FISPACT-II Extended exercises

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1 Exercise PULSES

This exercise examines the use of the `PULSES` keyword. The `PULSES` 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 `PULSES` keyword, we can model this using:

```
PULSES 10
  PULSES 5
    PULSES 2
      PULSES 8
        FLUX 1.0E14
        TIME 300 ATOMS
        FLUX 0.0
        TIME 1500 ATOMS
      ENDPULSES
      FLUX 0.0
    ENDPULSES
    FLUX 0.0
    TIME 8 HOURS ATOMS
  ENDPULSES
ENDPULSES
```

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

```
PULSES 50
  PULSES 16
    FLUX 1.0E14
    TIME 300 ATOMS
    FLUX 0.0
    TIME 1500 ATOMS
```

```
  ENDPULSES
  FLUX 0.0
  TIME 8 HOURS ATOMS
ENDPULSES
```

1.1 Example A

In order to convince yourself that PULSES 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 pulses keyword
2. Do the same as (1) but without the pulses 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** flag is included in the input file. These exercises will use the TENDL 2017 nuclear data set.

1. **pathways_exercise1.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. 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.

2. If the composition from exercise 1 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_exercise2.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_exercise1.o** and **pathways_exercise2.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_exercise2.o**.

(c) From the number of atoms of the daughter nuclides estimate how many atoms of ^{52}Cr are lost during from the pathways identified in exercise 2b. Why is this not possible to calculate from the number of ^{52}Cr atoms directly?

(d) Study the file **pathways_exercise1.json** outputted from this input. Use this to calculate the number of ^{52}Cr before and after irradiation. How does this compare to your previous results? What does this result suggest?

3. **pathways_exercise3.i** changes the composition of the material studied to what is seen below.

```
<< ----- 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 flux remains unchanged, but the irradiation scenario has been altered; the sample is irradiated for 1 year. The resulting pathways are much more complex.

(a) ^{99m}Tc, the most commonly used medical isotope, happens to be created during this irradiation. Extract the pathways which create and destroy ^{99m}Tc from the output file.

(b) Compare the pathways resulting ^{60}Co in this output and that from exercise 2. What has the increased irradiation time allowed to occur which has changed the ^{60}Co pathways.

(c) Most of ^{57}Co is created via either the $^{58}\text{Ni}(n, np)^{57}\text{Co}$ or $^{58}\text{Ni}(n, d)^{57}\text{Co}$ reactions. Estimate how many atoms of ^{57}Co are created from each reaction?

(d) Modify the input file by adding the **SORTDOMINATS** keyword. This will increase the number of dominant nuclides, and therefore possible pathways, outputted. Ensure that the output file includes the 40 dominant nuclides, run this file. By studying the new output file determine which nuclide present before irradiation is most commonly the source of the following nuclides present after irradiation:

- ^{95}Nb
- ^{124}Sb
- ^{60}Co
- ^{55}Fe

4 Pathways Analysis answers

1. Question 1

(a)

Quantity	Dominant	Reaction	Parent
Activity	^{55}Cr	(n,γ)	^{54}Cr
Dose Rate	^{52}V	(n,p)	^{52}Cr
Ingestion	^{56}Mn	(n,p)	^{56}Fe
Inhalation	^{62}Co	(n,p)	^{62}Ni

(b) Total number of ^{55}Fe atoms = 1.22199×10^{14}

- 1.082×10^{14} atoms
- 1.361×10^{14} atoms
- 1.774×10^{12} atoms

2. Question 2

(a) Added additional pathway, 3.081% created via $^{64}\text{Ni}(n,\alpha)^{61}\text{Fe}$ then β^- decay to ^{61}Co.

(b) ^{52}Cr is used to create:

- 99.547% of ^{52}V via $^{52}\text{Cr}(n,p)^{52}\text{V}$
- 1.557% of ^{51}Cr via $^{52}\text{Cr}(n,2n)^{51}\text{Cr}$

(c) ^{52}Cr :

$$\begin{aligned}\text{Atoms lost} &= \text{Atoms of } ^{52}\text{V created} + \text{Atoms of } ^{51}\text{Cr created}\\ &= (99.547\% \text{ of } 2.88571\times10^{12}) + (1.557\% \text{ of } 8.20952\times10^{16})\\ &= 1.281\times10^{15}.\end{aligned}$$

The difference is smaller than the accuracy printed in the output so no change is apparently seen.

(d) json gives atoms lost as 1.527135×10^{17}. This is larger than that calculated from the pathways analysis, suggesting that some ^{52}Cr is lost via other pathways which do not produce dominant nuclides or

output file is not accurate enough for such work. For small changes the output file does not provide the required accuracy, so use json files

3. Question 3

   (a) creation:

   ```
   Mo 98 ---(R)--- Mo 99 ---(d)--- Tc 99m---(S)---
   ```

   destruction :

   ```
   Mo 98 ---(R)--- Mo 99 ---(d)---
   Tc 99m---(b)--- Tc 99 ---(R)--- Tc100 ---(S)---
   ```

   (b) ^{59}Fe is allowed to decay so extra pathways are produced.

   (c) ^{57}Co atoms

   - $^{58}\mathrm{Ni}(n,np)^{57}\mathrm{Co}$ produces 8.185×10^{17} atoms
   - $^{58}\mathrm{Ni}(n,d)^{57}\mathrm{Co}$ produces 1.893×10^{16} atoms

   (d) most common source nuclides:

   - ^{95}Nb from ^{93}Nb
   - ^{124}Sb from ^{122}Sb
   - ^{60}Co from ^{60}Ni
   - ^{55}Fe from ^{54}Fe

5 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?

6 Exercise graphical plotting and library variations

This exercise explores some of the additional output files from FISPACT-II – ones more suited to plotting, as well as illustrating how to compare results with different nuclear data libraries. Both 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

7 Exercise compressxs

This example makes use of the *compress_xs_endf* tool, which can dramatically improve FISPACT-II run times when processing large nuclear data libraries, such as TENDL2017.

We will first do a simple inventory calculation using TENDL 2017, without compress. Run the input file *'simpleinventorywithoutcompress.i'*.

How long did it take to run? On my machine it took roughly 106 seconds. Most of the time was actual spent reading the TENDL 2017 cross section data.

Now we will run *compress_xs_endf* to compress the cross sectional data. The tool is a binary executable program, like FISPACT-II, and should reside in the same directory as the main FISPACT-II program. Again, you can set an environment variable to point to the binary.

```
[$] export COMPRESS=/path/to/compress_xs_endf
```

To run the tool, it requires a files file pointing to corresponding index and cross section data. It only requires these two paths, using the keys *ind_nuc* and *xs_endf*. No other entries should be required in the files file.
Can you construct this files file for TENDL2017 using neutron incident data? Name it files.tendl17_n.

No input file is required for the tool and just requires command line arguments. The command line arguments are then:

```
[$] $COMPRESS <name> <particle> <group> <option> <filesfile>
```

Here the name is the name of the binary file produced without the *.bin* extension, particle is the character indicating the incident particle (n, g, a, d, t, or p), group is the group structure (typically 709), option indicates whether to include uncertainties and covariances (option 5 does everything), and the files file should be the file we just created. Running *compress_xs_endf* will take some time, but it only needs to be performed once per host machine. A useful name would be *tal2017-n*. Try and run it and check the log to ensure no errors occurred.

In order to run the same inventory simulation but now with the newly compressed nuclear data library, we need to make a few changes to the input file and files file. The first step is to add an additional key and path to the files file. The key *xs_endfb* must now be added and point to our new binary file *tal2017-n.bin*. Secondly, in order for this path to be registered, the corresponding input file must be altered such that the *GETXS* keyword should have the 1 changed to -1 (this indicates to read from binary format). Note that without this, the standard text format will be used from the *xs_endf* path. Make these changes and create a new input file *simpleinventorywithcompress.i* based on the *simpleinventorywithoutcompress.i* but reading binary cross section data.

After running it what percent speed up do you get?
Hint: Use 'time' to precede the compress command to get the time taken in bash. On my machine it took roughly 64 seconds, almost 40% faster!

Check your output files have the same results.

We will now perform a more complex simulation, to highlight that the benefit of compress is diminished when enabling fission and using large irradiation schedules, as more time is spent solving the rate equation matrices and reading fission yield data, which is not included in the binary version. The input file *inventorywithoutcompress.i* reflects this added complexity using a fission case. Follow the same procedure as before and compare the runtimes and outputs. Again, check your output files have the same results, regardless of cross section format.

My runtime without compress was 181 seconds and with compress was 128 seconds - now only 30% speed up. The runtimes are very much machine specific.

A bash script exists which allows you to compress all versions of TENDL (14, 15, and 17) for all incident particles in one go (it will take a while). The script is aptly named *compress_all.sh*.

8 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*.

9 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

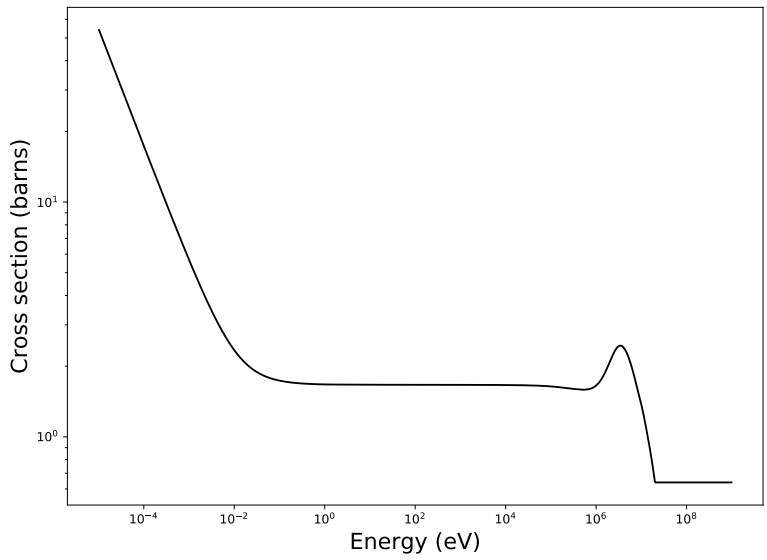

Figure 1: The energy dependent total cross section for tritium, from TENDL 2017 in 709 group.

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/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.

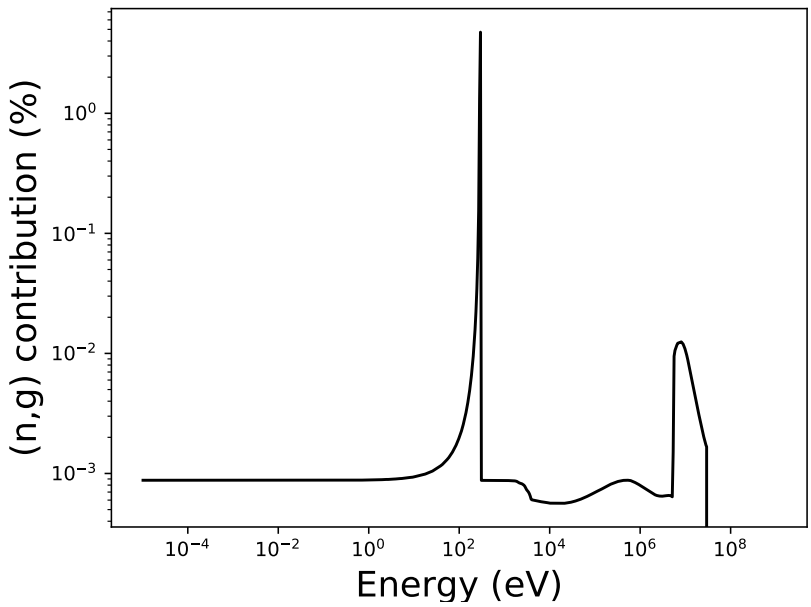

Figure 2: The energy dependent (n,g) contribution for Al^{24}, from TENDL 2017 in 709 group.

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.

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?

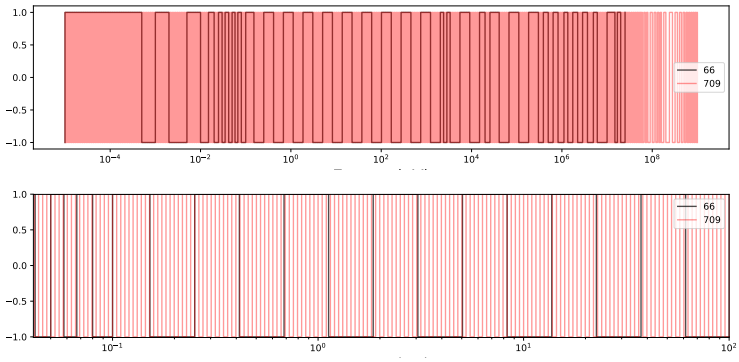

Figure 3: The energy group structure for group 66 and 709 used in FISPACT-II. The red lines indicate the 709 group and black lines indicate group 66 bounds. The upper plot shows the full range, whilst the lower plot focuses on a smaller range to show how the groups overlap.

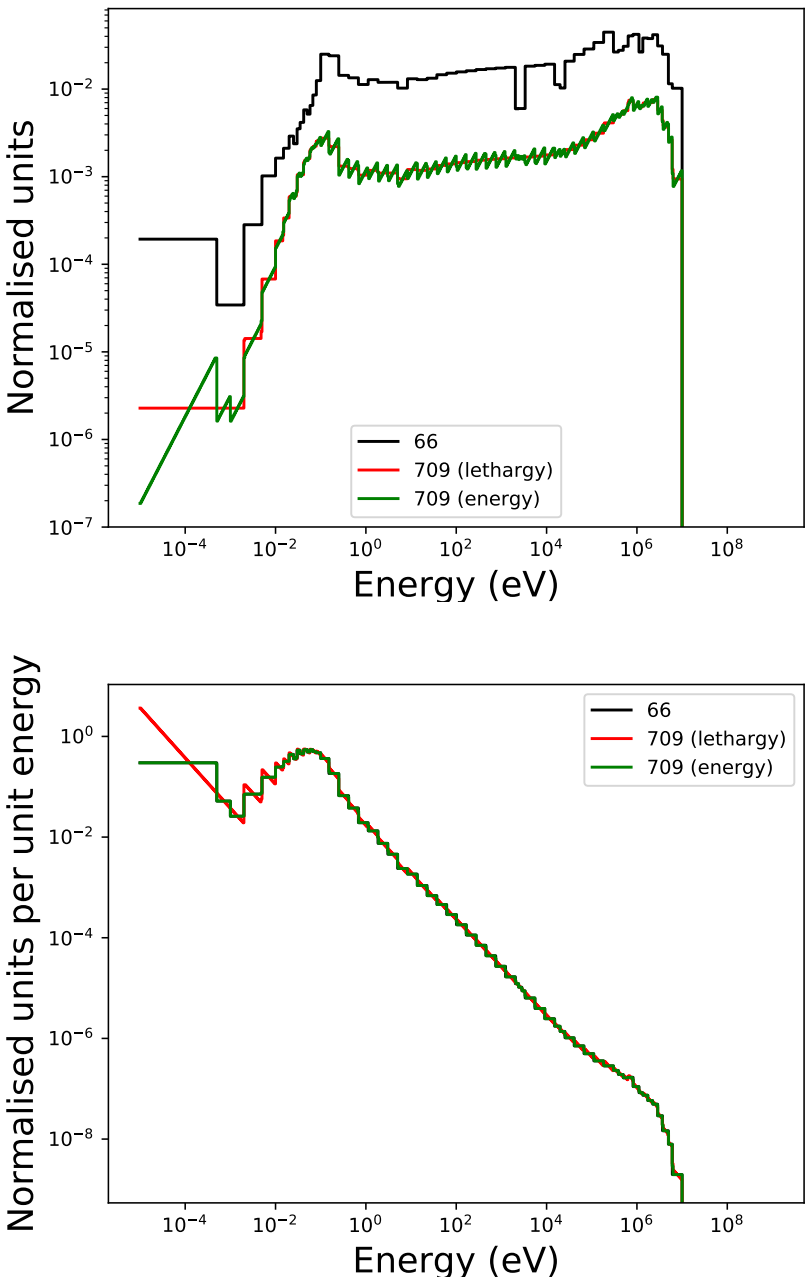

Figure 4: Upper: The incident particle energy spectra for an input arbitrary flux in a 66 group structure (black) compared to the corresponding 709 group energy spectra using equal lethargy conversion (red) and equal energy conversion (green). Lower: The incident particle energy spectra per unit energy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