A Study of the Covariance Data in ENDF/B VIII.0 for Low Z Isotopes

D. Kent Parsons – Group XCP-5, Los Alamos National Laboratory -- LA-UR-21-29001

Introduction

30 group covariance data have been produced for analysis and checking for H1, H2, He4, Li6, Li7, Be9, B10, B11, C12, C13, N15, O16, and the JENDL O16. (H3, He3, Be7, N14, O17, and O18 do not have any covariance data.) In processing these evaluations, cross section (MF 33) covariance data was produced for the cross sections given in the evaluations. NJOY routine ERRORR produces the multi-group covariances.

A big combined covariance matrix was also produced for each isotope. All of the processing calculations used "absolute" covariance matrices, not relative covariances (ie., relative to the means of the cross sections). Nor were correlation matrices (ie. using covariances and the standard deviations of the cross sections) used. The big combined covariance matrix is important, since it would be used to produce replica cross section data and libraries for all of the reactions with covariance data.

Testing the MF 33 Covariance Data

Two methods were used to test the covariance matrices. An eigenvalue decomposition was performed on the big combined covariance matrix for each isotope. For example, the big covariance matrix for Be9 is 240x240 with the following reactions included – total (mt 1), elastic (mt 2), n2n (mt 16), ng (mt 102), np (mt 103), nd (mt 104), nt (mt 105), and nalpha (mt 107). Each sub-block of the big matrix is 30x30. Quite a few of the sub-blocks are 0.0.

All of the isotopes listed above were free from any "large" negative eigenvalues. The negative eigenvalues were all close to 0.0 and several orders of magnitude smaller than the dominant large positive eigenvalues.

The other test was a check of the covariance restraint imposed by having a total cross section and a bunch of partial cross sections which sum to the total cross section. This covariance constraint requires that the covariance block of the total cross section be equal to the sum of all of the other cross sections' covariance block matrices.

In 30x30 sub-block matrix terms (using data from Be9), the covariance constraints can be expressed as:

cov11 – cov12 – cov116 –cov1102 – cov1103 – cov1104 – cov1105 – cov1107 = 0.0

cov21 – cov22 – cov216 – cov2102 – cov2103 – cov2104 – cov2105 – cov2107 = 0.0

cov161 – cov162 – cov1616 – cov16102 – cov16103 – cov16104 – cov16105 – cov16107 = 0.0

cov1021 – cov1022 – cov10216 – cov102102 – cov102103 – cov102104 – cov102105 – cov102107 = 0.0

cov1031 – cov1032 – cov10316 – cov103102 – cov103103 – cov103104 – cov103105 – cov103107 = 0.0

cov1041 – cov1042 – cov10416 – cov104102 – cov104103 – cov104104 – cov104105 – cov104107 = 0.0

cov1051 – cov1052 – cov10516 – cov105102 – cov105103 – cov105104 – cov105015 – cov105107 = 0.0

cov1071 – cov1072 – cov10716 – cov107102 – cov107103 – cov107104 – cov107105 – cov107107 = 0.0

where cov12 = the covariance between mt 1 and mt 2,

cov21 = the transpose of cov12,

cov11 = the covariance matrix of the 30g mt 1 cross sections with each other,

covnm = similarly for mt combinations of reactions n and m.

The zeros on the RHS of the equations are understood to be 30x30 block matrices will all elements equal to or nearly equal to 0.0.

These covariance constraints are satisfied for all 30 groups for H1, He4, Li7, Be9, B11, N15, and the Japanese O16. They are satisfied ONLY in the higher energy groups (and NOT in the lower energy groups) for H2, B10, and C12. The common factor in the B10, C12, and O16 evaluations is that the covariance for inelastic (mt 4) is defined as a combination of all of the other covariances.

The problem is that inelastic (mt 4) cross sections exist only above some threshold energy (for C12, it is 4.812 MeV) – and are 0.0 at lower energies. Therefore, the covariances for inelastic (mt 4) cross sections must also be 0.0 at lower energies. This means that ERRORR in NJOY can **NOT** impose the covariance constraint on any cross sections in the lower energies with an inelastic (mt 4) covariance definition. Similarly, H2 hits a similar threshold limitation since its covariance constraints are defined with n2n (mt 16) cross sections.

Li6 and C13 have a different covariance constraint problem. They do not specify any cross terms between reactions. In fact, Li6 only specifies (within reaction) covariance data for elastic (mt 2) and nt (mt 105). C13 only specifies elastic (mt 2) and inelastic (mt 51). Therefore, any user would have to make some sort of assumption about the across reaction correlations to use these data to sample cross sections (otherwise, the sampled cross sections will not balance between total and the sum of the partials).

For example, the user could allow changes in elastic (mt 2) and then impose exactly the same changes (in magnitude) into the total (mt 1) cross sections. Such a common-sense approach preserves cross section balance. A more general approach would be to change the evaluation file to define covariance data for the total (mt 1) cross section in terms of the other cross sections.

Covariance Data for mubar, MF 34, MT 2

Of all the low Z isotopes surveyed, only O16 and JO16 have MF 34, MT 2 mubar uncertainties, though the O16 has some very large pointwise values at energies in the MeV range. These uncertainties are larger than the maximum allowable range for mubar data (between -1.0 and 1.0). The ENDF/B VIII.0 version of O16 also has unrealistically high values of the covariance at lower energies. This low energy problem has been fixed at Los Alamos and a correction is being prepared for ENDF/B.

Summary

An extensive verification test of evaluated low Z reaction rate covariances has been carried out at Los Alamos. The good news was that there were no significant negative eigenvalues in any of the covariance data sets. The bad news was that some of the data sets do not preserve the covariance constraint condition that the total (mt 1) covariance matrix must be equal to the sum of all of the partial cross section covariance matrices. For Li6 and C13, two simple solutions are proposed which would satisfy the constraint. Covariances for H2, B10, C12, and O16 require further corrections to meet the constraint.