
Brookhaven
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U.S. DEPARTMENT OF
ENERGY
TSL MAT number problems
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Three open TSL library trackers

#1 - O in BeO U in UO2: MAT numbers for thermal scat.

#7 - MAT numbers for U(UO2) and O(UO2) do not agree with ENDF manual

#16 - Overloaded MAT numbers / misassigned MAT numbers for Al2O3

This is a simple fix, right?

right?

We ran out of MAT numbers

ENDF-102, page 12:

For mixtures, compounds, alloys, and molecules (evaluations using the thermal scattering law (TSL) formats in Chapter 7), MAT numbers between 1 and 99 are assigned on a special basis (see Appendix C).

but…

- ENDF/B-VIII.0 has 33 TSL evaluations
- ENDF/B-VIII.1 already has 50 TSL evaluations
- NCrystal database has 213 evaluations

What to do?

Option #1: stop using ENDF and cut over to GNDS

Option #2: kludge the MAT numbers

Kludging the MAT numbers

Current MAT numbers use the FORTRAN **`I4`** format

Option #2.1: we change to the FORTRAN **`A4`** format and reserve 0-99 and all alphanumeric MAT designators for TSL evaluations

- This is potentially disruptive, depending on how many legacy codes depend on MAT being an integer
- Allows 36^4-900=1,678,716 TSL MAT designators

Option #2.2: we allow TSL evaluations to use all numbers 0-9999

- This is similar to how we handle the same issue in the decay sublibrary
- Allows 9999 TSL MAT designators

Kludging the MAT numbers should work

MAT Numbers are used in surprisingly few places:

- End of line designators (so we can put the punchcards back in order)
- HSUB (because ENDF doesn't have proper metadata support)
- Cross material references in covariance matrices
  - As ENDF has no support for TSL covariances (unlike GNDS), we don't need to change anything here

The (sub)options

Option #2.1

- “MAT number” -> “MAT designator”
- Chapter 1, change all ENDF formats to use the FORTRAN **`A4`** format, plus associated discussion
- Update the HSUB format (it is free text already)
- Update the TSL example
- Add note in the covariance chapters about not changing MAT numbers here
- Appendix A summary table
- Appendix C now can be made to work

Option #2.2

- “MAT number” -> “MAT designator”
- Chapter 1 update rules
- Appendix C now can be made to work

The (sub)options

Option #2.1

- “MAT number” -> “MAT designator”
- Chapter 1, change all ENDF formats to use the FORTRAN **`A4`** format, plus associated discussion
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- Add note in the covariance chapters about not changing MAT numbers here
- Appendix A summary table
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Option #2.2

- “MAT number” -> “MAT designator”
- Chapter 1 update rules
- Appendix C now can be made to work

(Thank you for this one, Wim!)

Option #2.2 causes the least disruption…

Merge request #10 “A better MAT number rule”

0.4.1 Material (MAT, MOD)

A ***material*** may be a single nuclide, a natural element containing several isotopes, or a mixture of several elements (compound, alloy, molecule, *etc.*). A single isotope can be in the ground state or an excited (or isomeric) state. Each material in an ENDF library is assigned a unique identification number, designated by the symbol MAT, which ranges from 1 to 9999.[11]

The assignment of MAT numbers for ENDF/B libraries is made on a systematic basis assuming uniqueness of the four digit MAT number for a material. A material will have the same MAT number in each sub-library (incident neutrons, incident charged particles, *etc.*) with the exception of decay data (NSUB=4) and thermal neutron scattering (NSUB=12) sublibraries:

NSUB≠4,12: One hundred MAT numbers (Z01-Z99) have been allocated to each element Z, through Z = 98. Natural elements have MAT numbers Z00. The MAT numbers for isotopes of an element are assigned on the basis of increasing mass in steps of three, allowing for the ground state and two metastable states.[12] In the ENDF/B files, which are application oriented, the evaluations of neutron excess nuclides are of importance, since this category of nuclide is required for decay heat applications. Therefore, the

[11] The strategy for assigning MAT numbers for ENDF/B libraries is described here; other libraries may have different schemes.

[12] This procedure leads to difficulty for the nuclides of xenon, cesium, osmium, platinum, *etc.*, where more than 100 MAT numbers could be needed and some decay data where more than two isomeric states might be present.

11

lightest stable isotope is assigned the MAT number Z25 so that the formulation can easily accommodate all the neutron excess nuclides.

For the special cases of elements from einsteinium to lawrencium (Z≥ 99) MAT numbers 99xx are assigned, where xx = 30, 25, 20, 15, and 12 for elements 99 to 103 respectively; such a scheme covers all known nuclides with allowance for expansion.

NSUB=4 As the total number of known isotopes as given in the decay sublibrary exceeds what can be accomodated with the above scheme, we adopt a simpler scheme. All materials are ordered by Z*1000000 + A*1000 + LIS and the MAT number is the material's position in this list. For example, the neutron has MAT=1, ^{1}H has MAT=2, ^{2}H has MAT=3, etc.

NSUB=12 For mixtures, compounds, alloys, and molecules (evaluations using the thermal scattering law (TSL) formats in Chapter 7), all MAT numbers (1 - 9999) are assigned on a special basis (see Appendix C).

The above conventions are adopted in ENDF/B libraries and are recommended (but not mandatory) in other libraries in ENDF-6 format.

I have not revised appendix C, want to wait until know full scope of TSL changes…

I really hope you all like this format, since I accidentally merged it

The master branch is now locked so that I can’t do that again