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MCNP Intrinsic Source Constructor (MISC): A User's Guide

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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, 3, 4, 7]. 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 [6]
endf6.dk	decay chain	radioactive isotope decay chain information from ENDF/B-VI [7]
endf7.dk.xml	decay chain	radioactive isotope decay chain information from ENDF/B-VII.1 [4]
endf6.idx	particle emission	radioactive particle emission index built from data in ENDF/B-VI [7]
endf7.idx.xml	particle emission	radioactive particle emission index built from data in ENDF/B-VII.1 [4]

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.

Keyword	Use	Description
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 <i>endf6.dk.xml</i> and <i>endf7.dk.xml</i> .
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 <i>nist.na.xml</i> .
pelib	required	The “pelib” keyword specifies the particle emission library to be used for the calculation. Currently, the available values are <i>endf6</i> and <i>endf7</i> .
output	optional	The “output” keyword specifies the name of the output file. The default is <i>misc.out</i> .
srcout	optional	The “srcout” keyword specifies the name of the source distribution file suitable for cut and paste into MCNP. The default is <i>source.out</i> .
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 <i>pelib</i> 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 <i>decay_data_file</i> keyword has decay chain information (see Table 1).
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.

Keyword	Use	Description
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. Currently, the only available argument is “uniform” which produces a uniform biasing over the source distribution.
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.
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.

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

^awhere applicable, the integer and character designators correspond to the same integer used by MCNP

^bthe 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 j th daughter in the decay chain N_j after a time t can be expressed [8]

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

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

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

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 [2]

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

where W is a dimensionless unit of energy given as

$$W = \frac{E + m_o c^2}{m_o c^2}. \quad (4)$$

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

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

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 [5]

$$I(E_x)dE_x = CZ(E_e - E_x). \quad (6)$$

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

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

The constant C is a function of the Z -number and is tabulated for various Z 's by McCall [5]. 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

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

References

- [1] G. Erdtmann and Werner Soyka. *The Gamma Rays of the Radionuclides*. Verlag Chemie, 1979.
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- [3] R. Gunnick and J.F. Tinney. *Analysis of Fuel Rods by Gamma-Ray Spectroscopy*. UCRL-51086, Lawrence Livermore Laboratory, 1971.
- [4] 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.
- [5] G.H. McCall. Calculation of x-ray bremsstrahlung and characteristic line emission produced by a Maxwellian electron distribution. *Journal of Physics D: Applied Physics*, 15:823–831, 1982.
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- [7] 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.
- [8] 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 $0.5 \text{ y} = 1.58\text{e}7 \text{ s}$ (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
estobrem = 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/cm³

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/cm³

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

Material density: 1.89370e+01 g/cm³

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/cm³

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
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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/cm³

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/cm³

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
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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	cm ⁻³ s ⁻¹	g ⁻¹ s ⁻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	cm ⁻³ s ⁻¹	g ⁻¹ s ⁻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	cm ⁻³ s ⁻¹	g ⁻¹ s ⁻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