LLC, Oak Ridge National Laboratory (2011).