SCALE USER NOTICE
SCALE Criticality Safety Analysis Sequence 5S (CSAS5S) using continuous-energy cross sections with the legacy SOLN material input format can cause significant reactivity coefficient k_{eff} underprediction.

September 1, 2022

The SCALE legacy SOLN material composition input specification within the CSAS5S sequence in SCALE versions 6.2.2–6.2.4 [1] can cause significant k_{eff} underprediction only in continuous-energy (CE) calculations. Note that there is no discrepancy when using the contemporary "solution" material input format.

According to the requirements of the Quality Assurance Plan for the SCALE Code System [2], as well as the SCALE Procedure for Discrepancy Reports [3], this defect is being categorized as a *Significant Software Error* (SSE) as reported in this User Notice.

September 1, 2022

Director, SCALE Code Suite — Date

1. Summary

In SCALE 6.2.2–6.2.4, the use of the SOLN material composition input specification in the CSAS5S sequence with CE nuclear data can lead to significant underprediction of k_{eff}. This issue only occurs in the CSAS5**S** sequence, where the "S" denotes the search capability to find optimal moderation conditions. There is no issue with CSAS5, the standard criticality safety analysis, without the search capability. Additionally, this issue is triggered by the user's specification of the legacy SOLN input format instead of using the contemporary "solution … end solution" input approach. The use of the input shown in Figure 1 (left) leads to a significant underprediction of k_{eff}. **Note that there is no unexpected k_{eff} discrepancy when using the contemporary "solution" material input format or when performing multigroup (MG) transport. This user notice confirms the potential SSE that was identified to users via email from the SCALENEWS mailing list on May 13, 2022.**

2. Recommended Actions

Users should review their CSAS5S inputs; if they use a CE cross section library and the legacy SOLN material input specification, then their results may be affected. The k_{eff} calculation in the CSAS5S search can be confirmed by converting the input to CSAS5. If the k_{eff} results from the first CSAS5S calculation and CSAS5 are statistically equivalent, then the input is not affected by the issue.

3. Details

This defect was originally reported to scalehelp@ornl.gov by an external user. Below in Figure 1, a CSAS5S input (left) that is affected by this defect is shown next to its simplification to a CSAS5 input (right), which is not affected. The standard criticality analysis sequence, CSAS5 (without search), is never affected. To convert a CSAS5S input to CSAS5, users should need only to change the sequence name and remove the search block.

```
=csas5s
ISSUE WITH CSAS5S+CE+SOLN
ce_v7.1

read comp
' un
  solnuo2(no3)2  1  245 0 1 293.0 92235 6.5 92238 93.5  end
' h2o reflector
  h2o  2 1.00 293.0 end
end comp

read parameters
  gen=203
  npg=5000
  nsk=3
  htm=no
end parameters

read geometry
 global unit 1
  cuboid     1 1 50   0   4P1
  cuboid     2 1 1000 0   4P1
end geometry

read bounds
  all=refl
end bounds
end data

read search CRITICAL DIMENSION kef=0.89 more
  MODIFY unit=1 region=1 +x=1
' Constraints are multiplicative factors
  +con=10 -con=-0.999
end search
end
```

```
=csas5
NO ISSUE WITH CSAS5+CE+SOLN
ce_v7.1

read comp
' un
  solnuo2(no3)2  1  245 0 1 293.0 92235 6.5 92238 93.5  end
' h2o reflector
  h2o  2 1.00 293.0 end
end comp

read parameters
  gen=203
  npg=5000
  nsk=3
  htm=no
end parameters

read geometry
 global unit 1
  cuboid     1 1 50   0   4P1
  cuboid     2 1 1000 0   4P1
end geometry

read bounds
  all=refl
end bounds
end data
end
```

Figure 1. An erroneous CSAS5S sequence (left) and the equivalent functional CSAS5 sequence (right).

If the CSAS5S is defective, then the issue can first be observed in an erroneous mixing table, where hydrogen and oxygen elements are listed instead of their isotopes, as shown in Figure 2.

```
                                        mixing table

 mixture =     1          density(g/cc) =  1.3273             temperature(K) =    293.00
    nuclide   atom-dens.   wgt. frac.     za      awt          temp     nuclide title
       1000  6.16187E-02  7.77002E-02    1000     1.0079       293.00     h @ 293K
       7014  1.23607E-03  2.16542E-02    7014    14.0031       293.00     n-14 @ 293K
       7015  4.51573E-06  8.47418E-05    7015    15.0001       293.00     n-15 @ 293K
       8000  3.08094E-02  6.16682E-01    8000    15.9994       293.00     o @ 293K
       8016  4.96046E-03  9.92609E-02    8016    15.9949       293.00     o-16 @ 293K
       8017  1.88957E-06  4.01850E-05    8017    16.9991       293.00     o-17 @ 293K
      92235  4.08009E-05  1.19976E-02   92235   235.0439       293.00     u-235 @ 293K
      92238  5.79492E-04  1.72581E-01   92238   238.0508       293.00     u-238 @ 293K

 mixture =     2          density(g/cc) = 0.99820             temperature(K) =    293.00
    nuclide   atom-dens.   wgt. frac.     za      awt          temp     nuclide title
       1001  6.67431E-02  1.11899E-01    1001     1.0078       293.60     h-1 @ 293.6K
       1002  7.67722E-06  2.57227E-05    1002     2.0141       293.60     h-2 @ 293.6K
       8016  3.33627E-02  8.87716E-01    8016    15.9949       293.00     o-16 @ 293K
       8017  1.27087E-05  3.59385E-04    8017    16.9991       293.00     o-17 @ 293K
```

Figure 3. Faulty CSAS5S mixing table listing elemental hydrogen and oxygen (highlights added).

Because the elemental hydrogen and oxygen do not match data in the CE library, zero cross sections are introduced (i.e., listed as IN-MEMORY), providing further notice of unexpected and incorrect behavior. This results in dramatic loss of moderation and reactivity for this case, with a k_{eff} underprediction of ~45%. Only O-18 (8018) is expected to be listed as IN-MEMORY when using Evaluated Nuclear Data File (ENDF)/B-VII.0 or ENDF/B-VII.1 libraries distributed with SCALE.

```
Processing nuclide 1 of 10, ID= 1000 at T=  293.00K
 Temperature Independent CE XS File: IN-MEMORY
   Temperature Dependent CE XS File: IN-MEMORY
…
 Processing nuclide 4 of 10, ID= 8000 at T=  293.00K
 Temperature Independent CE XS File: IN-MEMORY
   Temperature Dependent CE XS File: IN-MEMORY
```

Figure 4. Erroneous CSAS5S cross section data edits for CE mode.

Table 1. Checklist for SSE notification

Item	Description
Software identification	- Code name: CSAS5S (CSAS5 Search Sequence) - Version impacted: SCALE 6.2 (CCC-834) updates 6.2.2, 6.2.3, 6.2.4
Data library	CE ENDF/B-VII.0, ENDF/B-VII.1 cross sections
Computing platform (Unix, Windows, Linux, etc.)	All
Description of the error	**For CE calculations performed using the legacy SOLN material format, the CSAS5S sequence in SCALE versions 6.2.2–6.2.4 may show significant k_{eff} underprediction. Note that there is no discrepancy in CSAS5, or when using the "solution … end solution" input format, or when using MG transport.**
How was the error identified?	An external user reported unexpected behavior. Further investigation uncovered the underlying defect.
When does this error occur?	The error occurs when using CSAS5S with the CE cross section library and the legacy SOLN material input specification.
Potential impact of this error	The magnitude of the error is problem dependent. Typically, in terms of reactivity and impact on k_{eff}, the amount of moderation (e.g., water) in the problem will drive the extent of k_{eff} underestimation.
Frequency/likelihood of this error occurring	This error can occur for any problem using CSAS5S with CE cross sections and the legacy SOLN material input format.
How can users determine whether this error affects their calculations?	The primary indication is the output containing elemental hydrogen and oxygen listed in the mixing table and zero IN-MEMORY cross sections being listed.
What action should users take if this error affects them?	Users affected by this error should assume underprediction in these systems. Users can evaluate the magnitude of the underprediction for their cases by converting the legacy SOLN material input to the contemporary "solution … end solution" material input format.
Is correction to code/data available?	Correction will not be available, as 6.2.4 was the last release in the 6.2 series. Also, please note that CSAS5S was removed from SCALE in the 6.3 series for two main reasons: (1) CSAS5S was one of the legacy sequences not fully modernized in SCALE 6.2, and the maintenance burden was high relative to the capabilities, and (2) the parametric study option in Sampler is the preferred way to investigate optimum moderation conditions, as it is both more robust and flexible.
How to obtain/install a correction	Convert from the legacy SOLN material input format to the contemporary "solution … end solution" format to correct the problem.

4. SCALE Quality Assurance Program

After SCALE 6.1 [4] was released in 2011, the SCALE Quality Assurance Program, the associated procedures, and the supporting infrastructure were substantially upgraded. These upgrades were implemented in 2013, and they represent an essential starting point for SCALE modernization activities. As part of the ongoing modernization initiative, the SCALE team is continually seeking means of 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).