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Title: MCNPs Easy Sources for (a,n) (MESA) 1.0: A User’s Guide

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MCNPs Easy Sources for (α,n) (MESA) 1.0: A User's Guide

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1 Introduction

MCNPs Easy Sources for Alpha,N (MESA) facilitates the construction of MCNP source definition cards for (α,n) sources. It is a complete re-write of the homogeneous, surface source, and three layer problem types from Sources4c[4]. Please refer to this reference for documentation on the cross-sections and neutron emission spectra. The one departure from Sources4c is the use of alpha energies and activities from the ISC ENDF VII[2] or VIII[1] library specified by the user.

2 Data Files

Table 1. MESA data file summary

File	Type	Description
nist.na.xml	abundance	natural abundance and masses of isotopes from the National Institute of Standards and Technology [3]
s4c.atxs.xml	total charged particle cross-sections	Fits to atomic and nuclear cross sections for charged particles imported from Sources4c `tape2`.
s4c.anxs.xml	(α,n) cross-sections	Cross sections imported from Sources4c `tape3`.
s4c.nem.xml	n-emission library	neutron emission as a function of excited level imported from Sources4c `tape4`.

3 Usage

3.1 Input Specification

The MESA utility takes a single command-line input-file parameter and produces a source output file (default name “alphan.sdef”) containing the source distributions suitable for copy-and-pasting into an MCNP input file. The MESA 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. 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**.

Table 2. Description of keywords of MESA input

Keyword	Use	Description
iscdata	required	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 precedence 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*, *endf8.dk.xml* and *am.dk.xml*.
pelib	required	The “pelib” keyword specifies the particle emission library to be used for the calculation. Currently, the available values are *endf6*, *endf7*, *endf8* ,*radsrc*, *irtape11e*, and *irtape11l*.
output_file	optional	The “output_file” keyword specifies the name of the output file that can be copied into MCNP. The default is *alphan.sdef*.
alpha_output_file	optional	The “alpha_output_file” keyword specifies the name of the alpha output file that can be copied into MCNP as a source. The default is *alpha_decay.sdef*.

Keyword	Use	Description
source_zaids	required	list of ZAIDs to be considered the source material for all problems and both the source and target for `homogeneous` problems.
source_fracs	required	list of isotope fractions to be considered the source material. Only atom fractions are allowed at this time. If values do not sum to one they will be normalized.
source_density	required for homogeneous	The "source_density" keyword specifies the density of the source material. Positive values are interpreted as atom densities (atom/barn-cm), 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).
min_neutron_energy	optional	minimum neutron energy to tabulate to (default = 0 MeV).
max_neutron_energy	optional	maximum neutron energy to tabulate to (default = 11 MeV).
neutron_energy_bins	optional	neutron energy groups to tabulate (default = 110).
alpha_energy_groups	optional	number of alpha energy groups to use (default = 4000)
min_alpha_energy_bin	optional	minimum energy to calculate alphas to (default = 1E-6 MeV).
cosine_groups	optional	number of cosine groups to use for transmission calculations in three-layer problems.
target_zaids	required	list of target material ZAIDs
target_fracs	required	list of target material atom fractions
target_density	required	density of target material. Positive for atom density negative for mass density.
target_isgas	optional	use gas cross section for stopping power (default = false). Must be lower case true/false or 1/0.
barrier_zaids	required	list of barrier material ZAIDs

Keyword	Use	Description
barrier_fracs	required	list of barrier material atom fractions
barrier_density	required	density of barrier material. Positive for atom density negative for mass density.
barrier_isgas	optional	use gas cross section for stopping power (default = false). Must be lower case true/false or 1/0.
thickness	required	thickness of barrier layer in cm.

3.2 Running MESA

MESA 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:

```
mesa source1.inp
```

If the user *has not* specified the "output_file" keyword in the input file, then the default output file "alphan.sdef" will be created. In addition an "alpha_decay.sdef" will be created that provides the initial alpha source used for the calculations.

4 Theory

This utility can calculate three different types of problems: homogeneous, interface, and three layer. The first type assumes a material of sufficient thickness that to first order all alphas stop in the material. Based on this approximation it calculates the density of states a given initial energy alpha particle will populate as it slows down and then the distribution of resulting neutron emission energies. The second type of problem assumes an effectively infinitely thick alpha source interacting with an effectively infinitely thick production material. For this approximation no source density is required. Finally the third problem type assumes a source material, a barrier layer, and a target material. In this problem type the source and target are assumed to be effectively infinitely thick while the barrier is finite. This problem calculates neutron production in both the barrier and the target layer. With the production in each being modified by the alpha energies reaching that material. Please see the Sources4c manual[4] for a detailed description of the approximations used to calculate the (α,n) production in all three cases.

5 Basic Homogeneous Example Input

The first example is intended to be nearly identical to the sample problem 1 from Sources4c. Note that Sources4c expects sources listed in atoms per cubic centimeter by isotope and seperately density and Z atom fraction of stopping materials. In contrast mesa uses a single unified material definiton for soures and stopping materials. It is therefore not possible to exactly translate one to the other due to rounding in the Sources4c problem definition. It is a standard PuBe source setup.

5.1 Input

```
[global]
# This is a nearly identical PuBe source to sample 1
# from Sources4c documented in LA-UR-02-1839
problem_type = homogeneous
source_zaids = 94237 94238 94239 94240 94241 94242 4009
source_fracs = 1.511e-19 8.106e-06 0.0669 0.00430 0.000190 1.403e-05  0.928571
source_density = .084
min_neutron_energy = 0
max_neutron_energy = 12
neutron_energy_bins = 48
```

6 Three-layer-input

This example is intended to be nearly identical to example 7 from Sources4c. It includes a plutonium source, an aluminum barrier layer, and a beryllium target layer.

6.1 Input

```
[global]
# This three layer problem is intended to be nearly identical
# to example 7 from sources 4c documented in LA-UR-02-1839
problem_type = three_layer
source_zaids = 94238 94239 94240 94241 94242 95241
source_fracs = 0.0005 0.9233 0.0650 0.0100 0.0010 0.0002
# Note: source_density in three-layer problems
barrier_zaids = 13027
barrier_fracs = 1.
barrier_density = .15
barrier_thickness = .00001
target_zaids = 4009
target_fracs = 1.
target_density = -1.86
min_neutron_energy = 0
max_neutron_energy = 10
neutron_energy_bins = 20
alpha_energy_groups = 400
```

References

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