DISCLAIMER:

The following appendix is taken from the Master of Nuclear Engineering project of Jesse C. Holmes, "Development of ENDF Thermal Neutron Scattering Libraries for Silicon Dioxide and MCNP Criticality Testing with an ICSBEP Benchmark," published in May 2011 at North Carolina State University under the direction of Dr. Ayman I. Hawari. The full document is available by request from Dr. Holmes (Jesse.Holmes@unnpp.gov). Minor edits to the original text have been made for clarity. This appendix describes issues with generating thermal neutron scattering data for mixed moderators in NJOY. All of the content refers to the most recent versions of the NJOY 99 code, modules, and manual available at the time of publication in May 2011. The full project document (with this appendix) was provided by request to the NJOY team at LANL in November 2013. Based on recent discussions with NJOY personnel and the nuclear data community at mini-CSWEG (BNL, May 7-8, 2015) and WPEC SG42 (OECD/NEA, Paris, France, May 18-19, 2015), the author believes it likely that the issues discussed here have not been resolved in any version of NJOY 99, NJOY 2012, or in any published updates. However, the author has not personally verified this by testing or by examining source code for recent versions and updates of NJOY and its modules.

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Appendix A

Notes on Using the NJOY Code for Mixed Moderators

Several problems exist with the LEAPR module of NJOY 99 that prevent the correct calculation of thermal neutron scattering cross section data for mixed moderators with stoichiometry other than 1:1. LEAPR uses a value of 1 for the secondary scatterer control flag MSS on Card 6, Entry 5, for the inelastic routine even if a value greater than 1 is entered. (The value for the MSS flag is printed correctly in the produced library tape, but it is not incorporated correctly in calculations). This entry should tell LEAPR how many secondary scatterer atoms exist in the molecule (or in a representative stoichiometric unit). For the mixed moderator SiO_2, normalized to silicon, there are two secondary scatterer atoms. For any mixed moderator, the values for $S(\alpha,\beta)$ and the subsequently calculated inelastic cross sections will be wrong unless there is actually only one secondary scatterer atom in the molecule (or stoichiometric unit). To compensate for this issue (without source code modification), it is necessary to scale the secondary scatterer free cross section inputted to LEAPR by the actual number of secondary scatterer atoms present. For inelastic scattering, this cross section is used in properly normalizing $S(\alpha,\beta)$ to the primary scatterer.

Another problem in LEAPR exists in the routine for calculating elastic cross sections. The Debye-Waller coefficient for a single atomic species j is given by $W_j = \frac{\lambda_j}{Ak_BT}$. The *effective* Debye-Waller coefficient for SiO_2 is given by $W = \frac{1}{3}\left(\frac{\lambda_{Si}}{A_{Si}k_BT}\right) + \frac{2}{3}\left(\frac{\lambda_O}{A_O k_BT}\right)$. The effective W for any molecule (or stoichiometric unit) within the interatomic structure must be calculated to appropriately weight the W_j values for each atom type j by stoichiometry such that W is

associated with a single "effective" atom. Currently, in calculating the effective W for mixed moderators, LEAPR automatically assumes 1:1 stoichiometry for a molecule (or stoichiometric unit) with two atoms types (regardless of the inputted values for NPR on Card 5, Entry 3, and MSS on Card 6, Entry 5, telling LEAPR how many primary and secondary scatterer atoms there are, respectively). LEAPR simply averages the two W_j values to solve for the effective W.

Information for the crystallographic structure factors f_i and other required parameters must be hard-coded into LEAPR to calculate coherent elastic cross sections for a particular crystal structure (this is not required for incoherent elastic cross sections). For a structure with non-1:1 stoichiometry, a special procedure must be used to ensure the elastic cross sections are calculated correctly (if the issue is not resolved through source code modification). The Card 13, Entry 3, value for TBETA for each atomic species must compensate for the 1:1 averaging of the W_j values. TBETA effectively multiplies λ_j by whatever value is inputted (the default is 1). For the case of SiO_2, TBETA for Si would need to be entered as 0.666667 and TBETA for O would need to be entered as 1.333333. LEAPR will then divide each W_j by two and add the results together. With the adjusted TBETAs, the correct value for the effective W will be generated. However, this procedure will cause the inelastic calculations to be wrong. To produce both elastic and inelastic data correctly (without source code modification), LEAPR must be run twice independently, once with TBETAs not scaled and once with TBETAs stoichiometrically scaled. The elastic cross section data in the form of $E\sigma(E)$ written by LEAPR will have to be cut from the output tape of the run with the scaled TBETAs and spliced into the output tape of the run with TBETAs not scaled, replacing the incorrect elastic data. A tape with correct elastic data and $S(\alpha,\beta)$ data will now exist that can be processed by THERMR. Care must be taken to manually verify and correct all flags and line numbers printed in the File 7 tape due to the splicing process.

Incorrect guidance exists for use of the Card 9, Entry 5, NMIX flag (number of atom types in a mixed moderator) in the ACER module. A non-default value of NMIX is only used for mixed moderator libraries such as benzene (C_6H_6), BeO, and now SiO_2. The output tape of THERMR is a full ENDF file for the primary scatterer with the mixed moderator thermal cross section data associated with the whole molecule (or the whole stoichiometric unit). The secondary scatterer is treated as having a zero cross section. The ACER manual states that NMIX specifies the number of different kinds of atoms found in the mixed moderator being evaluated. In other words, according to examples given in the manual, NMIX should equal 2 for both BeO and benzene (C_6H_6), since each has only two kinds of atoms, and NMIX should equal 1 (the default value) for all other materials (which are not mixed moderators). This guidance is misleading. NMIX should actually equal the total number of atoms in the molecule (or stoichiometric unit) divided by the number of primary scatterer atoms in the molecule (or stoichiometric unit). This is 2 for both BeO and benzene. Consequently, the misguidance has no impact in these cases. However, for SiO_2 (normalized to silicon), the value of NMIX should equal 3. ACER will properly read and process NMIX = 3. If SiO_2 is normalized to oxygen (which actually has a larger nuclear coherent cross section than silicon), then NMIX should equal 1.5. However, NMIX can only accept integer values without source code modification. Therefore, SiO_2 is normalized to silicon to avoid this issue.

The purpose of NMIX is to compensate for the fact that the scattering data tabulated in thermal ACE libraries is associated with every atom in the mixed moderator equivalently, regardless of its stoichiometry and identity as a primary or secondary scatterer. (Thermal ACE libraries do not separately treat the secondary scatterer atoms as having zero cross sections as THERMR does.) In other words, the same scattering data in the thermal ACE library is read

each time the library is called for any atom in the mixed moderator material. To adjust for this oversampling, ACER takes the THERMR cross sections for the mixed moderator and divides them by NMIX, which is 3 in the case of SiO_2. Thus, after appropriate adjustment, the ACE library actually contains cross sections that are $\frac{1}{NMIX}$ of the cross sections produced by THERMR. This will ensure that a neutronics code (such as MCNP) using the ACE library applies correct cross sections (when the cross sections are oversampled by a factor of NMIX).

Every published ENDF mixed moderator thermal library that was produced with LEAPR before SiO_2 (where oxygen is chosen to be the secondary scatterer for the reason discussed above) has had only one secondary scatterer atom in the molecule (or stoichiometric unit). In the case of benzene, the Gasket code was used, and the $S(\alpha, \beta)$ values for carbon and hydrogen were computed separately (where each was treated as a primary scatterer) and then appropriately weighted and combined to form mixed moderator $S(\alpha, \beta)$ data normalized to hydrogen. Therefore, the production of the SiO_2 mixed moderator thermal library with LEAPR may be the first instance where any of the discussed issues, including those for ACER, were relevant.