FISPACT-II Extended exercises

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1 Exercise PULSES

This exercise examines the use of the `PULSE` keyword. The `PULSE` keyword is a compact way of representing repetitive irradiation scenarios, for example ignoring the early startup phase of H and DD irradiation, we expect 2 shifts of 8 hours each, running pulses of 300 seconds duration followed by 1500 seconds of dwell (flux off), followed by 8 hours of decay, 5 days a week with weekends off, for say 10 years. Using the `PULSE` keyword, we can model this using:

```
PULSE 10
  PULSE 5
    PULSE 2
      PULSE 8
        FLUX 1.0E14
        TIME 300 ATOMS
        FLUX 0.0
        TIME 1500 ATOMS
      ENDPULSE
      FLUX 0.0
    ENDPULSE
    FLUX 0.0
    TIME 8 HOURS ATOMS
  ENDPULSE
ENDPULSE
```

Note the above example is more verbose than needed for clarity, one could do this more compactly but perhaps less clearly:

```
PULSE 50
  PULSE 16
    FLUX 1.0E14
    TIME 300 ATOMS
    FLUX 0.0
```

```
    TIME 1500 ATOMS
  ENDPULSE
  FLUX 0.0
  TIME 8 HOURS ATOMS
ENDPULSE
```

1.1 Example A

In order to convince yourself that PULSE works, look at the at the example pulses.i example and introduce a multilayer irradiation schedule problem. So, lets say that we want to do 10 days of irradation, where in a single day, we have 1 hour of irradiation, followed by 11 hours of decay, twice.

1. Construct your example using the pulse keyword
2. Do the same as (1) but without the pulse keyword

1.2 Example B

1. MAST Upgrade - a device at CCFE is expected to run 52 weeks a year, 5 days a week (with weekends off), there are pulses 8 hours per day, and in any given hour there will be 2 pulses of 5 seconds duration, with $\sim$ 30 mins between pulses. Using the file included complete the irradiation section that defines this irradiation schedule - compute the activity after 1 year of operation, at shutdown 1 hour and 10 years decay time
2. Compute the same as in (1) but ensure that the activity is calculated immediately following the last pulse
3. Compute the activity as in (2) but at the following decay times, 5 mins, 1 hour, 1 day, 30 days, 60 days, 90 days, 180 days, 1 year, 2 year, 3 year, 5 year, 10 year, 20 year, 30 year, 50 year and 100 year

2 Exercise Waste Classification

FISPACT-II is a natural tool for assessing the waste classification of a given sample under set irradiation conditions. The following exercises will demonstrate how this analysis can be performed with FISPACT-II. We will consider the example of a steel undergoing long term neutron irradiation, followed by cooling.

1. The FISPACT input file **waste_exercise1.i** contains an approximate traditional stainless steel composition:

   ```
   << ----- steel composition ----- >>
   DENSITY 7.9
   MASS 1 9
   ```

```
FE 62.395
C 0.03
MN 2.0
CR 18.5
NI 13.5
P 0.045
S 0.03
SI 1.0
MO 2.5
```

1kg of this 'steel' will be irradiated with a 709 group neutron flux (in the file **fluxes**) representative of that expected to be experienced by the DEMO fusion reactor's near-plasma components. This 'steel' is irradiated with an energy integrated flux of 2.49068×10^{14} $\mathrm{cm}^{-2}\mathrm{s}^{-1}$, (DEMO's maximum power) for 1 day. It is then allowed to cool for 500 years. Run FISPACT-II with this input file.

(a) The UK's Low Level Waste requirements are that a sample must have total α activity less than 4 MBq/kg and the total $\beta+\gamma$ activity less than 12 MBq/kg. Study the output file produced (**waste_exercise1.o**), when would this composition meet the UK's low level waste requirements?

(b) Spain's low level waste criteria uses the activities from several nuclides as well as total α and $\beta+\gamma$ activity to determine waste classification. Spain's limits for α activity is 1.85×10^5 Bq/kg and it's $\beta+\gamma$ limit is 3.7×10^7 Bq/kg. When would the steel achieve these limits?

(c) Determine when the sample would meet the following nuclide limits set by the Spanish Low Level Waste system:

- ^{60}Co activity below 3.7×10^6 Bq/kg
- ^{99}Tc activity below 1×10^6 Bq/kg
- ^{55}Fe activity below 3.7×10^7 Bq/kg

(d) This FISPACT-II output file contains the 20 dominant nuclides at each time step contributing to Activity, Heating and Dose rates. Study the 'Dominant Nuclides' at last cooling step in the output file generated in this example. How many of the dominant nuclides could could not of been present before irradiation?

2. Let us suppose that the idealised composition used in the previous example is discovered to truly contain additional impurities. Take its 'true' composition to be:

```
<< ----- steel composition ----- >>
DENSITY 7.9
MASS 1 13
```

```
FE 61.395
C 0.03
MN  2.0
CR 18.5
NI  12
P 0.035
S  0.03
SI  1.0
MO  2.3
O  1.2
N  1.0
NB  0.01
SN 0.5
```

The file **waste_exercise2.i** will irradiate 1kg of this composition under the same scenario as was used previously. From the generated output files determine:

(a) When would this composition meet UK and Spain's total α and $\beta+\gamma$ activity limits? How does this differ from the previous composition?

(b) Extract the specific activities (Bq/kg) of the following nuclides for both the previous composition (**waste_exercise1.o**) and the new composition (**waste_exercise2.o**) 100 years after irradiation.

- ^{14}C
- ^{94}Nb
- ^{63}Ni

How has the change in composition effected these activities? Are any of the changes surprising?

3. The previous exercises have assumed that the steel compositions only experience 12 hours of irradiation from DEMO. In reality almost all steel components of DEMO will experience years of irradiation.

(a) The input file **waste_exercise3.i** is identical to that used in exercise 2.

- Modify this file to irradiate the steel for 1 year rather than 1 day.
- Currently the input file cools for 500 years, increase this to 3000 years wit two 250 year time steps and 2 1000 year time steps.
- Run the modified input file.

When will the total β activity be less than 100 times the UK's $\beta+\gamma$ limit?

(b) Extract the activities for ^{60}Co, ^{99}Tc, ^{55}Fe for the cooling steps. When are they less than the limits given in exercise 1? Do any fail to ever meet the requirements?

(c) Study the specific activity (Bq/kg) from ^{14}C 3000 years after irradiation ceased. How does this compare to the results found in exercise 2 after 100 years? How much has the specific activity changed by?

(d) Based on the results of all 3 exercises, is it likely that traditional stainless steels will be called Low Level waste after use in a DEMO like fusion reactor?

3 Exercise Pathways Analysis

It is often required to understand how a given nuclide is created within a sample under irradiation. The following exercises will use FISPACT-II's pathways output to study this. FISPACT-II will print the reaction pathways to the output file if the **UNCERTAINTY** keyword is included in the input file. These exercises will use the TENDL 2017 nuclear data set.

1. **pathways_exercise1.i** irradiates a 1kg of Nickel, made up of 5 isotopes in natural abundances, for 1 year with a flux representative of that experienced by the near-plasma components of DEMO fusion reactor operating at 30% power.

   (a) How any unique nuclides have been added to the inventory during the irradiation?

   (b) By studying the pathways output determine the following:

   - How many pathways produce ^{59}Fe?
   - Which is the most likely pathway for the creation of ^{60}Co?

   (c) By studying the Uncertainty Estimates determine:

   - What is the error associated with Total Decay heat?
   - Of the quantities printed, which errors is the greatest and least percentage of the total?

2. **pathways_exercise2.i** irradiates a 1kg mixed sample of Fe (80%), C (2%), Cr (10%) and Ni (8%) for 1 minute with a 709 group flux representative of that experienced by the near-plasma components of DEMO fusion reactor operating at 30% power. The sample under goes no cooling steps. Run FISPACT-II with this input file.

   (a) Study the Dominant Nuclide tables and the pathways in **pathways_exercise1.o**. For the following quantities extract the dominant nuclide, the dominant reaction which created it and the parent nuclide for that reaction.

   - Activity
   - Dose Rate
   - Ingestion
   - Inhalation

(b) For this sample ^{55}Fe is created from multiple sources. Approximately how many atoms of ^{55}Fe have been created from the following sources:

- $^{54}\mathrm{Fe}(n,\gamma)\ ^{55}\mathrm{Fe}$.
- $^{56}\mathrm{Fe}(n,2n)\ ^{55}\mathrm{Fe}$.
- All other reactions.

3. If the composition from exercise 2 is irradiated for a longer time period the build up of new nuclides will allow new pathways to open. Run FISPACT-II with the input file **pathways_exercise3.i**. This subjects the same composition from question 1 to the same flux, but for 1 day rather than 1 minute.

   (a) Find the pathways for the creation of ^{61}Co in both **pathways_exercise2.o** and **pathways_exercise3.o**. What has the longer irradiation time changed about the available pathways?

   (b) ^{52}Cr is the most numerous (by number of atoms) isotope of Cr before irradiation. Identify the pathways and reactions which have ^{52}Cr as a parent nuclide in **pathways_exercise3.o**.

4 Exercise Self-Shielding

As described in the accompanying lecture, accounting for the influence of giant-resonances on both the transport of neutrons through a material and on the reaction rates of neutron-capture events is vital to correctly predict transmutation rates in some materials. This exercise will demonstrate how FISPACT-II can account for the latter (a 3D transport code must be relied upon to address the former). A number of different elements can be influenced by self-shielding, but here let's stick to the same tungsten as considered in the lecture.

1. **exercise_1/W_noSSF.i** performs a basic 10 year irradiation of pure W in a typical fusion first wall flux and uses TENDL-2017 nuclear libraries. Using the elemental breakdown of the material at the end of the 10 years (identified as "COMPOSITION OF MATERIAL BY ELEMENT" in the output file), what are the atom % concentrations of W, Re, and Os at the end of the irradiation?

2. **exercise_2/W_SSF.i** extends the basic simulation to include the required coding to self-shield all naturally occurring isotopes of W:

```
<< -----self-shielding correction----- >>
PROBTABLE 0 1
SSFCHOOSE 1 0
W
SSFMASS 1.0 1
W 100.0
```

The remainder of the file is identical to the first case. What are the W, Re, Os concentrations after 10 years this time?

3. If the concentration of a transmutation product becomes significant then its subsequent reactions must also be properly self-shielded. However, this is not a straightforward task since the composition is constantly changing. The file **exercise_3/W_SSF_ext.i** is identical to that used in exercise 2. Using the final composition from exercise 2 as an estimate, modify this input file to tell FISPACT-II to self-shield the isotopes of Re. How do the final concentrations of Re and Os differ compared to the previous case? Note that this approach to account for "secondary" self-shielding is only approximate – is there an alternative approach to produce a more realistic prediction?

5 Exercise graphical plotting

This exercise explores some of the additional output files from FISPACT-II – ones more suited to plotting, as well as a first illustrationg of how to compare results with different nuclear data libraries (the following exercise will build on this). These features are used extensively in the FISPACT-II validation & verification suites – including the fusion decay-heat benchmark discussed in the lecture.

1. **exercise_1/Zr.i** runs the 5-minute irradiation decay-heat benchmark simulation for pure zirconium. To rapidly access (and plot) the decay-heat evolution the `GRAPH` keyword is used to instruct FISPACT-II to output the evolution in this quantity in a separate **exercise_1/Zr.gra** file. After running FISPACT-II, there should be an accompanying **exercise_1/Zr.plt** file that can be invoked through `GNUPLOT` to produce a postscript plot. Options of the `GRAPH` keyword allow additional plots to be produce, as well as allowing the format of the **exercise_1/Zr.gra** to be modified to suit different needs. Explore these.

2. To understand the behaviour observed in the total decay-heat, FISPACT-II can provide an additional output that details the radionuclide breakdown to the total heat. This is controlled via the `NUCGRAPH` keyword.

   ```
   NUCGRAPH 1 1.0 1 2
   ```

   After running the simulation defined in **exercise_2/Zr.i** there should be a **exercise_2/Zr.grn file** that gives the decay-heat contributions from the dominant nuclides. A template gnuplot plot file **exercise_2/Zr.prn** is also produced, although this should only be used a as guide/example. As with the `GRAPH` keyword, there are various options that can be modified to change the style of output in **exercise_2/Zr.grn** and/or the radiological quantities considered. Explore these.

3. The results from the above 2 examples were all computed by FISPACT-II using the TENDL-2017 nuclear cross section data library and associated decay-2012 decay library. However, as was discussed in the lecture on the decay-heat benchmark, there can be significant variation in simulation results depending on the input nuclear data provided to FISPACT-II. The **exercise_3/Zr.i** is identical to that used in exercise 2, but the folders listed in **exercise_3/files** are instead those corresponding to the JEFF-3.3 international library (Joint Evaluated Fission and Fusion file) – some modification may be required to get this running.
   Using GNUPLOT or other, compare the TENDL-2017 results to those from JEFF-3.3. An additional file of experimental data points (**exercise_3/Zr_exp.dat**) is provided, but note the different units compared to those in the FISPACT-II output. Plot these experimental points on the same graph as the two simulation curves. Which library gives the best match to the experiment? Use `NUCGRAPH` to explore the reason behind any differences.

- Check http://fispact.ukaea.uk/wiki/Keyword:NUCGRAPH and http://fispact.ukaea.uk/wiki/Keyword:GRAPH for more details

6 Exercise library variations

This exercise explores how to run identical simulations with different input nuclear data and then how to compare the results. The examples here are taken from the decay heat benchmark already described in the lectures.

- **Ni-tendl17.i** & **tendl17.files** runs the 5-minute irradiation decay-heat benchmark simulation for pure nickel with the TENDL-2017 nuclear data libraries. As before the `GRAPH` and `NUCGRAPH` keywords are used to provide rapid access to the decay-heat quantities (totals and nuclide contributions).

- to run this example, you will need to specify the **tendl17.files** on the command line with the input file.

- repeat the simulation with the equivalent input files for the JEFF-3.3 and ENDF/B-VIII libraries

- the total decay-heat results can be plotted separately using the .plt files created by FISPACT-II, but can you modify this to plot the results from the different libraries. An experimental results file is also provided.

- notice that the different libraries produce different decay-heat evolutions; can you use the .grn files or similar to work out what is different about the libraries considered?

- example plotting scripts are provided to help you with this

7 Exercise extractxs

This example makes use of the *extract_xs_endf* tool, which can be used to get group wise energy dependent cross sectional data.

Similar to *compress_xs_endf* the tool does not take an input file and uses a reduced files file. The same files file and fluxes file from the compress exercise can also be used here - we will again use the TENDL2017 library.
Again, you can set an environment variable to point to the binary.

```
[$] export EXTRACT=/path/to/extract_xs_endf
```

The command line arguments are then:

```
[$] $EXTRACT <name> <particle> <group> \
<parent-nuclide> <mt-number> <daughter-nuclide> <filesfile>
```

MT numbers refer to that of the ENDF-6 format and can be found in the manual or on the FISPACT-II website `https://fispact.ukaea.uk/wiki/ENDF_file_definitions_and_supplied_nuclear_data`. When using total cross section (MT=1) the daughter-nuclide option can be anything, as it will be ignored.

Can you extract the total cross section for tritium (H3) and plot it? It should look like figure 1.

Can you plot the (n,g) contribution (MT=102) for Al^{24} as a function of energy? It should look like figure 2.

A bash script exists which allows you to extract data from TENDL 17 and is customisable for any reaction and any particle. The script is aptly named *runextract.sh*.

8 Exercise groupconvert

This example makes use of the *GRPCONVERT* keyword in FISPACT-II which allows users to convert incident particle energy spectra from an arbitrary group structure to a FISPACT-II group structure.

Using group convert there are two possible options. Convert from one group structure to another which is of different size, or convert within the same group size, but where the bin boundaries are altered. FISPACT-II uses a set of internal group structures which cover all the necessary structures for the nuclear data libraries shipped with FISPACT-II. If you are using a bespoke library with a different structure this can be catered for by using *GETXS 1 1* option (not covered here and not recommended). The internal group structures have a 66, 69, 100, 162, 172, 175, 211, 315, 351, 586, 616, 709, and 1102 size, the actual energy bounds of these groups can be found here `https://fispact.ukaea.uk/`

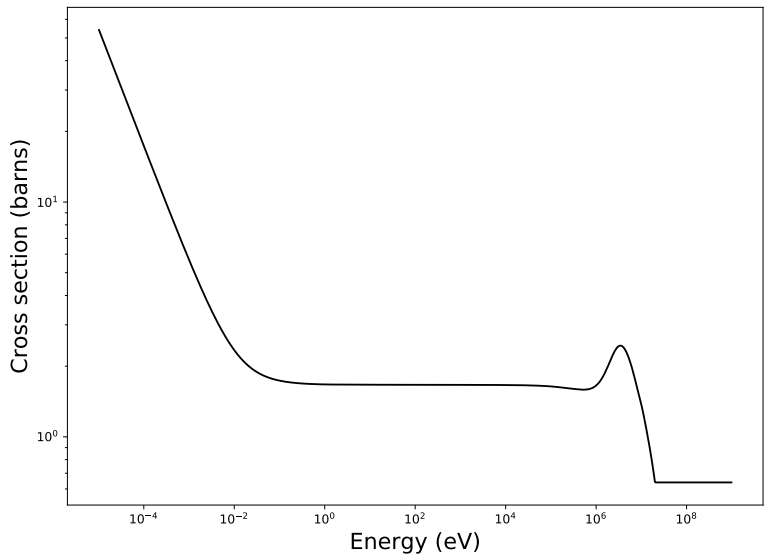

Figure 1: The energy dependent total cross section for tritium, from TENDL 2017 in 709 group.

`wiki/Keyword:GETXS`. The official python package *pypact* also has these ready to use. Note that group structures are typically defined in descending order, due to legacy reasons.

The first part of this exercise will convert a energy spectra from group 66 to group 709. The FISPACT-II group structures are shown for these two groups in figure 3.
Can you use the *fluxes66.in* file in the 'groupconvert' directory to convert to the FISPACT-II 709 group? An input file, *66.to.709.i* has been prepared to show you how to do this.

```
[1206][user1@fispact:~/exercises/extended/groupconvert] ls
    fluxes66.in   fluxes709.in    files.66.to.709    66.to.709.i
    66.to.709_2.i
```

The default conversion option uses equal lethargy, can you do the same conversion again but now using equal energy? You will need to use the keyword *CNVTYPE* to change the conversion type.

After doing the conversion both ways can you plot the three spectra (one input in 66 and two output in 709) and compare per unit energy? It should look like figure 4.

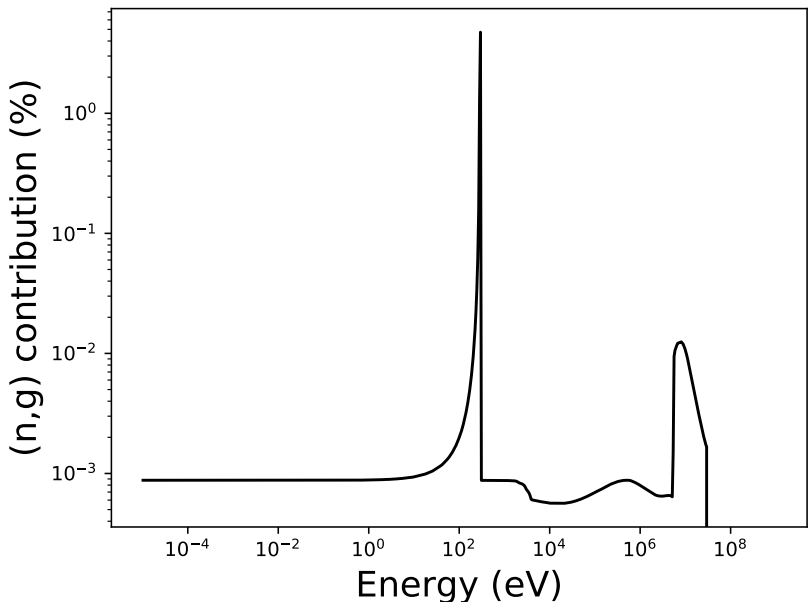

Figure 2: The energy dependent (n,g) contribution for Al^{24}, from TENDL 2017 in 709 group.

Extra effort: Can you convert the output 709 spectra to group 172 and then to group 66? Can you compare this with the original input? Do they match up?

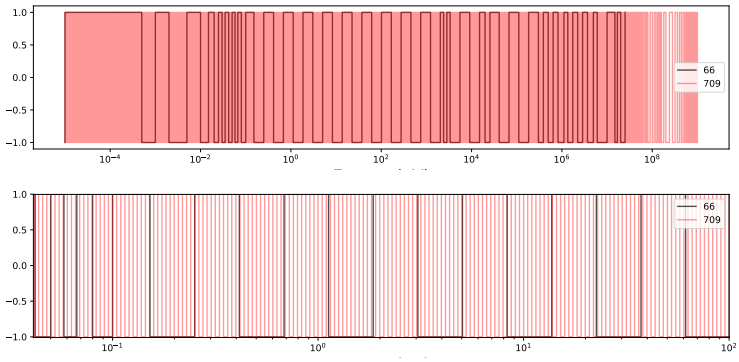

Figure 3: The energy group structure for group 66 and 709 used in FISPACT-II. The red lines indicate the 709 group and black lines indicate group 66 bounds. The upper plot shows the full range, whilst the lower plot focuses on a smaller range to show how the groups overlap.

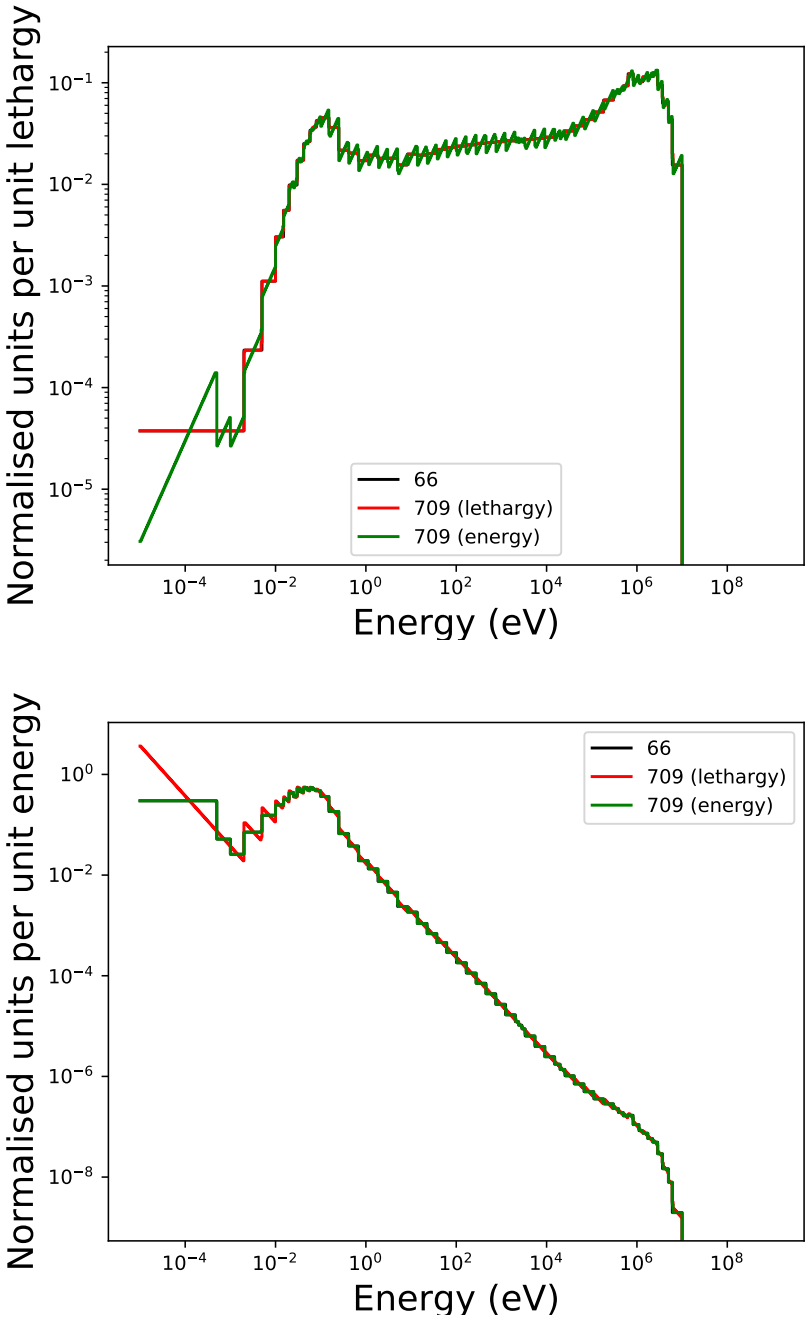

Figure 4: Upper: The incident particle energy spectra per unit lethargy for an input arbitrary flux in a 66 group structure (black) compared to the corresponding 709 group energy spectra using equal lethargy conversion (red) and equal energy conversion (green). Lower: The incident particle energy spectra per unit energy for an input arbitrary flux in a 66 group structure (black) compared to the corresponding 709 group energy spectra using equal lethargy conversion (red) and equal energy conversion (green).