SCALE User Notice

March 8, 2018

The KENO V.a Monte Carlo code in SCALE 6.1–6.2.2 does not include an input check to ensure compliance with the requirement that albedo boundary conditions other than vacuum (e.g., mirror, periodic, white) are only applied to cuboidal outer shapes. Users who do not follow this requirement per the user documentation may generate non-conservative k_{eff} results without warning.

Per the requirements of the *Quality Assurance Plan for the SCALE Code System* [1] and specifically the *SCALE Procedure for Discrepancy Reports* [2], this issue is being categorized as a *Significant Software Error* and is reported in this User Notice.

Summary

In all versions of SCALE, the Monte Carlo code KENO V.a only implements the use of non-vacuum albedo boundary conditions (e.g., mirror, periodic, white) when the outermost geometry region of the model is a cuboidal region. This limitation is noted in the user documentation in the section on *Albedo data,* where it is stated that "Albedo boundary conditions are applied only to the outermost region of a problem. In KENO V.a this geometry region must be a rectangular parallelepiped"[3][4].

It was recently discovered that—beginning with the release of SCALE 6.1 in 2011—KENO V.a will accept non-compliant input that specifies albedo boundary conditions for non-cuboidal outer shapes and will then attempt to complete the calculation. For example, a user can specify a cylinder as the outermost region and add a mirror boundary condition on the top or bottom to effectively double the volume of the system considered. A user could also add a mirror boundary condition to both the top and the bottom of the cylinder to simulate a bounding case of an infinite system. While these scenarios are accepted and perform as expected in KENO-VI, *KENO V.a requires the addition of a cuboidal region (typically an empty void region) to enable the use of these albedo boundary conditions*.

For calculations using KENO V.a in SCALE 6.1–6.2.2 with non-compliant input in which albedo boundary conditions are applied but *without* the required cuboidal outermost region, the calculation will proceed without warning, and an underestimation of k_{eff} often results. The magnitude of underestimation in k_{eff} can vary widely, depending on the system modeled and the desired boundary conditions, but it **can exceed several percent in k_{eff}**.

It is strongly recommended that users who rely on albedo boundary conditions in KENO V.a review their input models to ensure that the outermost region is a cube or cuboid, per the documentation requirement. Note that input models that were generated and applied with SCALE 6 and earlier versions that included the check for the cuboidal outer boundary will continue to produce the expected results with SCALE 6.1–6.2.2.

In testing the extent of this issue by placing mirror boundary conditions on non-cuboidal outer shapes, it was found that cylinders oriented along the x-, y-, or z-axis most often produce non-

conservative results without warning. The calculation will terminate prior to completion for cases in which a sphere is the outermost shape. The calculation will terminate with an error message for cases in which a hemicylinder or hemisphere is the outermost shape. The calculation performs as expected for cases in which a cube or cuboid is the outermost shape.

This issue applies to all SCALE 6.1–6.2.2 sequences that implement KENO V.a, including CSAS5, TSUNAMI-3D-K5, T5-DEPL, and STARBUCS. No other SCALE sequences are impacted by this issue. The error condition for the attempted use of albedo boundary conditions on non-cuboidal outer shapes in KENO V.a will be restored in the pending release of SCALE 6.2.3, thus preventing users from inadvertently entering non-compliant input.

Recommended Actions

Users should review all KENO V.a calculations performed with SCALE 6.1–6.2.2. **Models using spherical or cylindrical outer boundaries *and* non-vacuum albedo boundary conditions are non-compliant with the user documentation and must be considered for non-conservative k_{eff} results.** The addition of a void-filled cuboid as the outer boundary of the problem will result in the correct application of the requested boundary conditions. The results from the two models can be compared to evaluate the impact of the non-compliant input.

Details

KENO V.a supports the specification of boundary conditions via "face codes" and "albedo names." The face codes were developed with the requirement that a cuboid be used as the outer boundary of a KENO V.a model, thus allowing users an array of combinations of the ±X faces, the ±Y faces, and the ±Z faces. No face codes were ever implemented for spherical or cylindrical outer boundaries. The albedo names declare the boundary condition to be used on the specified face. This input is provided in the "BOUNDS" input block. An example specification for a mirror (reflective) boundary condition on the positive X face of a model is "+xb=mirror."

Beginning with SCALE 6.1, the KENO V.a input check for the cuboidal outer boundary when albedo boundary conditions are applied was partially disabled. Only spherical and cylindrical outer boundaries were excluded from the check; hemispheres and hemicylinders are still not allowed as the outer boundary of the model. The interpretation of the face codes for non-cuboid outer boundaries led to the potential that a user-specified non-vacuum boundary condition would not be applied.

Internal to the code, the face codes are stored in a data array in sequential order from 1–6, as: +X, -X, +Y, -Y, +Z, -Z—the same as the data ordering for the geometry specification of a cuboid. Because KENO V.a is designed exclusively for the boundary conditions to be applied as a six-sided cuboid, the face codes have a one-to-one correspondence to the geometry regions. When a non-vacuum boundary is erroneously applied to a non-cuboidal outer region, then the following behavior results.

1 The +X face code is applied to the surface of a sphere or the round surface of a cylinder.

2 A check in the code prevents the application of a reflective or periodic boundary condition to a round surface, preventing execution in this case.
3 The -X face code is applied to the "top" surface of a cylinder (+Z for zcylinder or cylinder, +X for xcylinder, +Y for ycylinder), and the +Y face code is applied to the "bottom" surface of a cylinder (-Z for zcylinder or cylinder, -X for xcylinder, -y for ycylinder).

These two face codes are ignored for a sphere, and the face codes for the -Y and ±Z faces are ignored for cylinders. In practice, attempting to specify the ends of the cylinder as reflective boundary conditions leads to the following scenarios:

- cylinder/zcylinder, with +Z and -Z set to reflective: no reflective boundary conditions
- ycylinder, with +Y and -Y set to reflective: the -Y face is reflective (by the +Y input), and the other two surfaces are vacuum
- xcylinder, with +X and -X set to reflective: the job exits and issues an error message because of the attempt to apply a reflective boundary condition to the side of a cylinder (via the +X input)

Checklist for Significant Software Error Notification

Item	Description
Software Identification	Code name: KENO V.a and associated computational sequences CSAS5, T5-DEPL, TSUNAMI-3D-K5, and STARBUCS Version impacted: SCALE 6.1 (CCC-785) and subsequent updates 6.1.1, 6.1.2, and 6.1.3 SCALE 6.2 (CCC-834) and subsequent updates 6.2.1 and 6.2.2 No other codes or versions are impacted
Data Library	Issue is not associated with a particular data library
Computing platform (Unix, Windows, Linux, etc.)	Generic to all computing platforms
Description of the error	KENO V.a in SCALE 6.1–6.2.2 does not include an input check to ensure compliance with the requirement that albedo boundary conditions other than vacuum (e.g., mirror, periodic, white) are only applied to cuboidal outer shapes, and users who do not follow this requirement per the user documentation may generate non-conservative k_{eff} results without warning.
How was the error identified?	A user submitted an inquiry to scalehelp@ornl.gov identifying this issue, which was subsequently confirmed by the SCALE team.
When does the error occur?	For calculations with KENO V.a in SCALE 6.1–6.2.2 with non-compliant input in which albedo boundary conditions are applied but *without* the required cuboidal outermost region, the calculation will proceed without warning, and an underestimation of k_{eff} often results.

Potential impact of error	The magnitude of underestimation in k_{eff} can vary widely, depending on the system modeled and the desired boundary conditions, but it can exceed several percent in k_{eff}.
Frequency / likelihood of error occurring	The error will never be encountered for input that is compliant with the user documentation. The error may occur when non-compliant input is provided by the user and not rejected by the code.
How can users determine if error affects their calculations?	Users can search for KENO V.a input files with non-vacuum face codes in the Boundary block. For cases in which non-vacuum face codes are applied, users should confirm that the outermost region of the geometry is a cube or cuboid. When non-vacuum albedo boundary conditions are applied *and* the outmost region is *not* a cube or cuboid, then the user's calculations may be affected.
What action should users take if error affects them?	The addition of a void-filled cuboid as the outer boundary of the problem will result in the correct application of the requested boundary conditions. The results from the two models can be compared to evaluate the impact of the non-compliant input.
Is correction to code/data available?	SCALE 6.2.3 will implement the required input data check to prevent any further use of non-compliant input. Users must correct any non-compliant input for the calculation to proceed.
How to obtain/install correction	Users can check for and correct any non-compliant input immediately. SCALE 6.2.3 will be announced to the user distribution list when it is released.

SCALE Quality Assurance Program

After the 2011 release of SCALE 6.1, 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. While no quality assurance program is foolproof, it is more likely that this issue would have been detected under the updated program prior to distribution.

References

1. 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).
2. 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).
3. *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).
4. B. T. Rearden and M. A. Jessee, Eds., *SCALE Code System*, ORNL/TM-2005/39, Version 6.2.2, UT-Battelle, LLC, Oak Ridge National Laboratory (2017).