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Author(s):	Solomon, Clell Jeffrey Jr. Bates, Cameron Russell Marcath, Matthew James
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MCNP Intrinsic Source Constructor (MISC): A User's Guide

Clell J. (C.J.) Solomon, XCP-2, csolomon@lanl.gov

Cameron R. Bates, XCP-7, batesca@lanl.gov

Matthew J. Marcath, XCP-7, marcath@lanl.gov

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1 Introduction

The *MCNP Intrinsic Source Constructor* (MISC) facilitates the construction of MCNP source definition cards for radioactive materials. Given a material nuclide specification, either weight or atom fractions of those nuclides, and either a weight or atom density of the material, MISC will construct the source spectrum distribution of a specified particle type. MISC also calculates the absolute number of particles emitted per second per unit mass or volume. Furthermore, if decay chain information is available in the data sets selected by the user, the initial isotopes specified by the user can be approximately decayed to the resulting isotopes after a specified amount of time.

2 Data Files

The data for radioactive particle emissions in MISC come from many sources [1, 2, 4, 5, 8]. Each source of data differs in the individual line intensities of the emitted radiation type. **The user should take precaution in that every data set may not applicable to their specific problem.** The current data files contained with the MISC utility are summarized in Table 1.

Three different types of data files exist for use with MISC: 1) natural abundance and mass data files, 2) radioactive decay chain data files, and 3) radioactive particle emission data files. The natural abundance and mass data files are used for proper conversion of specified mass/atom fraction information into atom/mass fractions. The radioactive decay chain data files contain the half lives, decay constants, daughter isotopes, and branching ratios of all isotopes in the library. The particle emission index files contain maps from an isotope to a file containing the particles emitted by that isotope when it decays. Not all of the decay chain data files contain the full set of decay chain information for all isotopes and therefore *cannot* be used to compute the fully aged isotopic specification of the material.

Table 1. MISC data file summary

File	Type	Description
nist.na.xml	abundance	natural abundance and masses of isotopes from the National Institute of Standards and Technology [7]
endf7.dk.xml	decay chain	radioactive isotope decay chain information from ENDF/B-VII.1 [5]
endf8.dk.xml	decay chain	radioactive isotope decay chain information from ENDF/B-VIII.0 [1]
endf7.idx.xml	particle emission	radioactive particle emission index built from data in ENDF/B-VII.1 [5]
endf8.idx.xml	decay chain	radioactive isotope decay chain information from ENDF/B-VIII.0 [1]

3 Usage

3.1 Input Specification

The MISC utility takes a single command-line input-file parameter and produces two files: 1) a summary output file (default name "misc.out") and 2) a source output file (default name "source.out") containing the source distributions suitable for copy-and-pasting into an MCNP input file. The MISC input file uses a *keyword-value* input form, namely:

```
keyword = value(s)
```

The "value" specified on a keyword may be composed of one or more input values. If multiple values are specified on a keyword requiring only one value, only the first is read and used by MISC. Lines with the "#" character occupying the **first** place on a line are comment lines. Lines containing five-or-more spaces before an entry are considered continuations of the previous line. **Input is case sensitive**. Currently, fifteen different keywords are available for the input specification to MISC, and they are summarized in Table 2.

Table 2. Description of keywords of MISC input

Keyword	Use	Description
ISCDATA	optional	The "ISCDATA" keyword specifies an optional path to the location of the data files described in Table 1. This keyword can also be specified through the ISCDATA environment variable. If omitted from the input and not specified as an environment variable, the value of ISCDATA defaults to the current working directory. The value in the input file takes precendence over the environment variable.
decayfile	required	The "decayfile" keyword specifies which decay data file to be used for the source calculation. The argument must be one of the decay data files given in Table 1. Currently, the available files are *endf6.dk.xml*, *endf7.dk.xml*, and *am.dk.xml*.
abundfile	required	The "abundfile" keyword specifies which natural abundance and mass data file to be used for the source calculation. The argument must be one of the abundance data files given in Table 1. Currently, the available files are *nist.na.xml*.
pelib	required	The "pelib" keyword specifies the particle emission library to be used for the calculation. Currently, the available values are *endf6*, *endf7*, *radsrc*, *irtape11e*, and *irtape11l.*
output	optional	The "output" keyword specifies the name of the output file. The default is *misc.out*.
srcout	optional	The "srcout" keyword specifies the name of the source distribution file suitable for cut and paste into MCNP. The default is *source.out*.
matspec	required	The "matspec" keyword is the input mechanism for the material specification. The values of the matspec keyword should be isotope/fraction pairs with the optional addition of a pelib override. As in MCNP, positive fractions are interpreted as atom fractions while negative fractions are interpreted as mass fractions. Mixing of atom and mass fractions is not allowed. The additional pelib override allows for a different particle emission library than that specified on the *pelib* keyword to be used for a specific isotope. See Appendix B for an example of the override.
density	required	The "density" keyword specifies the density of the material given on the matspec keyword. Again, positive values are interpreted as atom densities, while negative values are interpreted as mass densities.
age	optional	The "age" keyword specifies amount of time **in seconds** to age the material specification given on the matspec keyword. This keyword will only have an effect if the file specified on the decay_data_file keyword has decay chain information (see Table 1).

Keyword	Use	Description
format	optional	The "format" keyword specifies the formatting of the source.out file produced by MISC. Allowable values are "h" or "H" to produce MCNP distributions in the horizontal format or "v" or "V" to produce distributions in the vertical format.
particle	required	The "particle" keyword specifies the particle type for which the source distribution will be generated. The value should be the integer particle-type designator or character particle-type designator used by MCNP. See Table 3 for the list of available particle types.
brems	optional	The "brems" keyword indicates whether or not bremsstrahlung contributions should be added to a photon source. Possible values are "y" or "Y" to add the bremsstrahlung contribution or "n" or "N" not to add the bremsstrahlung contribution. The default is "y."
estobrems	optional	The "estobrems" keyword indicates whether or not a thick-target-bremsstrahlung (TTB) model should be used to convert electron source distributions into photon bremsstrahlung. Possible values are "y" or "Y" to convert electron distributions into photon bremsstrahlung or "n" or "N" not to convert electron distributions into photon bremsstrahlung. The default is "n." If estobrems is set to "y" but brems is set to "no" the contribution will not be added to the photon source.
bremsmult	optional	The "bremsmult" keyword allows the specification of an arbitrary scalar multiplier for the bremsstrahlung spectrum. The default value is one.
startdist	optional	The "startdist" keyword allows specification of the starting MCNP distribution number to be used. The default value is one.
biasing	optional	The "biasing" keyword allows source biasing to be applied to the MCNP source produced. There are four options for this keyword: "none", "uniform", "limited", and "butterworth". "uniform" produces a uniform biasing over the source distribution. "limited" limits the biasing of low probability lines (see details under "bias_limit"). "butterworth" implements a high-pass filter as a bias function on the probability (see "bias_limit" and "bias_order" for details).
ebins	optional	The "ebins" keyword changes the energy group structure on which the continuum histogram is computed. The values must be monotonically increasing and positive.

Keyword	Use	Description
collapse	optional	The "collapse" keyword allows the user to generate the source distributions as a function of isotope, that is, a separate distribution will be written for each daughter isotope that emits a particle of the type specified on the particle keyword. The default value "y" collapses all the isotopes into a single distribution. The value "n" on the collapse keyword will produce the distributions by isotope. WARNING: Use of the "n" option with inputs having long decay chains can produce large outputs.
intensity_ratio	optional	The "intensity_ratio" keyword allows the user to set a floating point value relative to the total intensity below which lines will be discarded. The speeds up source sampling routines in MCNP. Recommended value is between 1-1000/"nps". Default is `DBL_MIN`
bias_limit	optional	The "bias_limit" keyword behavior depends on the `biasing` keyword setting. It has no effect when `biasing` is "none" or "uniform". If the "limited" mode is used the bias is set to 1.0 for all lines with a emission probability greater than the limit and is set to probability/"bias_limit" for all other lines. This minimizes time spent sampling lines with low weight that will not contribute to the final spectrum. Recommended value is 1000/"nps". If the "butterworth" mode is used for `biasing` this sets the cutoff frequency(Energy) of the high pass butterworth filter in MeV. The filter transfer function at a given energy is multiplied by the emission probablity. This is often useful in cases where the absolute source intensity is dominated by low energy X-rays but there is sufficient shielding such that those X-rays do not make it to the tally location. For many scenarios a cutoff at 0.1 MeV is a good tradeoff between computational efficiency and accuracy. Default is `DBL_MIN`.
bias_order	optional	The "bias_order" keyword only has meaning when `biasing` is set to "butterworth". This keyword sets the order of the butterworth filter to be used. This order effects how steep the high pass rolloff is. The rolloff function is $\frac{1}{\sqrt{1+(\omega_c/\omega)^{2n}}}$ where n is the order of the filter ω_c is the value of "bias_limit" and ω is the energy of the line in MeV. The default value for this is 6.

3.2 Running MISC

MISC is executed on the command line with the input file name as the single command line parameter. For example, if the user's input file has the name "source1.inp," MISC would be executed as follows:

```
misc source1.inp
```

If the user *has not* specified "output" or "srcout" keywords in the input file, then the default output file "misc.out" and source file "source.out" will be created.

3.3 To Isomers and Beyond

In order to create a tool capable of truly capturing the decay emissions of aged isotopes, one must be inherently concerned with long lived isomers (a.k.a. metastable states). The conventional *Z-A* specification, e.g., 92238 for U-238, ceases to be an adequate representation of all nuclei when isomers are also required. Thus the conventional *Z-A* specification must be extended to an *S-Z-A* specification, where S indicates the isomeric state of the nucleus. The *S-Z-A* specification has the form

$$S \times 10^6 + Z \times 10^3 + A$$

The isomeric state should not to be confused with the actual excited state of the nucleus as the first isomeric state could correspond to the first, second, or higher excited state.

Using the above *S-Z-A* specifiers still allows for the specification of the ground state isotopes in the same historic *Z-A* form, that is, $S = 0$. However, now an isomeric state such as Pa-234m can be specified with the *S-Z-A* identifier 1091324. **While technically isotopes and isomers are not interchangeable terms, henceforth in this document they will be used interchangeably**.

4 Particle Types

The particle types available for source calculation are summarized in Table 3. If the user desires a specific particle source and no isotope in the material has data for the emission of that particle (this does not indicate that the isotopes does not emit the particle, only that the data is lacking), MISC will exit with an error to that effect.

Table 3. Particle types currently available for use with MISC

Particle Type	Integer Designator[a]	Character Designator[a]
Neutron	1	n
Photon	2	p
Bremsstrahlung[b]	-2	brems
Electron	3	e
Positron	8	f
Proton	9	h
Alpha	34	a

[a] where applicable, the integer and character designators correspond to the same integer used by MCNP

[b] the bremsstrahlung source results from either bremsstrahlung spectra in the data or from the TTB conversion of electrons into a photon source

5 Models

5.1 Decay Chain Solution

The decay of the radioactive nuclides specified in the material is accomplished by solution of the Bateman equations. When only a parent isotope X_1 is present, the solution of the Bateman equation for the atoms of the jth daughter in the decay chain N_j after a time t can be expressed [9]

$$N_j(t) = \frac{N_1(0)}{\lambda_j} \sum_{m=1}^{j} C_m e^{-\lambda_m t}, \tag{1}$$

where λ_j is the decay constant of the jth isotope and C_m is given as

$$C_m = \frac{\prod_{i=1}^{j} \lambda_j}{\prod_{i=1, i\neq m}^{j} (\lambda_i - \lambda_m)}. \tag{2}$$

Thus, this equation is solved for each initial parent nuclide specified in the material and the resulting daughters are summed to obtain the aged material specification.

5.2 Beta Particle Emissions

The beta particle (both electron and positron) energy distributions are calculated through application of Fermi theory of beta decay. The maximum energy that can be imparted to the beta particle is the Q-value for the radioactive decay. The spectrum of beta particles $n(W)$ for a fixed Q is given by [3]

$$n(W)dW = \left(\frac{16\pi m_o^5 c^4}{h^6}\right)(W^2 - 1)^2 (W_o - W)^2 F(Z, W) dW, \tag{3}$$

where W is a dimensionless unit of energy given as

$$W = \frac{E + m_o c^2}{m_o c^2}. \tag{4}$$

$F(Z, W)$ is a nuclear coulomb factor that accounts for deceleration of electrons and acceleration of positrons out of the nucleus and is given by

$$F(Z, W) = \left[\frac{4(1 + s/2)}{[\Gamma(3 + 2s)]^2}\left(\frac{4\pi R}{h/m_o c}\right)^{2s}\right] \times \left[(W^2 - 1)^{2s} e^{\pi y} |\Gamma(1 + s + iy)|^2\right], \tag{5}$$

where $s = \sqrt{1 - (Z\alpha)^2} - 1$ and $y = \pm Z\alpha W/(W^2 - 1)$ ($+Z$ for electrons and $-Z$ for positrons).

5.3 Thick-Target Bremsstrahlung

A model for converting electron emissions into thick-target bremsstrahlung (TTB) emission has been incorporated into MISC. The intensity $I(E_x)dE_x$ of bremsstrahlung photons emitted from a material with Z-number Z by an electron with energy E_e is given by [6]

$$I(E_x)dE_x = CZ(E_e - E_x). \tag{6}$$

Thus, because I = {number of quanta × energy of quanta}, the number of photons $N(E_x)$ emitted in dE_x about E_x is

$$N(E_x)dE_x = CZ\frac{E_e - E_x}{E_x}. \tag{7}$$

The constant C is a function of the Z-number and is tabulated for various Z's by McCall [6]. The TTB emission from the emission of a beta particle can be calculated by integrating the beta-particle emission spectrum with the TTB conversion function, namely

$$N_\beta(E_x)dE_x = CZ\int_0^{E_e^{max}} dE_e n(E_e)\frac{E_e - E_x}{E_x}. \tag{8}$$

References

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[5] T.D. Johnson, E.A. McCutchan, and A.A. Sonzogni, editors. *ENDF/B-VII.1 Radioactive Decay Data Files*. National Nuclear Data Center (www.nndc.bnl.gov), 2011.

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[7] National Institute of Standards and Technology. Atomic Weights and Isotopic Compositions. http://www.nist.gov/pml/data/comp.cfm, 2011.

[8] C.W. Reich, T.R. England, F.M. Mann, and F. Schmittroth. *ENDF/B-VI Radioactive Decay Data Files*. National Nuclear Data Center (www.nndc.bnl.gov), 1991.

[9] J.K. Shultis and R.E. Faw. *Fundamentals of Nuclear Science and Engineering*. Marcel Dekker, Inc., 2002.

A Basic Example Input

The following input specifies a material composed of the natural uranium isotopes. The uranium is aged for 0.5 y = 1.58e7 s (a sufficient amount of time for secular equilibrium of the daughters to be achieved). The electron emissions from the resulting isotopes are converted to bremsstrahlung emissions (estobrem = y) and the bremsstrahlung is added to the photon source (brems = y).

A.1 Input

```
# ISCDATA path from environment
# output file
output = xmpl1.out
# source file
srcout = xmpl1.src
# radioactive decay data file
decayfile = endf7.dk.xml
# natural abundance/mass data file
abundfile = nist.na.xml
# default particle emission library
pelib = endf7
# material specification
matspec = 92234  -.000055
          92235  -.0072
          92238  -.992745
# mass density
density = -18.937
# output format
format = v
# source particle type
particle = 2
# age the material (seconds)
age = 1.58e7
# add bremsstrahlung to photon source
brems = y
# convert electrons to bremsstrahlung
estobrems = y
# bremsstrahlung multiplier
bremsmult = 1.0
```

A.2 Output

```
USER INPUT MATERIAL SPECIFICATION:

      SZA   Isotope    Mass Frac
    92234     U-234  5.50000e-05
```

```
    92235     U-235  7.20000e-03
    92238     U-238  9.92745e-01

Material density: 1.89370e+01 g/cm^3

The material was aged for 1.58000e+07 s  using data from endf7.dk.xml

RESULTING MATERIAL SPECIFICATION:

      SZA   Isotope    Atom Frac    Mass Frac
    80206    Hg-206  1.62202e-34  1.40361e-34
    81205    Tl-205  9.48941e-49  8.17165e-49
    81206    Tl-206  5.13357e-33  4.44229e-33
    81207    Tl-207  4.73192e-24  4.11464e-24
    81210    Tl-210  5.55574e-29  4.90130e-29
    82206    Pb-206  5.81544e-24  5.03231e-24
    82207    Pb-207  4.96199e-20  4.31466e-20
    82209    Pb-209  7.07449e-31  6.21117e-31
    82210    Pb-210  1.19825e-20  1.05707e-20
    82211    Pb-211  3.59143e-23  3.18344e-23
    82214    Pb-214  5.45420e-24  4.90360e-24
    83209    Bi-209  2.13988e-28  1.87874e-28
    83210    Bi-210  6.57370e-24  5.79918e-24
    83211    Bi-211  2.12893e-24  1.88707e-24
    83214    Bi-214  4.04985e-24  3.64100e-24
    83215    Bi-215  1.00570e-29  9.08408e-30
    84210    Po-210  3.31744e-23  2.92656e-23
    84211    Po-211  2.36132e-29  2.09306e-29
    84214    Po-214  5.57161e-31  5.00905e-31
    84215    Po-215  2.95454e-29  2.66869e-29
    84218    Po-218  6.30806e-25  5.77751e-25
    85215    At-215  3.81552e-36  3.44636e-36
    85218    At-218  1.01809e-30  9.32457e-31
    85219    At-219  1.25684e-30  1.15642e-30
    86218    Rn-218  2.37553e-35  2.17570e-35
    86219    Rn-219  6.56932e-26  6.04441e-26
    86222    Rn-222  1.12112e-21  1.04571e-21
    87223    Fr-223  4.93763e-25  4.62629e-25
    88223    Ra-223  1.63827e-20  1.53496e-20
    88226    Ra-226  1.82007e-16  1.72829e-16
    89227    Ac-227  1.86283e-17  1.77674e-17
    90227    Th-227  3.22434e-20  3.07532e-20
    90230    Th-230  7.90726e-11  7.64165e-11
    90231    Th-231  3.01526e-14  2.92668e-14
    90234    Th-234  1.45362e-11  1.42929e-11
```

91231	Pa-231	3.56519e-12	3.46045e-12
91234	Pa-234	2.69386e-16	2.64875e-16
92234	U-234	5.59371e-05	5.50000e-05
92235	U-235	7.29143e-03	7.20000e-03
92238	U-238	9.92653e-01	9.92745e-01
1091234	Pa-234m1	4.85462e-16	4.77334e-16

Atom density: 4.79107e-02 a/b*cm
Mass density: 1.89370e+01 g/cm^3

TOTAL PARTICLE EMISSION RATES

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate
n	2.55316e-01	1.34824e-02	3.74045e-07
p	1.98288e+05	1.04709e+04	2.90498e-01
a	4.84292e+05	2.55738e+04	7.09502e-01
Total	6.82580e+05	3.60448e+04	1.00000e+00

ISOMER PARTICLE EMISSION RATES

80206, Hg-206:

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot
p	5.85364e-15	3.09112e-16	1.00000e+00	8.57577e-21
Total	5.85364e-15	3.09112e-16	1.00000e+00	8.57577e-21

81205, Tl-205:

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot
Total	0.00000e+00	0.00000e+00	0.00000e+00	0.00000e+00

81206, Tl-206:

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot
p	1.35706e-13	7.16619e-15	1.00000e+00	1.98814e-19
Total	1.35706e-13	7.16619e-15	1.00000e+00	1.98814e-19

81207, Tl-207:

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot
p	9.86585e-05	5.20983e-06	1.00000e+00	1.44538e-10
Total	9.86585e-05	5.20983e-06	1.00000e+00	1.44538e-10

81210, Tl-210:

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot
p	8.87105e-08	4.68451e-09	1.00000e+00	1.29964e-13
Total	8.87105e-08	4.68451e-09	1.00000e+00	1.29964e-13

82206, Pb-206:

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot
Total	0.00000e+00	0.00000e+00	0.00000e+00	0.00000e+00

82207, Pb-207:

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot
Total	0.00000e+00	0.00000e+00	0.00000e+00	0.00000e+00

82209, Pb-209:

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot
p	1.05695e-13	5.58141e-15	1.00000e+00	1.54847e-19
Total	1.05695e-13	5.58141e-15	1.00000e+00	1.54847e-19

82210, Pb-210:

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot
p	1.98760e-07	1.04959e-08	1.00000e+00	2.91190e-13
a	1.07920e-14	5.69889e-16	5.42965e-08	1.58106e-20
Total	1.98760e-07	1.04959e-08	1.00000e+00	2.91190e-13

82211, Pb-211:

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot
p	1.51884e-04	8.02050e-06	1.00000e+00	2.22515e-10
Total	1.51884e-04	8.02050e-06	1.00000e+00	2.22515e-10

82214, Pb-214:

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot
p	1.17406e-04	6.19983e-06	1.00000e+00	1.72004e-10
Total	1.17406e-04	6.19983e-06	1.00000e+00	1.72004e-10

83209, Bi-209:

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot
a	1.18472e-32	6.25614e-34	1.00000e+00	1.73566e-38
Total	1.18472e-32	6.25614e-34	1.00000e+00	1.73566e-38

83210, Bi-210:

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot
p	6.58550e-08	3.47759e-09	9.99990e-01	9.64796e-14
a	6.65453e-13	3.51403e-14	1.01047e-05	9.74908e-19
Total	6.58557e-08	3.47762e-09	1.00000e+00	9.64806e-14

83211, Bi-211:

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot
p	9.26983e-05	4.89509e-06	1.44434e-01	1.35806e-10
a	5.49104e-04	2.89964e-05	8.55566e-01	8.04455e-10
Total	6.41803e-04	3.38915e-05	1.00000e+00	9.40261e-10

83214, Bi-214:

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot
p	1.81509e-04	9.58490e-06	9.99870e-01	2.65917e-10
a	2.36473e-08	1.24873e-09	1.30265e-04	3.46440e-14
Total	1.81533e-04	9.58615e-06	1.00000e+00	2.65951e-10

83215, Bi-215:

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot
p	4.80832e-10	2.53911e-11	1.00000e+00	7.04433e-16
Total	4.80832e-10	2.53911e-11	1.00000e+00	7.04433e-16

84210, Po-210:

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot
p	9.62651e-13	5.08344e-14	1.04466e-05	1.41031e-18
a	9.21491e-08	4.86609e-09	9.99990e-01	1.35001e-13
Total	9.21501e-08	4.86614e-09	1.00000e+00	1.35003e-13

84211, Po-211:

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot
p	1.70893e-08	9.02429e-10	1.11200e-02	2.50364e-14
a	1.51972e-06	8.02513e-08	9.88880e-01	2.22644e-12
Total	1.53681e-06	8.11538e-08	1.00000e+00	2.25147e-12

84214, Po-214:

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot
p	1.18869e-08	6.27708e-10	1.05541e-04	1.74147e-14

```
         a  1.12616e-04  5.94689e-06  9.99894e-01  1.64986e-10
     Total  1.12628e-04  5.94752e-06  1.00000e+00  1.65004e-10

84215, Po-215:

   Particle   cm^-3 s^-1    g^-1 s^-1   Frac. Rate    Frac. Tot
         p  3.59196e-07  1.89680e-08  6.51392e-04  5.26233e-13
         a  5.51070e-04  2.91002e-05  9.99349e-01  8.07334e-10
     Total  5.51429e-04  2.91191e-05  1.00000e+00  8.07860e-10

84218, Po-218:

   Particle   cm^-3 s^-1    g^-1 s^-1   Frac. Rate    Frac. Tot
         p  1.52365e-09  8.04589e-11  1.35221e-05  2.23219e-15
         a  1.12677e-04  5.95009e-06  9.99986e-01  1.65075e-10
     Total  1.12678e-04  5.95017e-06  1.00000e+00  1.65077e-10

85215, At-215:

   Particle   cm^-3 s^-1    g^-1 s^-1   Frac. Rate    Frac. Tot
         p  6.52040e-13  3.44321e-14  5.14326e-04  9.55258e-19
         a  1.26710e-09  6.69115e-11  9.99486e-01  1.85634e-15
     Total  1.26776e-09  6.69459e-11  1.00000e+00  1.85730e-15

85218, At-218:

   Particle   cm^-3 s^-1    g^-1 s^-1   Frac. Rate    Frac. Tot
         p  2.02767e-08  1.07074e-09  4.73821e-01  2.97060e-14
         a  2.25173e-08  1.18907e-09  5.26179e-01  3.29886e-14
     Total  4.27940e-08  2.25981e-09  1.00000e+00  6.26945e-14

85219, At-219:

   Particle   cm^-3 s^-1    g^-1 s^-1   Frac. Rate    Frac. Tot
         p  4.54996e-12  2.40268e-13  6.25406e-03  6.66583e-18
         a  7.22972e-10  3.81777e-11  9.93746e-01  1.05918e-15
     Total  7.27522e-10  3.84180e-11  1.00000e+00  1.06584e-15

86218, Rn-218:

   Particle   cm^-3 s^-1    g^-1 s^-1   Frac. Rate    Frac. Tot
         p  2.86798e-14  1.51449e-15  1.27083e-03  4.20168e-20
         a  2.25392e-11  1.19022e-12  9.98729e-01  3.30206e-17
     Total  2.25679e-11  1.19173e-12  1.00000e+00  3.30626e-17
```

86219, Rn-219:

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot
p	1.12121e-04	5.92073e-06	1.69097e-01	1.64260e-10
a	5.50937e-04	2.90932e-05	8.30903e-01	8.07140e-10
Total	6.63058e-04	3.50139e-05	1.00000e+00	9.71400e-10

86222, Rn-222:

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot
p	8.84567e-08	4.67110e-09	7.84259e-04	1.29592e-13
a	1.12702e-04	5.95140e-06	9.99216e-01	1.65111e-10
Total	1.12790e-04	5.95607e-06	1.00000e+00	1.65241e-10

87223, Fr-223:

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot
p	8.50955e-06	4.49361e-07	9.99912e-01	1.24668e-11
a	7.45340e-10	3.93589e-11	8.75809e-05	1.09195e-15
Total	8.51030e-06	4.49401e-07	1.00000e+00	1.24678e-11

88223, Ra-223:

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot
p	5.83271e-04	3.08006e-05	5.14313e-01	8.54509e-10
a	5.50807e-04	2.90863e-05	4.85687e-01	8.06949e-10
Total	1.13408e-03	5.98869e-05	1.00000e+00	1.66146e-09

88226, Ra-226:

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot
p	5.50034e-06	2.90455e-07	4.39264e-02	8.05817e-12
a	1.19717e-04	6.32185e-06	9.56074e-01	1.75389e-10
Total	1.25217e-04	6.61231e-06	1.00000e+00	1.83447e-10

89227, Ac-227:

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot
p	4.38910e-05	2.31774e-06	7.73816e-01	6.43016e-11
a	1.28292e-05	6.77465e-07	2.26184e-01	1.87951e-11
Total	5.67201e-05	2.99520e-06	1.00000e+00	8.30967e-11

90227, Th-227:

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot

p	5.70692e-04	3.01363e-05	4.61635e-01	8.36081e-10
a	6.65549e-04	3.51455e-05	5.38365e-01	9.75050e-10
Total	1.23624e-03	6.52818e-05	1.00000e+00	1.81113e-09

90230, Th-230:

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot
n	3.83601e-13	2.02567e-14	3.21622e-13	5.61987e-19
p	9.04633e-02	4.77707e-03	7.58472e-02	1.32532e-07
a	1.10224e+00	5.82058e-02	9.24153e-01	1.61482e-06
Total	1.19271e+00	6.29828e-02	1.00000e+00	1.74735e-06

90231, Th-231:

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot
p	1.04527e+04	5.51975e+02	1.00000e+00	1.53136e-02
Total	1.04527e+04	5.51975e+02	1.00000e+00	1.53136e-02

90234, Th-234:

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot
p	3.73590e+04	1.97280e+03	1.00000e+00	5.47321e-02
Total	3.73590e+04	1.97280e+03	1.00000e+00	5.47321e-02

91231, Pa-231:

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot
n	5.87502e-13	3.10240e-14	3.28382e-12	8.60709e-19
p	6.54515e-02	3.45628e-03	3.65839e-01	9.58885e-08
a	1.13457e-01	5.99127e-03	6.34161e-01	1.66217e-07
Total	1.78908e-01	9.44755e-03	1.00000e+00	2.62106e-07

91234, Pa-234:

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot
p	1.41828e+03	7.48948e+01	1.00000e+00	2.07783e-03
Total	1.41828e+03	7.48948e+01	1.00000e+00	2.07783e-03

92234, U-234:

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot
n	7.33710e-06	3.87448e-07	2.71422e-11	1.07491e-11
p	3.05463e+04	1.61305e+03	1.13000e-01	4.47512e-02
a	2.39775e+05	1.26617e+04	8.87000e-01	3.51277e-01
Total	2.70321e+05	1.42747e+04	1.00000e+00	3.96028e-01

92235, U-235:

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot
n	1.46789e-06	7.75142e-08	5.91176e-11	2.15050e-12
p	1.40601e+04	7.42468e+02	5.66256e-01	2.05985e-02
a	1.07698e+04	5.68720e+02	4.33744e-01	1.57782e-02
Total	2.48300e+04	1.31119e+03	1.00000e+00	3.63766e-02

92238, U-238:

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot
n	2.55307e-01	1.34819e-02	1.00061e-06	3.74032e-07
p	2.14061e+04	1.13039e+03	8.38954e-02	3.13606e-02
a	2.33746e+05	1.23433e+04	9.16104e-01	3.42445e-01
Total	2.55152e+05	1.34737e+04	1.00000e+00	3.73806e-01

1091234, Pa-234m1:

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot
p	8.30451e+04	4.38534e+03	1.00000e+00	1.21664e-01
Total	8.30451e+04	4.38534e+03	1.00000e+00	1.21664e-01

B Example Input with a *pelib* Override

The following input file demonstrates an override of the particle emission library used for the U-238 isotope. The particle emission library specified on the *pelib* keyword is endf7 and will be applied to the U-234, U-235, and U-236 isotopes, as well as, all daughters, **including those of U-238**, from the decay calculation. The output file reflects the use of the irtape11e library for U-238 and the endf7 library for all other isotopes.

B.1 Input

```
# ISCDATA path from environment
# output file
output = xmpl2.out
# source file
srcout = xmpl2.src
# radioactive decay data file
decayfile = endf7.dk.xml
# natural abundance/mass data file
abundfile = nist.na.xml
# default particle emission library
pelib = endf7
# material specification with U-238 pelib override
matspec = 92234  -.000055
          92235  -.0072
          92238  -.992745    irtape11e
# mass density
density = -18.937
# output format
format = v
# source particle type
particle = 2
# age the material (seconds)
age = 1.58e7
# add bremsstrahlung to photon source
brems = y
# convert electrons to bremsstrahlung
estobrems = y
# bremsstrahlung multiplier
bremsmult = 1.0
```

B.2 Output

```
USER INPUT MATERIAL SPECIFICATION:

      SZA   Isotope    Mass Frac
```

```
    92234     U-234  5.50000e-05
    92235     U-235  7.20000e-03
    92238     U-238  9.92745e-01

Material density: 1.89370e+01 g/cm^3

The material was aged for 1.58000e+07 s  using data from endf7.dk.xml

RESULTING MATERIAL SPECIFICATION:

      SZA   Isotope    Atom Frac    Mass Frac
    80206    Hg-206  1.62202e-34  1.40361e-34
    81205    Tl-205  9.48941e-49  8.17165e-49
    81206    Tl-206  5.13357e-33  4.44229e-33
    81207    Tl-207  4.73192e-24  4.11464e-24
    81210    Tl-210  5.55574e-29  4.90130e-29
    82206    Pb-206  5.81544e-24  5.03231e-24
    82207    Pb-207  4.96199e-20  4.31466e-20
    82209    Pb-209  7.07449e-31  6.21117e-31
    82210    Pb-210  1.19825e-20  1.05707e-20
    82211    Pb-211  3.59143e-23  3.18344e-23
    82214    Pb-214  5.45420e-24  4.90360e-24
    83209    Bi-209  2.13988e-28  1.87874e-28
    83210    Bi-210  6.57370e-24  5.79918e-24
    83211    Bi-211  2.12893e-24  1.88707e-24
    83214    Bi-214  4.04985e-24  3.64100e-24
    83215    Bi-215  1.00570e-29  9.08408e-30
    84210    Po-210  3.31744e-23  2.92656e-23
    84211    Po-211  2.36132e-29  2.09306e-29
    84214    Po-214  5.57161e-31  5.00905e-31
    84215    Po-215  2.95454e-29  2.66869e-29
    84218    Po-218  6.30806e-25  5.77751e-25
    85215    At-215  3.81552e-36  3.44636e-36
    85218    At-218  1.01809e-30  9.32457e-31
    85219    At-219  1.25684e-30  1.15642e-30
    86218    Rn-218  2.37553e-35  2.17570e-35
    86219    Rn-219  6.56932e-26  6.04441e-26
    86222    Rn-222  1.12112e-21  1.04571e-21
    87223    Fr-223  4.93763e-25  4.62629e-25
    88223    Ra-223  1.63827e-20  1.53496e-20
    88226    Ra-226  1.82007e-16  1.72829e-16
    89227    Ac-227  1.86283e-17  1.77674e-17
    90227    Th-227  3.22434e-20  3.07532e-20
    90230    Th-230  7.90726e-11  7.64165e-11
    90231    Th-231  3.01526e-14  2.92668e-14
```

```
    90234    Th-234  1.45362e-11  1.42929e-11
    91231    Pa-231  3.56519e-12  3.46045e-12
    91234    Pa-234  2.69386e-16  2.64875e-16
    92234     U-234  5.59371e-05  5.50000e-05
    92235     U-235  7.29143e-03  7.20000e-03
    92238     U-238  9.92653e-01  9.92745e-01
  1091234  Pa-234m1  4.85462e-16  4.77334e-16

Atom density: 4.79107e-02 a/b*cm
Mass density: 1.89370e+01 g/cm^3

TOTAL PARTICLE EMISSION RATES

   Particle   cm^-3 s^-1    g^-1 s^-1   Frac. Rate
          n  8.80499e-06  4.64962e-07  1.42590e-11
          p  3.66956e+05  1.93777e+04  5.94259e-01
          a  2.50546e+05  1.32305e+04  4.05741e-01
      Total  6.17502e+05  3.26082e+04  1.00000e+00

ISOMER PARTICLE EMISSION RATES

80206, Hg-206:

   Particle   cm^-3 s^-1    g^-1 s^-1   Frac. Rate    Frac. Tot
          p  5.85364e-15  3.09112e-16  1.00000e+00  9.47956e-21
      Total  5.85364e-15  3.09112e-16  1.00000e+00  9.47956e-21

81205, Tl-205:

   Particle   cm^-3 s^-1    g^-1 s^-1   Frac. Rate    Frac. Tot
      Total  0.00000e+00  0.00000e+00  0.00000e+00  0.00000e+00

81206, Tl-206:

   Particle   cm^-3 s^-1    g^-1 s^-1   Frac. Rate    Frac. Tot
          p  1.35706e-13  7.16619e-15  1.00000e+00  2.19766e-19
      Total  1.35706e-13  7.16619e-15  1.00000e+00  2.19766e-19

81207, Tl-207:

   Particle   cm^-3 s^-1    g^-1 s^-1   Frac. Rate    Frac. Tot
          p  9.86585e-05  5.20983e-06  1.00000e+00  1.59770e-10
      Total  9.86585e-05  5.20983e-06  1.00000e+00  1.59770e-10

81210, Tl-210:
```

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot
p	8.87105e-08	4.68451e-09	1.00000e+00	1.43660e-13
Total	8.87105e-08	4.68451e-09	1.00000e+00	1.43660e-13

82206, Pb-206:

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot
Total	0.00000e+00	0.00000e+00	0.00000e+00	0.00000e+00

82207, Pb-207:

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot
Total	0.00000e+00	0.00000e+00	0.00000e+00	0.00000e+00

82209, Pb-209:

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot
p	1.05695e-13	5.58141e-15	1.00000e+00	1.71166e-19
Total	1.05695e-13	5.58141e-15	1.00000e+00	1.71166e-19

82210, Pb-210:

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot
p	1.98760e-07	1.04959e-08	1.00000e+00	3.21878e-13
a	1.07920e-14	5.69889e-16	5.42965e-08	1.74769e-20
Total	1.98760e-07	1.04959e-08	1.00000e+00	3.21878e-13

82211, Pb-211:

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot
p	1.51884e-04	8.02050e-06	1.00000e+00	2.45966e-10
Total	1.51884e-04	8.02050e-06	1.00000e+00	2.45966e-10

82214, Pb-214:

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot
p	1.17406e-04	6.19983e-06	1.00000e+00	1.90131e-10
Total	1.17406e-04	6.19983e-06	1.00000e+00	1.90131e-10

83209, Bi-209:

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot
a	1.18472e-32	6.25614e-34	1.00000e+00	1.91858e-38
Total	1.18472e-32	6.25614e-34	1.00000e+00	1.91858e-38

83210, Bi-210:

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot
p	6.58550e-08	3.47759e-09	9.99990e-01	1.06648e-13
a	6.65453e-13	3.51403e-14	1.01047e-05	1.07765e-18
Total	6.58557e-08	3.47762e-09	1.00000e+00	1.06649e-13

83211, Bi-211:

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot
p	9.26983e-05	4.89509e-06	1.44434e-01	1.50118e-10
a	5.49104e-04	2.89964e-05	8.55566e-01	8.89235e-10
Total	6.41803e-04	3.38915e-05	1.00000e+00	1.03935e-09

83214, Bi-214:

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot
p	1.81509e-04	9.58490e-06	9.99870e-01	2.93941e-10
a	2.36473e-08	1.24873e-09	1.30265e-04	3.82951e-14
Total	1.81533e-04	9.58615e-06	1.00000e+00	2.93979e-10

83215, Bi-215:

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot
p	4.80832e-10	2.53911e-11	1.00000e+00	7.78673e-16
Total	4.80832e-10	2.53911e-11	1.00000e+00	7.78673e-16

84210, Po-210:

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot
p	9.62651e-13	5.08344e-14	1.04466e-05	1.55894e-18
a	9.21491e-08	4.86609e-09	9.99990e-01	1.49229e-13
Total	9.21501e-08	4.86614e-09	1.00000e+00	1.49230e-13

84211, Po-211:

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot
p	1.70893e-08	9.02429e-10	1.11200e-02	2.76749e-14
a	1.51972e-06	8.02513e-08	9.88880e-01	2.46108e-12
Total	1.53681e-06	8.11538e-08	1.00000e+00	2.48875e-12

84214, Po-214:

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot

p	1.18869e-08	6.27708e-10	1.05541e-04	1.92500e-14
a	1.12616e-04	5.94689e-06	9.99894e-01	1.82374e-10
Total	1.12628e-04	5.94752e-06	1.00000e+00	1.82393e-10

84215, Po-215:

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot
p	3.59196e-07	1.89680e-08	6.51392e-04	5.81693e-13
a	5.51070e-04	2.91002e-05	9.99349e-01	8.92418e-10
Total	5.51429e-04	2.91191e-05	1.00000e+00	8.93000e-10

84218, Po-218:

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot
p	1.52365e-09	8.04589e-11	1.35221e-05	2.46744e-15
a	1.12677e-04	5.95009e-06	9.99986e-01	1.82472e-10
Total	1.12678e-04	5.95017e-06	1.00000e+00	1.82475e-10

85215, At-215:

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot
p	6.52040e-13	3.44321e-14	5.14326e-04	1.05593e-18
a	1.26710e-09	6.69115e-11	9.99486e-01	2.05198e-15
Total	1.26776e-09	6.69459e-11	1.00000e+00	2.05304e-15

85218, At-218:

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot
p	2.02767e-08	1.07074e-09	4.73821e-01	3.28367e-14
a	2.25173e-08	1.18907e-09	5.26179e-01	3.64652e-14
Total	4.27940e-08	2.25981e-09	1.00000e+00	6.93019e-14

85219, At-219:

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot
p	4.54996e-12	2.40268e-13	6.25406e-03	7.36834e-18
a	7.22972e-10	3.81777e-11	9.93746e-01	1.17080e-15
Total	7.27522e-10	3.84180e-11	1.00000e+00	1.17817e-15

86218, Rn-218:

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot
p	2.86798e-14	1.51449e-15	1.27083e-03	4.64450e-20
a	2.25392e-11	1.19022e-12	9.98729e-01	3.65006e-17
Total	2.25679e-11	1.19173e-12	1.00000e+00	3.65471e-17

86219, Rn-219:

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot
p	1.12121e-04	5.92073e-06	1.69097e-01	1.81572e-10
a	5.50937e-04	2.90932e-05	8.30903e-01	8.92204e-10
Total	6.63058e-04	3.50139e-05	1.00000e+00	1.07378e-09

86222, Rn-222:

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot
p	8.84567e-08	4.67110e-09	7.84259e-04	1.43249e-13
a	1.12702e-04	5.95140e-06	9.99216e-01	1.82512e-10
Total	1.12790e-04	5.95607e-06	1.00000e+00	1.82655e-10

87223, Fr-223:

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot
p	8.50955e-06	4.49361e-07	9.99912e-01	1.37806e-11
a	7.45340e-10	3.93589e-11	8.75809e-05	1.20702e-15
Total	8.51030e-06	4.49401e-07	1.00000e+00	1.37818e-11

88223, Ra-223:

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot
p	5.83271e-04	3.08006e-05	5.14313e-01	9.44565e-10
a	5.50807e-04	2.90863e-05	4.85687e-01	8.91993e-10
Total	1.13408e-03	5.98869e-05	1.00000e+00	1.83656e-09

88226, Ra-226:

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot
p	5.50034e-06	2.90455e-07	4.39264e-02	8.90741e-12
a	1.19717e-04	6.32185e-06	9.56074e-01	1.93873e-10
Total	1.25217e-04	6.61231e-06	1.00000e+00	2.02780e-10

89227, Ac-227:

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot
p	4.38910e-05	2.31774e-06	7.73816e-01	7.10783e-11
a	1.28292e-05	6.77465e-07	2.26184e-01	2.07759e-11
Total	5.67201e-05	2.99520e-06	1.00000e+00	9.18542e-11

90227, Th-227:

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot
p	5.70692e-04	3.01363e-05	4.61635e-01	9.24195e-10
a	6.65549e-04	3.51455e-05	5.38365e-01	1.07781e-09
Total	1.23624e-03	6.52818e-05	1.00000e+00	2.00200e-09

90230, Th-230:

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot
n	3.83601e-13	2.02567e-14	3.21622e-13	6.21214e-19
p	9.04633e-02	4.77707e-03	7.58472e-02	1.46499e-07
a	1.10224e+00	5.82058e-02	9.24153e-01	1.78500e-06
Total	1.19271e+00	6.29828e-02	1.00000e+00	1.93150e-06

90231, Th-231:

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot
p	1.04527e+04	5.51975e+02	1.00000e+00	1.69275e-02
Total	1.04527e+04	5.51975e+02	1.00000e+00	1.69275e-02

90234, Th-234:

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot
p	3.73590e+04	1.97280e+03	1.00000e+00	6.05002e-02
Total	3.73590e+04	1.97280e+03	1.00000e+00	6.05002e-02

91231, Pa-231:

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot
n	5.87502e-13	3.10240e-14	3.28382e-12	9.51418e-19
p	6.54515e-02	3.45628e-03	3.65839e-01	1.05994e-07
a	1.13457e-01	5.99127e-03	6.34161e-01	1.83735e-07
Total	1.78908e-01	9.44755e-03	1.00000e+00	2.89729e-07

91234, Pa-234:

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot
p	1.41828e+03	7.48948e+01	1.00000e+00	2.29681e-03
Total	1.41828e+03	7.48948e+01	1.00000e+00	2.29681e-03

92234, U-234:

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot
n	7.33710e-06	3.87448e-07	2.71422e-11	1.18819e-11
p	3.05463e+04	1.61305e+03	1.13000e-01	4.94675e-02
a	2.39775e+05	1.26617e+04	8.87000e-01	3.88298e-01

Total	2.70321e+05	1.42747e+04	1.00000e+00	4.37765e-01

92235, U-235:

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot
n	1.46789e-06	7.75142e-08	5.91176e-11	2.37714e-12
p	1.40601e+04	7.42468e+02	5.66256e-01	2.27693e-02
a	1.07698e+04	5.68720e+02	4.33744e-01	1.74410e-02
Total	2.48300e+04	1.31119e+03	1.00000e+00	4.02103e-02

92238, U-238:

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot
p	1.90074e+05	1.00372e+04	1.00000e+00	3.07812e-01
Total	1.90074e+05	1.00372e+04	1.00000e+00	3.07812e-01

1091234, Pa-234m1:

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot
p	8.30451e+04	4.38534e+03	1.00000e+00	1.34486e-01
Total	8.30451e+04	4.38534e+03	1.00000e+00	1.34486e-01

C Example Input with a *pelib* Override of a Daughter

The following input file demonstrates an override of the particle emission library used for the U-238 isotope and the Pa-234m (S-Z-A = 1092234) daughter, which has no initial concentration. For this example the *pelib* value is endf7 and therefore the endf7 particle emission library is used for all isotopes other than U-238 and Pa-234m. The endf6 particle emission library will be used for U-238 and the irtape11e particle emission library will be used for Pa-234m.

C.1 Input

```
# ISCDATA path from environment
# output file
output = xmpl3.out
# source file
srcout = xmpl3.src
# radioactive decay data file
decayfile = endf7.dk.xml
# natural abundance/mass data file
abundfile = nist.na.xml
# default particle emission library
pelib = endf7
# material specification with U-238 pelib override to endf6
# and a Pa-234m pelib override to irtape11e
matspec = 92234  -.000055
          92235  -.0072
          92238  -.992745  endf6
        1091234  0.0       irtape11e
# mass density
density = -18.937
# output format
format = v
# source particle type
particle = 2
# age the material (seconds)
age = 1.58e7
# add bremsstrahlung to photon source
brems = y
# convert electrons to bremsstrahlung
estobrems = y
# bremsstrahlung multiplier
bremsmult = 1.0
```

C.2 Output

```
USER INPUT MATERIAL SPECIFICATION:
```

```
      SZA   Isotope    Mass Frac
    92234     U-234  5.50000e-05
    92235     U-235  7.20000e-03
    92238     U-238  9.92745e-01
  1091234  Pa-234m1  0.00000e+00

Material density: 1.89370e+01 g/cm^3

The material was aged for 1.58000e+07 s  using data from endf7.dk.xml

RESULTING MATERIAL SPECIFICATION:

      SZA   Isotope    Atom Frac    Mass Frac
    80206    Hg-206  1.62202e-34  1.40361e-34
    81205    Tl-205  9.48941e-49  8.17165e-49
    81206    Tl-206  5.13357e-33  4.44229e-33
    81207    Tl-207  4.73192e-24  4.11464e-24
    81210    Tl-210  5.55574e-29  4.90130e-29
    82206    Pb-206  5.81544e-24  5.03231e-24
    82207    Pb-207  4.96199e-20  4.31466e-20
    82209    Pb-209  7.07449e-31  6.21117e-31
    82210    Pb-210  1.19825e-20  1.05707e-20
    82211    Pb-211  3.59143e-23  3.18344e-23
    82214    Pb-214  5.45420e-24  4.90360e-24
    83209    Bi-209  2.13988e-28  1.87874e-28
    83210    Bi-210  6.57370e-24  5.79918e-24
    83211    Bi-211  2.12893e-24  1.88707e-24
    83214    Bi-214  4.04985e-24  3.64100e-24
    83215    Bi-215  1.00570e-29  9.08408e-30
    84210    Po-210  3.31744e-23  2.92656e-23
    84211    Po-211  2.36132e-29  2.09306e-29
    84214    Po-214  5.57161e-31  5.00905e-31
    84215    Po-215  2.95454e-29  2.66869e-29
    84218    Po-218  6.30806e-25  5.77751e-25
    85215    At-215  3.81552e-36  3.44636e-36
    85218    At-218  1.01809e-30  9.32457e-31
    85219    At-219  1.25684e-30  1.15642e-30
    86218    Rn-218  2.37553e-35  2.17570e-35
    86219    Rn-219  6.56932e-26  6.04441e-26
    86222    Rn-222  1.12112e-21  1.04571e-21
    87223    Fr-223  4.93763e-25  4.62629e-25
    88223    Ra-223  1.63827e-20  1.53496e-20
    88226    Ra-226  1.82007e-16  1.72829e-16
    89227    Ac-227  1.86283e-17  1.77674e-17
```

```
    90227    Th-227  3.22434e-20  3.07532e-20
    90230    Th-230  7.90726e-11  7.64165e-11
    90231    Th-231  3.01526e-14  2.92668e-14
    90234    Th-234  1.45362e-11  1.42929e-11
    91231    Pa-231  3.56519e-12  3.46045e-12
    91234    Pa-234  2.69386e-16  2.64875e-16
    92234     U-234  5.59371e-05  5.50000e-05
    92235     U-235  7.29143e-03  7.20000e-03
    92238     U-238  9.92653e-01  9.92745e-01
  1091234  Pa-234m1  4.85462e-16  4.77334e-16

Atom density: 4.79107e-02 a/b*cm
Mass density: 1.89370e+01 g/cm^3

TOTAL PARTICLE EMISSION RATES

   Particle   cm^-3 s^-1    g^-1 s^-1   Frac. Rate
          n  8.80499e-06  4.64962e-07  1.46250e-11
          p  1.17523e+05  6.20600e+03  1.95205e-01
          a  4.84525e+05  2.55862e+04  8.04795e-01
      Total  6.02048e+05  3.17922e+04  1.00000e+00

ISOMER PARTICLE EMISSION RATES

80206, Hg-206:

   Particle   cm^-3 s^-1    g^-1 s^-1   Frac. Rate    Frac. Tot
          p  5.85364e-15  3.09112e-16  1.00000e+00  9.72288e-21
      Total  5.85364e-15  3.09112e-16  1.00000e+00  9.72288e-21

81205, Tl-205:

   Particle   cm^-3 s^-1    g^-1 s^-1   Frac. Rate    Frac. Tot
      Total  0.00000e+00  0.00000e+00  0.00000e+00  0.00000e+00

81206, Tl-206:

   Particle   cm^-3 s^-1    g^-1 s^-1   Frac. Rate    Frac. Tot
          p  1.35706e-13  7.16619e-15  1.00000e+00  2.25407e-19
      Total  1.35706e-13  7.16619e-15  1.00000e+00  2.25407e-19

81207, Tl-207:

   Particle   cm^-3 s^-1    g^-1 s^-1   Frac. Rate    Frac. Tot
          p  9.86585e-05  5.20983e-06  1.00000e+00  1.63871e-10
```

```
      Total  9.86585e-05  5.20983e-06  1.00000e+00  1.63871e-10

81210, Tl-210:

   Particle   cm^-3 s^-1    g^-1 s^-1   Frac. Rate    Frac. Tot
          p  8.87105e-08  4.68451e-09  1.00000e+00  1.47348e-13
      Total  8.87105e-08  4.68451e-09  1.00000e+00  1.47348e-13

82206, Pb-206:

   Particle   cm^-3 s^-1    g^-1 s^-1   Frac. Rate    Frac. Tot
      Total  0.00000e+00  0.00000e+00  0.00000e+00  0.00000e+00

82207, Pb-207:

   Particle   cm^-3 s^-1    g^-1 s^-1   Frac. Rate    Frac. Tot
      Total  0.00000e+00  0.00000e+00  0.00000e+00  0.00000e+00

82209, Pb-209:

   Particle   cm^-3 s^-1    g^-1 s^-1   Frac. Rate    Frac. Tot
          p  1.05695e-13  5.58141e-15  1.00000e+00  1.75559e-19
      Total  1.05695e-13  5.58141e-15  1.00000e+00  1.75559e-19

82210, Pb-210:

   Particle   cm^-3 s^-1    g^-1 s^-1   Frac. Rate    Frac. Tot
          p  1.98760e-07  1.04959e-08  1.00000e+00  3.30140e-13
          a  1.07920e-14  5.69889e-16  5.42965e-08  1.79255e-20
      Total  1.98760e-07  1.04959e-08  1.00000e+00  3.30140e-13

82211, Pb-211:

   Particle   cm^-3 s^-1    g^-1 s^-1   Frac. Rate    Frac. Tot
          p  1.51884e-04  8.02050e-06  1.00000e+00  2.52279e-10
      Total  1.51884e-04  8.02050e-06  1.00000e+00  2.52279e-10

82214, Pb-214:

   Particle   cm^-3 s^-1    g^-1 s^-1   Frac. Rate    Frac. Tot
          p  1.17406e-04  6.19983e-06  1.00000e+00  1.95011e-10
      Total  1.17406e-04  6.19983e-06  1.00000e+00  1.95011e-10

83209, Bi-209:
```

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot
a	1.18472e-32	6.25614e-34	1.00000e+00	1.96782e-38
Total	1.18472e-32	6.25614e-34	1.00000e+00	1.96782e-38

83210, Bi-210:

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot
p	6.58550e-08	3.47759e-09	9.99990e-01	1.09385e-13
a	6.65453e-13	3.51403e-14	1.01047e-05	1.10531e-18
Total	6.58557e-08	3.47762e-09	1.00000e+00	1.09386e-13

83211, Bi-211:

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot
p	9.26983e-05	4.89509e-06	1.44434e-01	1.53972e-10
a	5.49104e-04	2.89964e-05	8.55566e-01	9.12060e-10
Total	6.41803e-04	3.38915e-05	1.00000e+00	1.06603e-09

83214, Bi-214:

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot
p	1.81509e-04	9.58490e-06	9.99870e-01	3.01486e-10
a	2.36473e-08	1.24873e-09	1.30265e-04	3.92781e-14
Total	1.81533e-04	9.58615e-06	1.00000e+00	3.01525e-10

83215, Bi-215:

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot
p	4.80832e-10	2.53911e-11	1.00000e+00	7.98660e-16
Total	4.80832e-10	2.53911e-11	1.00000e+00	7.98660e-16

84210, Po-210:

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot
p	9.62651e-13	5.08344e-14	1.04466e-05	1.59896e-18
a	9.21491e-08	4.86609e-09	9.99990e-01	1.53059e-13
Total	9.21501e-08	4.86614e-09	1.00000e+00	1.53061e-13

84211, Po-211:

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot
p	1.70893e-08	9.02429e-10	1.11200e-02	2.83853e-14
a	1.51972e-06	8.02513e-08	9.88880e-01	2.52425e-12
Total	1.53681e-06	8.11538e-08	1.00000e+00	2.55263e-12

84214, Po-214:

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot
p	1.18869e-08	6.27708e-10	1.05541e-04	1.97441e-14
a	1.12616e-04	5.94689e-06	9.99894e-01	1.87055e-10
Total	1.12628e-04	5.94752e-06	1.00000e+00	1.87075e-10

84215, Po-215:

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot
p	3.59196e-07	1.89680e-08	6.51392e-04	5.96623e-13
a	5.51070e-04	2.91002e-05	9.99349e-01	9.15325e-10
Total	5.51429e-04	2.91191e-05	1.00000e+00	9.15921e-10

84218, Po-218:

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot
p	1.52365e-09	8.04589e-11	1.35221e-05	2.53078e-15
a	1.12677e-04	5.95009e-06	9.99986e-01	1.87156e-10
Total	1.12678e-04	5.95017e-06	1.00000e+00	1.87158e-10

85215, At-215:

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot
p	6.52040e-13	3.44321e-14	5.14326e-04	1.08304e-18
a	1.26710e-09	6.69115e-11	9.99486e-01	2.10465e-15
Total	1.26776e-09	6.69459e-11	1.00000e+00	2.10574e-15

85218, At-218:

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot
p	2.02767e-08	1.07074e-09	4.73821e-01	3.36795e-14
a	2.25173e-08	1.18907e-09	5.26179e-01	3.74012e-14
Total	4.27940e-08	2.25981e-09	1.00000e+00	7.10807e-14

85219, At-219:

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot
p	4.54996e-12	2.40268e-13	6.25406e-03	7.55747e-18
a	7.22972e-10	3.81777e-11	9.93746e-01	1.20085e-15
Total	7.27522e-10	3.84180e-11	1.00000e+00	1.20841e-15

86218, Rn-218:

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot

p	2.86798e-14	1.51449e-15	1.27083e-03	4.76371e-20
a	2.25392e-11	1.19022e-12	9.98729e-01	3.74375e-17
Total	2.25679e-11	1.19173e-12	1.00000e+00	3.74851e-17

86219, Rn-219:

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot
p	1.12121e-04	5.92073e-06	1.69097e-01	1.86232e-10
a	5.50937e-04	2.90932e-05	8.30903e-01	9.15105e-10
Total	6.63058e-04	3.50139e-05	1.00000e+00	1.10134e-09

86222, Rn-222:

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot
p	8.84567e-08	4.67110e-09	7.84259e-04	1.46926e-13
a	1.12702e-04	5.95140e-06	9.99216e-01	1.87197e-10
Total	1.12790e-04	5.95607e-06	1.00000e+00	1.87344e-10

87223, Fr-223:

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot
p	8.50955e-06	4.49361e-07	9.99912e-01	1.41343e-11
a	7.45340e-10	3.93589e-11	8.75809e-05	1.23801e-15
Total	8.51030e-06	4.49401e-07	1.00000e+00	1.41356e-11

88223, Ra-223:

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot
p	5.83271e-04	3.08006e-05	5.14313e-01	9.68810e-10
a	5.50807e-04	2.90863e-05	4.85687e-01	9.14888e-10
Total	1.13408e-03	5.98869e-05	1.00000e+00	1.88370e-09

88226, Ra-226:

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot
p	5.50034e-06	2.90455e-07	4.39264e-02	9.13605e-12
a	1.19717e-04	6.32185e-06	9.56074e-01	1.98849e-10
Total	1.25217e-04	6.61231e-06	1.00000e+00	2.07985e-10

89227, Ac-227:

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot
p	4.38910e-05	2.31774e-06	7.73816e-01	7.29027e-11
a	1.28292e-05	6.77465e-07	2.26184e-01	2.13092e-11
Total	5.67201e-05	2.99520e-06	1.00000e+00	9.42119e-11

90227, Th-227:

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot
p	5.70692e-04	3.01363e-05	4.61635e-01	9.47917e-10
a	6.65549e-04	3.51455e-05	5.38365e-01	1.10547e-09
Total	1.23624e-03	6.52818e-05	1.00000e+00	2.05339e-09

90230, Th-230:

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot
n	3.83601e-13	2.02567e-14	3.21622e-13	6.37159e-19
p	9.04633e-02	4.77707e-03	7.58472e-02	1.50259e-07
a	1.10224e+00	5.82058e-02	9.24153e-01	1.83082e-06
Total	1.19271e+00	6.29828e-02	1.00000e+00	1.98108e-06

90231, Th-231:

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot
p	1.04527e+04	5.51975e+02	1.00000e+00	1.73620e-02
Total	1.04527e+04	5.51975e+02	1.00000e+00	1.73620e-02

90234, Th-234:

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot
p	3.73590e+04	1.97280e+03	1.00000e+00	6.20531e-02
Total	3.73590e+04	1.97280e+03	1.00000e+00	6.20531e-02

91231, Pa-231:

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot
n	5.87502e-13	3.10240e-14	3.28382e-12	9.75839e-19
p	6.54515e-02	3.45628e-03	3.65839e-01	1.08715e-07
a	1.13457e-01	5.99127e-03	6.34161e-01	1.88451e-07
Total	1.78908e-01	9.44755e-03	1.00000e+00	2.97166e-07

91234, Pa-234:

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot
p	1.41828e+03	7.48948e+01	1.00000e+00	2.35576e-03
Total	1.41828e+03	7.48948e+01	1.00000e+00	2.35576e-03

92234, U-234:

Particle	cm^-3 s^-1	g^-1 s^-1	Frac. Rate	Frac. Tot

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          n  7.33710e-06  3.87448e-07  2.71422e-11  1.21869e-11
          p  3.05463e+04  1.61305e+03  1.13000e-01  5.07372e-02
          a  2.39775e+05  1.26617e+04  8.87000e-01  3.98265e-01
      Total  2.70321e+05  1.42747e+04  1.00000e+00  4.49002e-01

92235, U-235:

   Particle   cmˆ-3 sˆ-1    gˆ-1 sˆ-1   Frac. Rate    Frac. Tot
          n  1.46789e-06  7.75142e-08  5.91176e-11  2.43815e-12
          p  1.40601e+04  7.42468e+02  5.66256e-01  2.33538e-02
          a  1.07698e+04  5.68720e+02  4.33744e-01  1.78887e-02
      Total  2.48300e+04  1.31119e+03  1.00000e+00  4.12425e-02

92238, U-238:

   Particle   cmˆ-3 sˆ-1    gˆ-1 sˆ-1   Frac. Rate    Frac. Tot
          p  1.89614e+04  1.00129e+03  7.49638e-02  3.14948e-02
          a  2.33980e+05  1.23557e+04  9.25036e-01  3.88639e-01
      Total  2.52941e+05  1.33570e+04  1.00000e+00  4.20134e-01

1091234, Pa-234m1:

   Particle   cmˆ-3 sˆ-1    gˆ-1 sˆ-1   Frac. Rate    Frac. Tot
          p  4.72506e+03  2.49515e+02  1.00000e+00  7.84831e-03
      Total  4.72506e+03  2.49515e+02  1.00000e+00  7.84831e-03
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