

# User Manual

## ACTYS

*A Nuclear Activation Code*



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# 1 ACTYS

Nuclear activation is defined as the generation of radioactive isotopes via the process of nuclear reactions (transmutations) or radioactive decay. It is governed by the first-order linear differential equation, known as the Bateman equation [1]. In a homogeneous, infinite and infinitely dilute material, the time evolution rate of nuclides ‘i’ can be written as: [2]

$$\frac{dN_i}{dt} = -(\lambda_{ii} + \bar{\sigma}_{ii}\Phi)N_i + \sum_{j \neq i} (\lambda_{ij} + \sigma_{ij}\Phi)N_j \quad (1)$$

The first term on the R.H.S is the loss term for nuclide  $N_i$ .  $\lambda_{ii}$  is the total decay coefficient and  $\bar{\sigma}_{ii}$  is the total loss due to transmutation. The second term on the R.H.S is the gain term, the production of nuclide  $N_i$  from various other nuclides  $N_j$ .  $\lambda_{ij}$  is the decay of isotope  $N_j$  to isotope  $N_i$  and  $\sigma_{ij}$  is the average transmutation probability of isotope  $N_j$  to isotope  $N_i$ . The time evolution rate for all the ‘n’ isotopes in the material is a set of ‘n’ coupled first-order linear differential equations. Since  $\lambda_{ij}$  and  $\sigma_{ij}$  are independent of  $N_j$ , these can be written in a matrix form [3]:

$$\frac{d\mathbf{N}}{dt} = -\Lambda\mathbf{N}(t) \quad (2)$$

where  $\mathbf{N}$  is the matrix containing the concentration of all isotopes at time  $t$  and  $\Lambda$  is the matrix of coefficients given as

$$\Lambda_{ij} = \lambda_{ij} + \sigma_{ij}\Phi \quad (3)$$

The solution of the above equation is:

$$\mathbf{N}(t) = e^{-\Lambda t}\mathbf{N}(0) \quad (4)$$

ACTYS is a single point activation code, developed at ITER-India, IPR [4, 5]. It calculates the time evolution of the nuclide inventory and radioactivity of isotopes in a material when irradiated with the constant neutron spectrum using the analytical linear chain method. ACTYS forms the initial transfer matrix, given by the equation 3, for the system of N-nuclides. Linear chains starting from a parent nuclide, are then extracted from the matrix system using inverse tree-search in-depth mechanism. As the branching in the tree structure increases, each level is identified as ‘rank’, starting with rank=1 for parent and rank=2 for subsequent daughter nuclides. Successive increment in rank is coherent with branching level.

While tree structure is being developed starting from a parent nuclide, the branches are opened up into simplified linear chains. Analytical method (sum of exponentials) is applied to solve the linear chain for a nuclide at rank=m in the chain. The chain is further extended to include subsequent daughters at rank=(m+1) after it passes successfully through ‘chain termination’ checks. Numerical corrections are automatically applied for ‘loops’ in the chains. Special technique based on ‘taylor expansion’ is used if the analytical solution breaks-down. Solution convergence is

then obtained in most of the cases. Any non-convergence through this technique for specific chains are reported. Once all the significant chains from a given parent are followed successfully and terminated, the solution shifts to the next parent nuclide and the process begins once again till all parent nuclides are covered. The derivation of the Linear Chain method is given in Appendix A. ACTYS also calculates the nuclear responses like activity, gamma dose rate, decay heat, prompt and decay gamma spectrum, radwaste index, gas production and pathways for radioactive isotopes present in the activated material.

## 1.1 Getting ACTYS

The executable file and DATA folder of ACTYS can be obtained by emailing at [actys@iter-india.org](mailto:actys@iter-india.org). To keep record of users of the code, the intended user must provide details of the computer including MAC number and operating system of the system on which ACTYS will be used. Upon verification of request ACTYS package may be given to the user along with a license file. ACTYS package contains actys.exe or actys (executable for Linux systems), License file and a DATA folder.

To run ACTYS following are the prerequisite.

- Create a folder to keep ACTYS executable file and the license file and data folder.
- Run sample input files and compare the outputs generated with the sample output given and report if any discrepancy is found.

## 1.2 Data Libraries

1. ACTYS uses external libraries of cross sections and decay data to calculate the inventory of nuclides following irradiation and at various decay times.
2. The point-wise neutron cross-section data in standard 'ENDF-6' format is presently sourced from EAF-2007 and 2010 distributions(data libraries). These raw data files are then processed using data-processing software 'PREPRO' to obtain group-condensed libraries. The format of processed files is also maintained as 'ENDF-6'.
3. Possibility to use other known data libraries like JEFF, ENDF/B, JENDL, TENDL, FENDL etc is also foreseen, provided the data is in ENDF-6 format.
4. The standard energy-group structures distributed with the code are DABL69(46), WIMS (69), GAM-II (100), VITAMIN-J (175).
5. Decay data for all nuclides is taken from JEFFRDD3.1.2 data file.
6. The neutron spectrum input to the code should be available in one of the standard energy structures given in point 4. Conversion of an arbitrary group

flux into one of the standard structures is not yet possible in ACTYS and is a subject of future developments.

7. ACTYS can handle nuclides for the elements hydrogen ( $Z = 1$ ) to fermium ( $Z = 100$ ). List of nuclides is given in a ‘isotope list’ file
8. The light nuclides (1H, 2H, 3H, 3He and 4He) which are produced from reactions such as (n,Xp), (n,Xd), (n,Xt), (n,Xh) and (n,X $\alpha$ ), where X can signify multiplicity or any other outgoing particle or by protons and alpha decays are included in the inventories, in addition to their formation as the daughters of a reaction.

### 1.3 Preparation of Input File

There are several keywords used in ACTYS. These are given below:

---

ISO	material description is given isotope wise. Eg: Fe56 1.00E25
ELE	material description will be given element wise. Eg Fe 100
CROP	=0, Inventory Table at each time step will be printed =1, Inventory Table at each time step will not be printed
PATHWAY	=0, Pathways for will not be printed for any dominant isotopes >0, Pathways for will be printed for isotopes =1 contributing most towards activity =2 contributing most towards contact dose rate =3 contributing most towards decay heat =4 for isotopes listed under ANDRA radwaste classification =5 all above radiological quantities
GRP	Neutron Group Number
PATH	Prints the major pathways of any desired nuclide. Eg PATH n, in the next ‘n’ lines write the name of each ‘n’ isotopes
PPATH	Prints the pathways of all the significant daughters of a parent nuclide. Eg PPATH n, in the next ‘n’ lines write the name of each n isotopes
WARN	=0, Will not print any warning messages =1, Will print some important warning messages for debugging
FFILE	Write the name of Flux file next to it
TIME	time step for irradiation. can be given in (S)seconds, (M)minutes, (H)hours, (D)days and (Y)years.

---

The general structure of input file is given below. The numbers on the left represent the line number in the input file. Repetition of a line number implies that the user can chose between the two options given on the line numbers.

01. **ACTYS** Header for the input file (Can be anything)
02. **C:/ACTYS/Data** Address and name of DATA folder

03. Empty Line before material description
04. **ELE 1.0 KG** ELE- elemental composition and quantity in Kg
04. **ISO -1 AD** ISO- isotopic composition and AD for Atomic density
05. 1 Number of Elements or isotopes in the input material
06. **Cr 100** Element name and its weight fraction
06. **Cr50 1.0E25** Isotope name and its number of atoms
07. Empty Line before keywords
08. **CROP 0** CROP 1: isotopic inventory and related radiological quantities not printed
09. **GRP 175** Neutron spectrum group number
10. **DEBUG 0** Debugger. Takes values 0,1,2,3
11. **PATHWAY 0** Prints pathways for dominating isotopes
12. **PATH 1** Pathway for given isotopes
13. **Cr51**
14. **PPATH 2** Pathways for the daughter of given isotopes
15. **Cr50**
16. **Cr52**
17. **FLUX\_FILE C:\ ACTYS\ EU-FW** Neutron spectrum file name and address
18. Empty line before time scenario
19. **INTR 7** INTR followed by number of time steps
20. **TIME 2.00E+00 Y FLUX 2.68E+16** time step with duration and total flux value
21. **PULSE 2** Pulsed time scenario
22. **OFF 4.54E-02 D FLUX 0.00E+00**
23. **ON 4.63E-03 D FLUX 7.00E+18**
24. **STOP**
25. **TIME 1.00E+00 D FLUX 0.00E+00**
26. **TIME 1.00E+11 S FLUX 0.00E+00**

Another file required as input is the FLUX\_FILE. This file contains groupwise neutron spectrum. First column contains the average energy of the neutron group and the second column contains the neutron flux in  $n/cm^2 s^{-1}$ . The spectrum is given in the order of lowest to highest energy. General Structure of the file is given in Figure 1.

## 1.4 How to Run

1. **For Windows**
  - (a) Open Command window
  - (b) Go to the location where actys.exe is kept.
  - (c) Check the address of data folder and flux file given in input file is correct.
  - (d) run actys.exe by typing actys.exe in the command window.
  - (e) the program will ask for the name of the input file. If the location of input file and executable is same, write the name of the input file only.

1.00E-07	2.00E+10
4.14E-07	2.30E+10
5.32E-07	2.88E+10
6.83E-07	3.59E+10
8.76E-07	4.49E+10
1.13E-06	5.62E+10
1.45E-06	7.02E+10
1.86E-06	8.77E+10
2.38E-06	1.10E+11
3.06E-06	1.37E+11
3.93E-06	1.71E+11
5.04E-06	2.14E+11
6.48E-06	2.68E+11
8.32E-06	3.35E+11
1.07E-05	1.00E+12

Figure 1: sample neutron spectrum

If not write the complete address where the input file is located.

- (f) wait for the activation run to finish
- (g) two files with same name as input file but with extension .out and .path will be created. The location of these two files is the same as the input file.

## 2. For Linux

- (a) Open Terminal
- (b) Go to the location where actys executable is kept.
- (c) Check the address of data folder and flux file given in input file is correct.
- (d) run actys by typing ./actys in the Terminal.
- (e) the program will ask for the name of the input file. If the location of input file and executable is same, write the name of the input file only.  
If not write the complete address where the input file is located.
- (f) wait for the activation run to finish
- (g) two files with same name as input file but with extension .out and .path will be created. The location of these two files is the same as the input file.

## 1.5 List of Error Messages

During the ACTYS run, the program can terminate if there is some mistake in input file preparation. If this happens the run will be terminated and following message will be displayed on the screen.

---

Error Message	Wrong MATERIAL FORM identifier. Either ELE or ISO
Solution	Check the entry at line number 4 in input file
Error Message	Wrong MAT description. Only AD/KG accepted
Solution	Check the entry at line number 4 in input file
Error Message	Number of isotopes/elements cannot be negative
Solution	Check the entry on line number 5 in input file

---

Error Message	Weight fraction cannot be negative or zero
Solution	Check the weight fraction of each element in the input file
Error Message	Atomic fraction cannot be negative or zero
Solution	Check the atomic fraction of each element in the input file
Error Message	UNEQUAL NUMBER OF ISOTOPES IN THE MATERIAL DESCRIPTION
Solution	Number entered in line 5 does not match the number of elements/isotopes provided in the material description
Error Message	UNDEFINED ISOTOPE IN THE MATERIAL DESCRIPTION
Solution	Check the names of isotopes listed in material description section of input file
Error Message	UNDEFINED ELEMENT IN THE MATERIAL DESCRIPTION
Solution	Check the names of elements listed in material description section of input file
Error Message	NO FLUX FILE PROVIDED
Solution	Check the Keyword FLUX_FILE and the flux file name
Error Message	Check Keyword
Solution	Check the spelling of the Keywords entered in the input file
Error Message	WRONG INPUT KEYWORD
Solution	Check the number adjacent to the keywords in the input file
Error Message	Time and Flux value cannot be negative
Solution	Check the numbers entered adjacent to TIME, ON, OFF and FLUX keywords
Error Message	Wrong TIME PERIOD identifier
Solution	Check Time period identifier, it can only take values INTR and CONT
Error Message	UNIDENTIFIED TIME UNIT
Solution	Check the time identifier. It can only take S,D,M and Y as inputs
Error Message	Insufficient number of time steps
Solution	Number after INTR or CONT does not match the time steps entered in the input file
Error Message	Error in Flux file format
Solution	Check the flux file format
WARNING	chains not converged

If any other error is encountered by the user that leads to termination of program, user can check using WARN 1. All the errors excluding the above, should be reported back to actys@iter-india.org.

## 1.6 Output File

If the input file name is **example** then the output files created by ACTYS are known as **example.out** and **example.path**. **example.out** contains the isotopic inventory at each time step (if CROP=0), radiological quantities produced by each isotope (if CROP=0), Gamma spectrum (groupwise and element wise), radwaste index and list of dominating isotopes for each radiological quantity for each time step mentioned in the input file. At the end of the all time steps a final table is created with total values of each radiological quantity for each time steps. Figure 2 are the screen shots of the output file.

- (a) Header for the output file, it contains ACTYS logo, date and time for the creation of output file, library details and material description.

(b) After header, the time scenario, calculated isotopic concentration of material, PATHWAYS creation status, total neutron flux is listed.

```

56 Total neutron flux from the "flux file" : 1.30206E+16
57 #
58 *****FINAL CONCENTRATION after DELTA TIME STEP 6.3115E+07 seconds*****
59
60 FLUX 2.68000E+16 --- Irradiation
61
62
63 -----
64 NUCLIDE HALF LIFE ATOMS MASS ACTIVITY DOSE a-HEATING b-HEATING g-HEATING
65 seconds Bq Sv/hr KW KW KW
66 -----
67 H1 Stable 4.78933E+23 8.01513E-01 0 0 0 0 0
68 H2 Stable 1.21336E+22 4.05806E-02 0 0 0 0 0
69 H3 3.89105E+08 2.63115E+19 1.31775E-04 4.68710E+10 0.00000E+00 0.00000E+00 4.28601E-08 0.00000E+00
70 He3 Stable 4.27777E+17 2.14241E-06 0 0 0 0 0
71 He4 Stable 9.21931E+22 6.12760E-01 0 0 0 0 0
72 Cl4 1.79874E+11 3.44379E+00 8.00780E-23 1.32707E-11 0.00000E+00 0.00000E+00 1.05194E-28 0.00000E+00
73 O16 Stable 2.15050E+01 5.71177E-22 0 0 0 0 0
74 O17 Stable 5.71234E+01 1.61246E-21 0 0 0 0 0
75 O18 Stable 7.18279E+01 2.14681E-21 0 0 0 0 0
76 F19 Stable 9.11232E+01 2.87472E-21 0 0 0 0 0
77 Ne20 Stable 4.67185E+03 1.55907E-19 0 0 0 0 0
78 Ne21 Stable 2.01299E+04 7.01752E-19 0 0 0 0 0
79 Ne22 Stable 5.88747E+04 3.51879E-18 0 0 0 0 0

```

(c) For a particular time step the isotopic inventory and the related radiological quantities are listed.

```

radiological quantities are listed.

226   NI58    2.20903E+28  3.61149E+03  3.47440E-19  1.13321E-25  0.00000E+00  0.00000E+00  3.49631E-41  0.00000E+00
227   NI59    2.39838E+12  8.81581E+06  8.62741E-16  2.54783E-06  1.22067E-18  0.00000E+00  1.88691E-24  1.03845E-24
228   NI60    Stable     9.10170E+08  9.05779E-14  0          0          0          0          0          0
229   NI61    Stable     3.41546E+08  3.45571E-14  0          0          0          0          0          0
230   NI62    Stable     7.77201E+05  7.99231E-17  0          0          0          0          0          0
231
232
233 Number of isotopes for which inventory is listed 164 out of 376 considered
234
235
236 Net activity of the material is 1.339400E+16 Bq or 3.619729E+05 Curie
237 Total Contact Dose is 1.675671E+06 Sv/hr
238      Total Decay heat 1.583901E+00 KW
239
240 Total material mass : 9.99394E+02 g
241 Specific activity : 1.34011E+16 Bq/Kg
242 -----Material Mass composition (grams)-----
243 H3      0.84223
244 He      0.61276
245 Ca      0.01600
246 Sc      0.00696
247 Ti      9.37928
248 V5      66.85786
249 Cr      921.59940
250 Mn      0.07685
251 Fe      0.00250
252
253
254
255 -----DOMINANT RADIONUCLIDES-----
256   NUCLIDE      Bq      % Activity | NUCLIDE      Sv/hr      % Dose | NUCLIDE      KW      % Decay heat
257
258   1  Cr51      9.15560E+15  68.361 | V52        5.149310E+06  89.104 | V52        1.39977E+00  88.375
259   2  V52       3.47701E+15  25.961 | Cr51       5.13257E+06  39.063 | V53        5.161678E-02  3.546
260   3  V49       3.50882E+14  2.620 | V53        5.02932E+04  3.001 | Cr51       5.33585E-02  3.369
261   4  V52       1.71985E+14  1.229 | S=48       4.12686E+04  2.462 | S=48       2.50270E-02  1.580

```

(d) After the isotopic inventory and the related radiological quantities, total radiological quantities, elemental mass composition and list of dominating isotopes are listed.

```

277 20 Sc45m    3.88055E+11      0.003 | K46      5.38265E+00      0.000 | Ca45     1.12930E-05      0.001
278
279
280 -----
281   TYPE   Isotope      Bq/kg
282   B      H3          4.68994E+10
283   B      Mn54         1.10779E+12
284 Material is TYPE B (a/c to ANDRA Classification)  4.62E+11
285 -----
286
287 *-----Gamma Spectrum-----*
288 1  1.05624E+13  1.68153E+13
289 2  4.21861E+04  2.23867E+04
290 3  1.49524E+06  3.40061E+05
291 4  7.56131E+11  8.02507E+10
292 5  2.88914E+12  1.53317E+11
293 6  4.75973E+11  1.51550E+10
294 7  3.21241E+14  7.30594E+12
295 8  1.96806E+13  3.13315E+11
296 9  2.00960E+12  2.28520E+10
297 10 9.12352E+13  8.06925E+11
298 11 2.06089E+14  1.47790E+12
299 12 5.11044E+15  3.05858E+13
300 13 9.09521E+12  4.67083E+10
301 14 8.18256E+12  3.55919E+10
302 15 1.70894E+13  6.04586E+10
303 16 4.05179E+12  1.17281E+10
304 17 2.07569E+12  4.72071E+09
305 18 4.03822E+08  7.14316E+05
306 19 6.33893E+07  8.77528E+04
307 20 2.14427E+03  2.35426E+00
308 21 2.32950E+02  2.06031E-01
309 22 0.00000E+00  0.00000E+00
310 23 0.00000E+00  0.00000E+00
311 24 0.00000E+00  0.00000E+00
312 *-----*

```

(e) After the list of dominating isotopes, groupwise gamma spectrum is listed.

```

315
316 *----Isotope wise Gamma Source (MeV/s)----*
317 Na22      1.64267E-06
318 Na24      1.28176E+00
319 Mg27      6.09847E+01
320 Mg28      4.79463E-02
321 Mg29      1.43160E+00
322 Al28      4.88368E+02
323 Al29      1.92555E+01
324 Al30      2.18377E+02
325 Si31      3.79862E+01
326 Si33      1.13730E+04
327 P30       9.95410E+00
328 P32       3.20711E+01
329 P34       3.844452E+04
330 P35       7.64812E+03
331 P36       4.26385E+04
332 S37       5.73182E+06
333 S38       3.424464E+03
334 S39       2.35377E+05
335 Cl34      2.58797E+02
336 Cl34m     7.14169E+02
337 Cl36      3.41997E-05
338 Cl38      3.24785E+07
339 Cl38m     4.26503E+06
340 Cl39      3.94296E+06
341 Cl40      6.92036E+06
342 Cl41      8.47190E+03
343 Cl42      1.13904E+06
344 Ar37      7.00215E+02

```

(f) Isotopic total gamma emission.

```

406 Co57      1.19644E+00
407 Co58      1.71181E+03
408 Co58m     5.31921E+00
409 Co60      2.58212E+02
410 Co60m     1.08131E+01
411 Co61      4.09722E+00
412 *-----*
413 *****END OF TIME STEP*****
414
415
416                                     Total CPU Time =      19.047 sec
417
418
419
420
421 #           2
422 *****FINAL CONCENTRATION after DELTA TIME STEP  3.9226E+03  seconds*****
423
424 FLUX  0.00000E+00 --- Decay
425

```

(g) After the end of all the above outputs for first time step, all the above outputs are listed for other time steps as well.

```

2231 *****END OF TIME STEP*****
2232
2233
2234 Total CPU Time = 19.141 sec
2235
2236
2237
2238
2239 -----PROBLEM SOLUTION TABLE-----
2240   TIME(s)    CUMLTVE TIME(y)    FLUX(n/cm2/s)    ACTIVITY(Bq/Kg)    Dose(mSv/h)    Heating(KW)    H3 Activity
2241
2242   1       6.31E+07      2.00E+00      2.68E+16      1.34E+16      1.68E+09      1.58E+00      4.69E+10      B
2243   2       3.92E+03      2.00E+00      0.00E+00      9.59E+15      1.05E+08      8.84E-02      4.69E+10      B
2244   3       4.00E+02      2.00E+00      7.00E+18      7.19E+17      2.95E+11      2.80E+02      4.70E+10      B
2245   4       3.92E+03      2.00E+00      0.00E+00      1.01E+16      1.53E+08      1.49E-01      4.70E+10      B
2246   5       4.00E+02      2.00E+00      7.00E+18      7.19E+17      2.95E+11      2.80E+02      4.72E+10      B
2247   6       8.64E+04      2.00E+00      0.00E+00      9.90E+15      1.19E+08      9.61E-02      4.71E+10      B
2248   7       1.00E+11      3.17E+03      0.00E+00      1.98E+04      5.04E-06      2.36E-14      0.00E+00      A
2249
2250
2251 Total Irradiation Time = 1.000632E+11 s
2252 Total Fluence = 1.403567E+30 n/cm2
2253 Neutrons produced = 11637
2254

```

- (h) At the end of output file a final table of all the total radiological quantities produced at each time step is given. Along with total fluence, total time taken for activation run and number of neutrons produced during the activation process.

Figure 2: Screen shots of sample output file

## 1.7 Path File

This files contains all the different pathways requested by the user. Screenshots from sample path file are given in the figure 3

```

1 -----time step          1 -----
2
3
4
5
6
7 -----BASED ON DoseRate
8
9
10 <V52>
11 1.127E+18(final) = 0.0000E+00(after loss) + 1.127E+18(gain)
12
13 0.103% Cr53 --->[(n,2n):1.00E+00] Cr52 --->[(n,g):8.13E-03] [(b+):9.92E-01] V51 --->[(n,g):1.00E+00] V52
14 0.037% Cr50 --->[(n,p):1.00E+00] V50 --->[(n,g):1.00E+00] V51 --->[(n,g):1.00E+00] V52
15 0.087% Cr52 --->[(n,p):1.00E+00] V52 --->[(b-):1.00E+00] Cr52 --->[(n,2n):1.00E+00] Cr51 --->[(n,p):8.13E-03] [(b+):9.92E-01] V51 --->[(n,g):1.00E+00] V52
16 2.051% Cr53 --->[(n,2n):1.00E+00] Cr52 --->[(n,p):1.00E+00] V52
17 83.684% Cr52 --->[(n,p):1.00E+00] V52
18 0.029% Cr52 --->[(n,np):9.42E-01] [(n,d):5.78E-02] V51 --->[(n,g):1.00E+00] V52 --->[(b-):1.00E+00] Cr52 --->[(n,p):1.00E+00] V52
19 1.786% Cr52 --->[(n,p):1.00E+00] V52 --->[(b-):1.00E+00] Cr52 --->[(n,p):1.00E+00] V52
20 0.034% Cr52 --->[(n,2n):1.00E+00] Cr51 --->[(n,p):8.13E-03] [(b+):9.92E-01] V51 --->[(n,g):1.00E+00] Ti51 --->[(b-):1.00E+00] V51 --->[(n,g):1.00E+00] V52
21 0.034% Cr53 --->[(n,2n):1.00E+00] Cr52 --->[(n,np):9.42E-01] [(n,d):5.78E-02] V51 --->[(n,g):1.00E+00] V52
22 0.023% Cr53 --->[(n,2n):1.00E+00] Cr52 --->[(b-):1.00E+00] Cr52 --->[(n,p):1.00E+00] V52
23 2.643% Cr52 --->[(n,np):9.42E-01] [(n,d):5.78E-02] V51 --->[(n,g):1.00E+00] V52
24 0.095% Cr52 --->[(n,g):1.00E+00] Cr53 --->[(n,2n):1.00E+00] Cr52 --->[(n,p):1.00E+00] V52
25 0.287% Cr53 --->[(n,np):4.68E-01] [(n,d):5.32E-01] V52
26 8.439% Cr52 --->[(n,2n):1.00E+00] Cr51 --->[(n,p):8.13E-03] [(b+):9.92E-01] V51 --->[(n,g):1.00E+00] V52
27 0.317% Cr50 --->[(n,p):1.00E+00] Cr51 --->[(n,np):8.13E-03] [(b+):9.92E-01] V51 --->[(n,g):1.00E+00] V52
28 0.029% Cr52 --->[(n,g):1.00E+00] Cr53 --->[(n,np):4.68E-01] [(n,d):5.32E-01] V52
29 0.087% Cr52 --->[(n,2n):1.00E+00] Cr51 --->[(n,p):8.13E-03] [(b+):9.92E-01] V51 --->[(n,g):1.00E+00] V52 --->[(b-):1.00E+00] Cr52 --->[(n,p):1.00E+00] V52
30 0.053% Cr54 --->[(n,2n):1.00E+00] Cr53 --->[(n,2n):1.00E+00] Cr52 --->[(n,p):1.00E+00] V52
31 0.019% Cr52 --->[(n,p):1.00E+00] V52 --->[(b-):1.00E+00] Cr52 --->[(n,p):1.00E+00] V52 --->[(b-):1.00E+00] Cr52 --->[(n,p):1.00E+00] V52
32 0.029% Cr52 --->[(n,p):1.00E+00] V52 --->[(b-):1.00E+00] Cr52 --->[(n,np):9.42E-01] [(n,d):5.78E-02] V51 --->[(n,g):1.00E+00] V52
33
34 Contribution from enlisted Pathways : 99.8646%

```

(a) Pathways for dominating isotopes

```

216 -----
217          PATHWAYS FOR REQUESTED NUCLIDES
218 -----
219 <Cr51>
220 3.162E+22(final) = 0.0000E+00(after loss) + 3.162E+22(gain)
221
222 2.153% Cr53 --->[(n,2n):1.00E+00] Cr52 --->[(n,2n):1.00E+00] Cr51
223 3.256% Cr50 --->[(n,g):1.00E+00] Cr51
224 0.023% Cr52 --->[(n,2n):1.00E+00] Cr51 --->[(n,2n):1.00E+00] Cr50 --->[(n,g):1.00E+00] Cr51
225 0.016% Cr52 --->[(n,2n):1.00E+00] Cr51 --->[(n,g):1.00E+00] Cr52 --->[(n,2n):1.00E+00] Cr51
226 0.003% Cr50 --->[(n,g):1.00E+00] Cr51 --->[(n,p):8.13E-03] [(b+):9.92E-01] V51 --->[(n,g):1.00E+00] V52 --->[(b-):1.00E+00] Cr52 --->[(n,2n):1.00E+00] Cr51
227 0.004% Cr53 --->[(n,g):1.00E+00] Cr54 --->[(n,2n):1.00E+00] Cr53 --->[(n,2n):1.00E+00] Cr52 --->[(n,2n):1.00E+00] Cr51
228 0.053% Cr54 --->[(n,2n):1.00E+00] Cr53 --->[(n,2n):1.00E+00] Cr52 --->[(n,2n):1.00E+00] Cr51
229 0.023% Cr53 --->[(n,2n):1.00E+00] Cr52 --->[(n,p):1.00E+00] V52 --->[(b-):1.00E+00] Cr52 --->[(n,2n):1.00E+00] Cr51
230 0.028% Cr52 --->[(n,np):9.42E-01] [(n,d):15.78E-02] V51 --->[(n,g):1.00E+00] V52 --->[(b-):1.00E+00] Cr52 --->[(n,2n):1.00E+00] Cr51
231 0.085% Cr52 --->[(n,2n):1.00E+00] Cr51 --->[(n,p):8.13E-03] [(b+):19.92E-01] V51 --->[(n,g):1.00E+00] V52 --->[(b-):1.00E+00] Cr52 --->[(n,2n):1.00E+00] Cr51
232 0.011% Cr53 --->[(n,p):1.00E+00] V53 --->[(b-):1.00E+00] Cr53 --->[(n,2n):1.00E+00] Cr52 --->[(n,2n):1.00E+00] Cr51
233 0.021% Cr52 --->[(n,p):1.00E+00] V52 --->[(b-):1.00E+00] Cr52 --->[(n,p):1.00E+00] V52 --->[(b-):1.00E+00] Cr52 --->[(n,2n):1.00E+00] Cr51
234 1.865% Cr52 --->[(n,p):1.00E+00] V52 --->[(b-):1.00E+00] Cr52 --->[(n,2n):1.00E+00] Cr51
235 0.007% Cr53 --->[(n,np):4.68E-01] [(n,d):5.32E-01] V52 --->[(b-):1.00E+00] Cr52 --->[(n,2n):1.00E+00] Cr51
236 92.349% Cr52 --->[(n,2n):1.00E+00] Cr51
237 0.094% Cr52 --->[(n,g):1.00E+00] Cr53 --->[(n,2n):1.00E+00] Cr52 --->[(n,2n):1.00E+00] Cr51
238
239 Contribution from enlisted Pathways : 99.9917%

```

(b) Pathways for isotopes requested through keyword PATH

```

248 -----
249          PATHWAYS FOR DAUGHTERS OF Cr50
250 -----
251
252
253 H1 -----> 4.79E+23
254 8.19E+22 Cr50 --->[(n,np):2.70E-01] [(n,p):7.27E-01] H1
255 2.29E+20 Cr50 --->[(n,p):1.00E+00] V50 --->[(n,2n):1.00E+00] V49 --->[(n,np):4.58E-01] [(n,p):5.41E-01] H1
256 2.40E+20 Cr50 --->[(n,g):1.00E+00] Cr51 --->[(n,p):8.13E-03] [(b+):9.92E-01] V51 --->[(n,g):1.00E+00] V52 --->[(b-):1.00E+00] Cr51
257 2.18E+20 Cr50 --->[(n,a):1.00E+00] T147 --->[(n,np):8.79E-02] [(n,np):1.29E-02] H1
258 1.54E+21 Cr50 --->[(n,np):9.51E-01] [(n,d):4.92E-02] V49 --->[(n,np):4.58E-01] [(n,p):5.41E-01] H1
259 1.52E+21 Cr50 --->[(n,p):1.00E+00] V50 --->[(n,np):5.03E-01] [(n,p):4.97E-01] H1
260
261 H2 -----> 1.21E+22
262 1.42E+19 Cr50 --->[(n,np):2.70E-01] [(n,p):7.27E-01] H1 --->[(n,g):1.00E+00] H2
263 1.11E+21 Cr50 --->[(n,d):1.00E+00] [(n,nd):1.14E-14] H2
264 7.85E+19 Cr50 --->[(n,p):5.09E-12] [(n,d):1.00E+00] H2
265 3.37E+19 Cr50 --->[(n,np):9.51E-01] [(n,d):4.92E-02] V49 --->[(n,d):1.00E+00] [(n,da):5.36E-20] H2
266 1.27E+19 Cr50 --->[(n,g):1.00E+00] Cr51 --->[(n,p):8.13E-03] [(b+):9.92E-01] V51 --->[(n,d):1.00E+00] H2
267 5.05E+18 Cr50 --->[(n,p):1.00E+00] V50 --->[(n,2n):1.00E+00] V49 --->[(n,d):1.00E+00] [(n,da):5.36E-20] H2
268
269 H3 -----> 2.63E+19
270 7.20E+16 Cr50 --->[(n,np):9.51E-01] [(n,d):4.52E-02] V49 --->[(n,g):1.00E+00] V50 --->[(n,t):1.00E+00] H3
271 1.78E+17 Cr50 --->[(n,p):1.00E+00] V50 --->[(n,t):1.00E+00] H3 --->[(b-):1.00E+00] He3 --->[(n,p):1.00E+00] H3
272 4.60E+16 Cr50 --->[(n,h):1.00E+00] He3 --->[(n,p):1.00E+00] H3
273 1.08E+17 Cr50 --->[(n,g):1.00E+00] Cr51 --->[(n,p):8.13E-03] [(b+):9.92E-01] V51 --->[(n,2n):1.00E+00] V50 --->[(n,t):1.00E+00] H3
274 9.61E+16 Cr50 --->[(n,np):9.51E-01] [(n,d):4.92E-02] V49 --->[(n,t):1.00E+00] H3
275 7.47E+18 Cr50 --->[(n,p):1.00E+00] V50 --->[(n,t):1.00E+00] H3
276

```

(c) All the different pathways through which isotope requested under keyword PPATH will produce its daughters. All the significant daughters of the nuclide are listed

Figure 3: Screen shots of sample path file

## 1.8 Test cases

The second international Activation calculation benchmark comparison study, carried out by IAEA in 1994 [6] is used as sample test case for ACTYS.

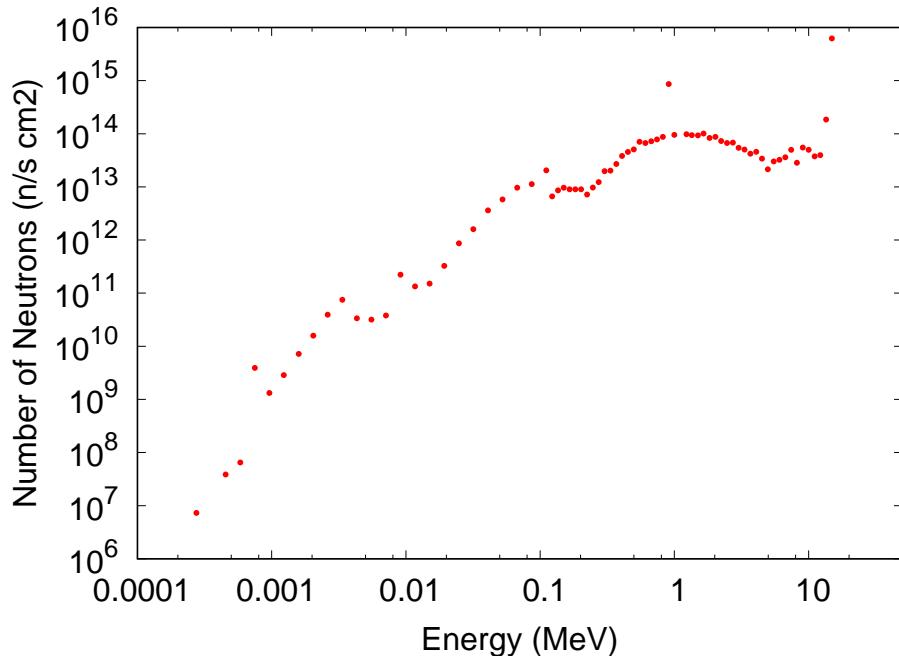


Figure 4: Neutron spectrum in 100 group structure (Normalized to  $5 \text{ MW/m}^2$  Wall loading)

1. 1kg of natural iron irradiated for 1 year using the GAM-II 100 group neutron spectrum, as given in figure: 4.
2.  $1.0 \times 10^{25}$  atoms of Cr – 50 irradiated for 1 year using the GAM-II 100 group neutron spectrum, as given in figure: 4.

A python program will be given along with the ACTYS executable. For first time users it will run the ACTYS executable for the above test cases and report the results to the user in a file. If no discrepancy is found user can continue using ACTYS for their purpose. If the test fails, user should report the error to [actys@iter-india.org](mailto:actys@iter-india.org).

The input file for both the cases are given below. Keywords are given in blue color and user inputs are given in pink. The entries in pink can be edited by the user. Also, more keywords can be added that are given in the Section 1.3.

---

**ACTYS**  
C:/ACTYS/Data

**ISO -1.0 AD**

1  
Cr50 1.00E25

**CROP 0**

**GRP 100**

**DEBUG 0**

**PATHWAY 0**

**FLUX\_FILE C:/ACTYS/flux**

**INTR 1**

**TIME 1 Y FLUX 4.41899E+15**

---

**ACTYS**  
C:/ACTYS/Data

**ELE 1.0 KG**

1  
Fe 100

**CROP 0**

**GRP 100**

**DEBUG 0**

**PATHWAY 0**

**FLUX\_FILE C:/ACTYS/flux**

**INTR 1**

**TIME 1 Y FLUX 4.41899E+15**

---

## 2 ACTYS-1-GO

ACTYS-1-GO is the extension of ACTYS which can do activation calculation for given materials at multiple neutron spectrum in one single run. To reduce the time of multipoint activation calculation in complex geometries, the concept of Superlist is developed and implemented in ACTYS-1-GO. This captures the essence of an entire material placed at multiple locations and experiencing different neutron spectrum in a small set of isotopes called the superlist. The details how this method works is given in article [7] and Appendix-D.

### 2.1 Input file preparation

To run ACTYS-1-GO, you need to prepare input files for each material as given in section 1.3. Along with that you need two additional input files, **fmat** and a file containing all neutron spectrum file. The first line of file **fmat** contains the name of file where all the neutron spectrum are stored, number of input material and the names of all input material along with the cell number where they are located. The **fmat** file will look like:

```
zone.txt 2
SS 3
1
3
6
W 2
2
4
```

---

<b>zone.txt</b>	<b>2</b>
name of neutron spectrum file	<b>number of materials file</b>
<b>SS</b>	<b>3</b>
name of material input file 1	number of cells the input material is located
<b>1</b>	
SS is located at cell number 1	
<b>3</b>	
SS is located at cell number 3	
<b>6</b>	
SS is located at cell number 6	
<b>W</b>	<b>2</b>
name of material input file 1	number of cells the input material is located
<b>2</b>	
W is located at cell number 2	
<b>4</b>	
W is located at cell number 4	

---

ACTYS-1-GO reads the entire set of neutron spectrum at each mesh location given as report file of ATTILA or in the format given in figure 5. The first word can be anything, the number gives the cell number identifier used in **fmat** file. For each cell/interval/mesh the spectrum is given from high energy to low energy.

```

int      1
0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
0.00000E+00 5.86479E+02 8.78499E+02 1.45604E+03 3.77965E+02 2.45423E+02
4.57573E+02 3.51105E+02 3.14498E+02 2.76094E+02 2.36317E+02 2.28536E+02
2.26934E+02 2.02088E+02 1.78292E+02 1.67403E+02 1.66455E+02 1.65260E+02
5.55326E+01 1.07476E+02 1.57125E+02 1.53139E+02 1.52700E+02 1.56791E+02
1.56272E+02 1.60469E+02 1.63087E+02 3.38427E+02 3.60990E+02 3.99509E+02
2.27127E+02 2.59667E+02 2.82738E+02 3.09677E+02 3.57439E+02 3.49049E+02
2.67556E+02 7.88082E+01 8.69383E+01 1.50338E+02 3.25101E+02 4.97658E+02
4.92244E+02 5.09996E+02 5.31574E+02 6.49724E+02 7.19558E+02 7.22742E+02
7.47474E+02 7.63156E+02 8.90203E+02 8.64984E+02 8.97314E+02 1.23904E+03
1.28006E+03 2.43094E+03 9.57190E+02 1.89861E+03 1.64456E+03 1.92005E+03
1.95916E+03 2.03029E+03 2.60866E+03 2.94358E+03 3.69514E+03 4.37673E+03
5.18679E+03 4.79212E+03 4.89267E+03 4.84714E+03 9.54175E+03 7.36651E+03
4.01418E+03 5.27243E+03 1.21184E+04 1.37546E+04 1.95721E+03 6.94919E+02
1.43903E+03 3.03216E+03 5.26865E+03 1.33192E+04 6.73056E+03 6.52891E+03
6.10354E+03 5.98056E+03 4.83859E+03 5.23422E+03 8.22934E+03 5.95399E+03
6.79108E+03 6.49589E+03 4.12199E+03 4.71437E+03 7.71704E+03 8.10801E+03
8.79432E+03 7.73825E+03 1.30708E+04 1.46003E+04 3.39446E+03 6.18356E+03
9.14455E+03 1.01137E+04 2.12929E+04 7.72844E+03 1.72349E+04 1.37262E+04
1.62296E+04 6.84501E+03 4.63346E+03 1.81185E+03 4.08893E+03 6.99661E+03
5.58730E+03 4.36991E+03 1.07256E+04 1.49090E+04 1.60713E+04 2.56198E+04
8.33326E+03 1.03907E+04 1.92266E+04 1.95670E+04 1.91523E+04 1.32927E+04
9.91609E+03 9.89651E+03 9.08831E+03 2.29867E+03 2.16558E+03 6.41133E+03
2.55639E+03 2.64679E+04 2.49104E+04 1.94166E+04 2.03702E+04 1.83589E+04
1.22541E+04 9.59340E+03 1.46491E+04 1.47517E+04 1.47013E+04 1.22427E+04
1.50388E+04 1.52527E+04 1.52197E+04 1.53578E+04 1.19981E+04 1.30009E+04
1.34937E+04 1.36720E+04 1.36813E+04 1.35019E+04 1.33357E+04 1.30823E+04
1.27490E+04 1.23363E+04 1.18691E+04 1.13310E+04 1.07324E+04 1.00741E+04
9.36482E+03 8.62063E+03 7.84385E+03 7.05389E+03 6.26402E+03 1.09372E+04
1.07859E+04

int      2
0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
0.00000E+00 5.83203E+02 8.74374E+02 1.45023E+03 3.76573E+02 2.44538E+02
4.56030E+02 3.49995E+02 3.13527E+02 2.75277E+02 2.35650E+02 2.27909E+02
2.26329E+02 2.01581E+02 1.77868E+02 1.67018E+02 1.66079E+02 1.64893E+02

```

Figure 5: sample neutron spectrum file for ACTYS-1-GO

## 2.2 Output file

For each material and cell number individual output files are generated using **CROP 0** keyword. Additionally a file is generated in which for each material at each different cell number the total activity, dose rate decay heat and gamma spectrum at each step is written.

## 2.3 Plot file

If the geometry file is available, for example the model file of ATTILA. Another output file is also generated for each material. This contains the location of the mesh/cell along with all the radiological quantities at each time step. This file can be plotted using python subroutine provided with ACTYS-1-GO executable [8]. Some of the outputs of this file is given below:

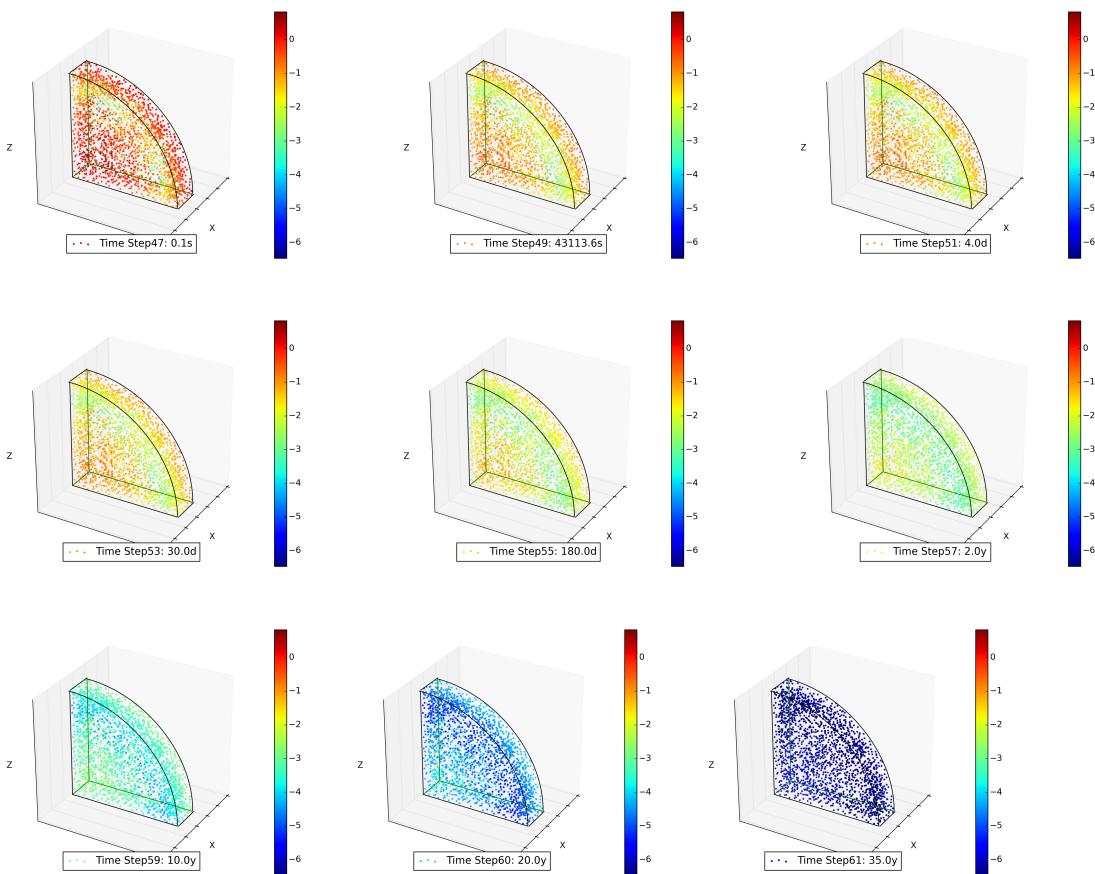


Figure 6: Contact dose rate(Sv/hr) calculated at each mesh location at various time steps after shutdown in quarter steel plate

These plots can also be converted into mp4 movie for easy visualization of time evolution of radiological quantities throughout the device.

## 2.4 Test Case

The FENDL Activation Benchmark study reported in the article [9] is used as a test case for ACTYS-1-GO. The IAEA FENDL Activation Benchmark is based on the reference steel/water shielding blanket design in ITER outline design, including materials from inboard magnet to the outboard vacuum vessel as given in figure 7

[9].

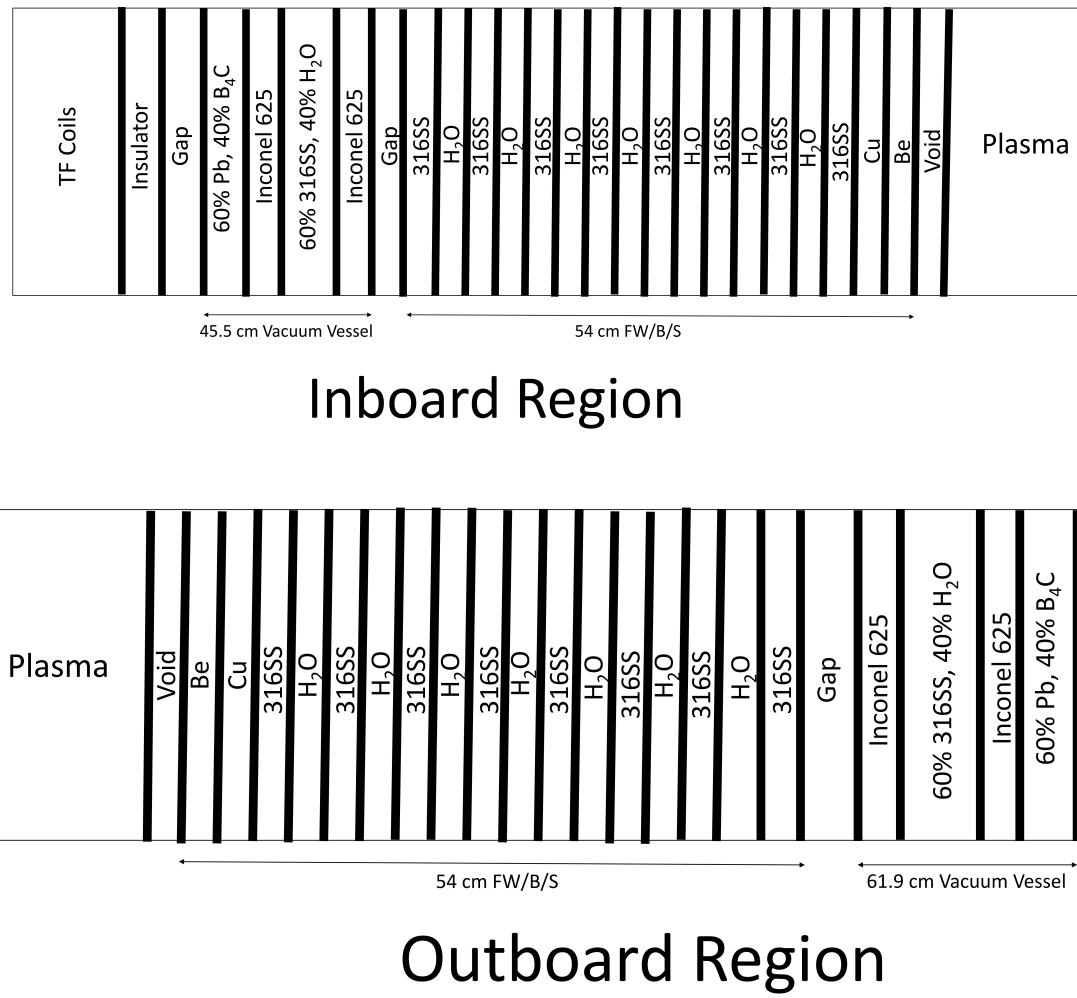


Figure 7: Geometrical model of FENDL Activation Benchmark Study based on the reference steel/water shielding blanket design of ITER.

The design includes:

- 14 mm thick first wall consisting of 8 mm thick Beryllium coating and 5 mm Copper attached to 1 mm thick Stainless steel.
- Shielding blanket is of 526 mm thickness with alternating layers of 316 SS and water.
- A double-wall Inconel 625 vacuum vessel is used with single size water-cooled 316 SS balls. The vacuum vessel walls are 50 mm thick. A 50 mm thick back shield zone made of lead and boron carbide is used at the back of it. The total vacuum vessel thickness is 455 mm in the inboard region and 619 mm in the outboard region.

The design is a 1-D toroidal cylindrical model with inboard and outboard regions modeled simultaneously. The model includes 51 zones, as given in figure 7, which is

further divided into 468 intervals. In the study out of these 468 intervals, only 317 are occupied by 9 different materials, rest are void. A uniform 14.1 MeV isotropic neutron source is used in the plasma zone. The neutron spectrum is obtained from reference [10] in the VITAMIN-J 175 group structure for each of the 468 intervals (fine meshes) included in the 51 zones (coarse meshes). These fluxes were calculated in the study using ONEDANT deterministic neutron transport code with a 14.1MeV isotropic neutron source normalized to inboard and outboard neutron wall loading of 1 and 1.5  $MW/m^2$ , respectively.

A python program given along with the ACTYS-1-Go executable will run the above test case and report the results to the user in a file. If no discrepancy is found user can continue using ACTYS-1-Go for their purpose. If the test fails, user should report the error to [actys@iter-india.org](mailto:actys@iter-india.org).

## APPENDIX-A

### Derivation of chain solution for Bateman Equation

The Bateman equation can be derived from the radioactive decay law in the following manner. For a radioactive isotope, **A** with initial concentration  $N_A(0)$  decaying to isotope **B** with decay constant  $\lambda_{AB}$  and initial concentration  $N_B(0) = 0.0$ , the Bateman equation is given as:

$$\frac{dA}{dt} = -\lambda_{AB}A \quad (5)$$

The solution of the above equation is :

$$N_A(t) = e^{-\lambda_{AB}t}N_A(0) \quad (6)$$

Likewise, if isotope **B** is also radioactive and would decay into isotope **C**, with decay constant  $\lambda_{BC}$  and initial concentration  $N_C(0) = 0.0$ , the rate of decay of isotope **B** will be given as:

$$\frac{dB}{dt} = \lambda_{AB}A - \lambda_{BC}B \quad (7)$$

The concentration of isotope B as a function of time can be written as:

$$N_B(t) = \lambda_{AB}N_A(0) \left[ \frac{e^{-\lambda_{AB}t}}{\lambda_{BC} - \lambda_{AB}} + \frac{e^{-\lambda_{BC}t}}{\lambda_{AB} - \lambda_{BC}} \right] \quad (8)$$

Hence for a chain of 'n' isotopes the rate equation of each isotope 'i' can be written as:

$$\frac{dN_i}{dt} = \lambda_{i-1}N_{k-1} - \lambda_iN_i \quad (9)$$

where,  $\lambda_i$  is the decay constant of the  $i^{th}$  nuclide, and  $N_i$  is the number of atoms of isotope at time 't', with the assumption that  $N_i(0) = 0.0$ . Now, the concentration of  $n^{th}$  isotope can be written as:

$$N_n(t) = \frac{N_1(0)}{\lambda_n} \sum_{i=1}^n \lambda_i \alpha_i \exp[-\lambda_i t] \quad (10)$$

where

$$\alpha_i = \prod_{j=1, j \neq i}^n \frac{\lambda_j}{(\lambda_j - \lambda_i)} \quad (11)$$

The equation 10 can be arranged in a recursive algorithm and is used to calculate the isotopic inventory at any time 't' for a given neutron spectrum. To accommodate the neutron-induced reactions  $\sigma_{ij} * \phi$  is added to the decay constant  $\lambda_i$ . ACTYS solves this equation based on the analytical linear chain solution method forming progressively growing linear continuous-time Markov chains starting from

each parent nuclide and solving them as they grow in length with careful checks for termination. It follows that each parent and its subsequent linear chain development is completely independent of other parent nuclides in the material. This is a direct outcome due to the inherent property of a nuclide's decay and transmutation in nature. Special routines are written in the program to take care of loop formation, chain termination, and chain weighing.

## Chain Termination Algorithm

The chain termination is treated by defining chain ‘passage’  $P_n$  at each  $n^{th}$  isotope in the linear chain .

$$P_n = \int_0^t d_n \cdot N_n(t) dt = \sum_{k=n+1} N_k \quad (12)$$

The passage  $P_n$  refers to the total production of all isotopes in the subtree through the  $n^{th}$  isotope in the chain. The chain is terminated when either the daughter nuclide has very low ( $d_n < 10^{-24}$ ) destruction coefficient or if the passage is less than a pre-determined cutoff value. It therefore represents maximum possible atom loss through this isotope. Chain termination occurs when

$$P_n < (cutoff * N_o + ll) \quad (13)$$

where,  $ll$  stands for lower limit and  $N_o$  is parent isotope nuclide density. A limiting condition of passage for continuation of linear chain

$$(N_o * cutoff + ll) \leq P_n \leq N_o(1 - e^{-d_1 t}) \quad (14)$$

The term  $(1 - e^{-d_1 t})$  can be used to define an appropriate cutoff. More details can be found in [5]

## APPENDIX-B

### Radiological quantities calculated by ACTYS

The radioactive nuclides generated in a material after neutron irradiation, would emit ionizing radiations like  $\alpha$ ,  $\beta$  and  $\gamma$  rays. These radiations affect materials and living beings differently and to different extents. Hence to quantify the radio-toxicity in an activated material typical parameters are defined. These parameters can be used for radioactivity level assessments, accident analyses, radiation dose assessments, decommission studies, etc. Typical activation parameters calculated by ACTYS are given below:

#### Activity

Activity is defined as the number of decays per unit time of radioactive isotope. The activity of any material is equal to the sum of activity of all its radioactive isotopes. It is used to measure the radioactivity of a material. The unit of activity is the Becquerel (Bq).  $1\text{Bq} = 1\text{disintegration/s}$ . The Specific activity is usually used to characterize the radioactivity of the material and is defined as the ratio of the activity to the mass, in units of Bq/kg. Activity can be further classified into alpha, beta and gamma activity depending upon the various decay modes of the isotope.

#### Gamma Spectrum

Gamma Spectrum is the relative intensity or the probability of emission and energy of discrete gamma, x-rays and bremsstrahlung radiation (all EM radiation will be referred under the common name gamma) emitted from decay process is grouped according to energy bins.

ACTYS reads gamma emission probability and relative intensity from JEFF-3.1.1 and JEFF-2.2 decay data library. Gamma spectrum is then calculated using in following steps:

- Based on the decay spectrum type, discrete energy lines are read along with their absolute and relative intensities.
- Using the Discrete energy of gamma (or X-ray) radiation, the energy lines are divided into standard 24 and 42 group structure given in APPENDIX-C.
- All the information regarding spectrum and energy grouping is written in a file name "SPECTRUM".

Gamma Spectrum is then read during the activation process from the pre-processed file "SPECTRUM". It is then used as an input for the dose rate, Gamma source

and nuclear heating calculation in ACTYS. Discrete gamma rays generated from individual isotope is summed according to 24/42-energy group structure to evaluate total gamma emission from an activated material, using the following formula:

$$\gamma_i = \sum_j P_i E_i A_j \quad (15)$$

Where,  $\gamma_i$  is the intensity of gamma ray emitted in the energy group 'i',  $P_i$  is probability of emission of gamma in energy group 'i',  $E_i$  is energy of emitted discrete gamma line in energy group 'i',  $A_j$  is Activity of isotope 'j'.

## Decay Heat

Once a material is activated, heat will be produced through deposition of energetic particles or radiations emitted from decay of radioactive isotopes. This heat is known as Decay heat. It is the main heat source in nuclear materials during periods of reactors shutdown. Thus, is the main safety concern in fusion devices. This decay heat( $H_i$ ) generated in an activated material is calculated by ACTYS using the formula:

$$H_i = A_i * E_i * C \quad (16)$$

where  $A_i$  is the activity of the isotope 'i',  $E_i$  is the energy of the emitted radiation ( $\alpha$ ,  $\beta$  or  $\gamma$ ) and C is the conversion factor from MeV/s to KW/hr.

## Contact Dose Rate

The ionizing radiations emitted from activated material in fusion systems can be absorbed by living and non living matter. To quantify the effects of radiation after being absorbed, various dose rates are defined. Absorbed dose is the measure of the energy deposited in matter by ionizing radiation per unit mass. The SI unit of measure is the gray (Gy), which is defined as one Joule of energy absorbed per kilogram of matter. To incorporate the biological effects of the radiation "Equivalent" and "Effective" dose are defined. The Equivalent dose gives the stochastic health effects of low levels of ionizing radiation on the human body. The SI unit of measure for equivalent dose is the sievert,  $1Sv = 1Joule/kg$ . Gamma Dose rate defined for fusion systems is the measure of biological( equivalent dose rate) received by the exposure to gamma radiation and is measured in  $Sv/hr$ . Gamma equivalent dose rate (gamma dose rate) is the most relevant radiological quantity in relation to health of the workers in reactors and locals in the nearby area. Contact dose rate is the measure of gamma dose rate received at the surface of the activated material.

Formula for dose rate used in ACTYS is derived from the book Engineering Compendium on Radiation Shielding. It assumes that the material is homogeneous and the isotope under consideration is the only active radiation source in the material emitting mono-energetic photons. The calculated dose is the dose at the surface

of a semi-infinite uniform volume source. Then contact dose for each isotope is calculated by:

$$D_i = C \frac{B}{2} \sum_g \frac{\mu_a}{\mu_m} E_g \frac{A_i}{M} \quad \text{where} \quad \mu_m = \sum \frac{m_i}{M} \mu_i \quad (17)$$

Where  $C = 5.767^{-10}$  is the conversion factor from Mev/s to Sv/hr,  $B = 2$  is the buildup factor,  $\mu_a$  is the attenuation coefficient in air,  $\mu_m$  is the attenuation coefficient in material,  $E_g$  is the energy of the emitted gamma radiation in the group 'g',  $A_i$  is the activity of the isotope and  $M$  is the mass of the material.

## Radwaste Index

After irradiation the material does not decay to background levels, rather the long lived radio-nuclides give it a prolonged activity. These material are referred to as Rad-Waste. A proper classification and disposal of these waste is mandatory to prevent radiation leakage and other harmful effects. There are two major rad-waste classification scheme. These are Clearance Index, classification scheme defined under IAEA guidelines and ANDRA Classification, rad-waste classification scheme defined under French guidelines.

Since ANDRA classification scheme is being used for rad-waste that would be produced in ITER, ACTYS uses ANDRA Classification scheme radwaste that is defined under French guidelines. According to ANDRA, nuclides are classified into 3 main types:

- Intermediate-level and long-lived radwaste (Type B) mainly from in-vessel component replacement.
- Purely tritiated waste (not irradiated by neutron, but contaminated by tritium) from tritium plant and fuelling system operation and maintenance
- Low-level solid and liquid radwaste (Type A) from process and housekeeping operations
- Very low-level radwaste (TFA)

IRAS index is also defined under this scheme. It is given as:

$$IRAS = \sum \frac{A_i}{10^{C_i}} \quad (18)$$

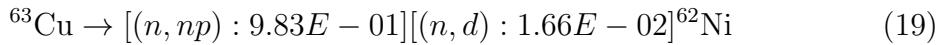
where  $A_i$  is the activity of radioisotope,  $C_i$  is the class.

In ACTYS isotopes listed under ANDRA classification are read and stored in a file along with their class and LMA values. The final inventory calculated by ACTYS is then scanned for such isotopes. If an isotope listed under ANDRA is present, its specific activity is calculated. If specific activity of any isotope is more than

its LMA value, material is classified as TYPE B Rad-Waste. If all the isotopes have specific activity less than LMA value, IRAS index is calculated on the basis of class of the nuclide. If IRAS index is found to be less than 1, then the material is classified as TFA waste, else the material is TYPE A category waste. ANDRA classification along with IRAS index is mentioned in ACTYS output file at the end of every irradiation/decay scenario.

## Pathways

Pathway analysis plays a crucial role in nuclear analysis for determining parents and reactions that contribute towards production of radioactive isotopes, gas and gamma spectrum in the material. Calculation of pathways according to different reactions and decay channels and their contribution are calculated by ACTYS. A sample pathway generated by ACTYS is:



ACTYS can print pathways with multiple competing reaction channels that would produce the same daughter product along with relative probability of each reaction channel. Such pathways can also illustrate the likelihood for the creation of daughter isotopes from parent isotopes through a nuclear reaction or radioactive decay. This information provides key insights into the nuclear process happening in the material.

## APPENDIX-C

### Gamma group structures used in ACTYS

VITAMIN-J (42)					
grp	Lower Bound	Upper Bound	grp	Lower Bound	Upper Bound
1	1.00E-03	1.00E-02	22	1.34E+00	1.50E+00
2	1.00E-02	2.00E-02	23	1.50E+00	1.66E+00
3	2.00E-02	3.00E-02	24	1.66E+00	2.00E+00
4	3.00E-02	4.50E-02	25	2.00E+00	2.50E+00
5	4.50E-02	6.00E-02	26	2.50E+00	3.00E+00
6	6.00E-02	7.00E-02	27	3.00E+00	3.50E+00
7	7.00E-02	7.50E-02	28	3.50E+00	4.00E+00
8	7.50E-02	1.00E-01	29	4.00E+00	4.50E+00
9	1.00E-01	1.50E-01	30	4.50E+00	5.00E+00
10	1.50E-01	2.00E-01	31	5.00E+00	5.50E+00
11	2.00E-01	3.00E-01	32	5.50E+00	6.00E+00
12	3.00E-01	4.00E-01	33	6.00E+00	6.50E+00
13	4.00E-01	4.50E-01	34	6.50E+00	7.00E+00
14	4.50E-01	5.10E-01	35	7.00E+00	7.50E+00
15	5.10E-01	5.12E-01	36	7.50E+00	8.00E+00
16	5.12E-01	6.00E-01	37	8.00E+00	1.00E+01
17	6.00E-01	7.00E-01	38	1.00E+01	1.20E+01
18	7.00E-01	8.00E-01	39	1.20E+01	1.40E+01
19	8.00E-01	1.00E+00	40	1.40E+01	2.00E+01
20	1.00E+00	1.33E+00	41	2.00E+01	3.00E+01
21	1.33E+00	1.34E+00	42	3.00E+01	5.00E+01

(24)					
grp	Lower Bound	Upper Bound	grp	Lower Bound	Upper Bound
1	0.00E+00	1.00E-02	13	1.44E+00	1.66E+00
2	1.00E-02	2.00E-02	14	1.66E+00	2.00E+00
3	2.00E-02	5.00E-02	15	2.00E+00	2.50E+00
4	5.00E-02	1.00E-01	16	2.50E+00	3.00E+00
5	1.00E-01	2.00E-01	17	3.00E+00	4.00E+00
6	2.00E-01	3.00E-01	18	4.00E+00	5.00E+00
7	3.00E-01	4.00E-01	19	5.00E+00	6.50E+00
8	4.00E-01	6.00E-01	20	6.50E+00	8.00E+00
9	6.00E-01	8.00E-01	21	8.00E+00	1.00E+01
10	8.00E-01	1.00E+00	22	1.00E+01	1.20E+01
11	1.00E+00	1.22E+00	23	1.20E+01	1.40E+01
12	1.22E+00	1.44E+00	24	1.40E+01	

## APPENDIX-D

### Multi-point calculation strategy and Superlist

In multi-point calculations, the entire computational domain of the nuclear device is divided into small sections called meshes. Each mesh contains a different set of material and neutron spectrum, with a general possibility of the same material spanning over various meshes. Each mesh will be a unique combination of one neutron spectra and one material. For such a system, the Bateman equation can be rewritten as:

$$\frac{dN_{ik}}{dt} = -(\lambda_{ii} + \sum_g (\sigma_{ii}^g \Phi_k^g)) N_{ik} + \sum_{j \neq i} (\lambda_{ij} + \sum_g (\sigma_{ij}^g \Phi_k^g)) N_{jk} \quad (20)$$

Where  $\phi_k^g$  is the groupwise neutron spectrum at  $k^{th}$  mesh and  $N_{ik}$  and  $N_{jk}$  are isotopic concentrations of parent nuclides at  $k^{th}$  mesh. We know that during the activation process isotopes present in the material form a tree-like structure. Also, the production of the next isotope in the tree depends on the value of transmutation coefficient ( $\sum_g (\sigma_{ij}^g * \Phi^g)$  and/or decay constant  $\lambda_{ij}$ ) of the parent and daughter isotopes, which in turn depends on the incident spectrum ( $\Phi^g$ ). This fact is used to develop the present formulation for multipoint activation calculation. The improvement in multipoint activation is achieved by three steps:

1. A common coefficient matrix is created for the material for one irradiation scenario by performing activation calculation at the groupwise highest neutron spectrum. This fictitious spectrum is calculated from all the neutron spectra experienced by the material, by taking the highest value from each group for all the neutron spectra.
2. A superlist is created such that it only includes the dominant isotopes contributing to the radiological responses of interest, from the isotopes listed in the common coefficient matrix.
3. The sparsity of the coefficient matrix is reduced by separating it into two terms so that the common matrix is separated as:

$$L_{ij} = \lambda_{ij} \quad \text{and} \quad S^g = \sigma_{ij}^g \quad \text{for } i, j \in \text{superlist} \quad (21)$$

Further, only  $L_{ij}$  and  $S^g$  for isotopes in the superlist are stored to perform activation calculation for the material and mesh locations where it is located. This formulation is included in the code ACTYS-1-GO for a faster and accurate activation calculation. More details can be found in [7, 8, 11]

## References

- [1] H. Bateman, Ed., *Solution of a system of differential equations occurring in the theory of radioactive transformations*, vol. 15. Proceedings of Cambridge Philosophical Society, Mathematics and Physical Sciences, 1910, pages 423-427.
- [2] R. A. Forrest, *FISPACT-2007:User manual*, Culham Science Centre, EURATOM/UKAEA Fusion Association, Culham Science Centre, Abingdon, Oxfordshire OX14 3DB, UK, 3 2007.
- [3] J. Cetnar, “General solution of bateman equations for nuclear transmutations,” *Annals of Nuclear Energy*, vol. 33, no. 7, pp. 640 – 645, 2006. [Online]. Available: <http://www.sciencedirect.com/science/article/pii/S0306454906000284>
- [4] “Actys webpage,” <https://www.iter-india.org/ACTYS/HomePage.html>.
- [5] S. C. Tadepalli, P. Kanth, G. Indauliya, I. Saikia, S. P. Deshpande, and P. V. Subhash, “Development and validation of actys, an activation analysis code,” *Annals of Nuclear Energy*, vol. 107C, pp. 71–81, 2017.
- [6] E. Cheng, R. Forrest, and A. Pashchenko, “Report on the second international activation calculation benchmark comparision study,” International Atomic Energy Agency, IAEA Nuclear Data Section, Wagramerstrasse 5, A-1400 Vienna, Tech. Rep., 2 1994.
- [7] P. Kanth, S. C. Tadepalli, R. Srinivasan, and P. Subhash, “Actys-1-go: A faster and accurate algorithm for multipoint nuclear activation calculations,” *Fusion Engineering and Design*, vol. 122, pp. 154 – 162, 2017. [Online]. Available: <http://www.sciencedirect.com/science/article/pii/S0920379617307998>
- [8] P. Kanth and P. V. Subhash, “Actys-asg, tool for coupling actys-1-go with attila,” *Fusion Engineering and Design*, vol. 129, pp. 196 – 201, 2018. [Online]. Available: <http://www.sciencedirect.com/science/article/pii/S0920379618302011>
- [9] M. E. Sawan, “Fendl activation benchmark: Specifications for calculation for the calculation activtaion benchmark,” International Atomic Energy Agency, IAEA Nuclear Data Section, Wagramerstrasse 5, A-1400 Vienna, Tech. Rep., 12 1994.
- [10] “Fendl-2 benchmarks sublibrary,” <https://www-nds.iaea.org/fendl2/validation/benchmarks/wisconsin/>.
- [11] P. Kanth, S. C. Tadepalli, and P. V. Subhash, “Composition optimization strategy based on multiple radiological responses for materials in spatially and temporally varying neutron fields,” *Nuclear Fusion*, vol. 58, no. 12, p. 126019, 2018. [Online]. Available: <http://stacks.iop.org/0029-5515/58/i=12/a=126019>