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 pro- cess of nuclear reactions (transmutations) or radioactive decay. It is governed by the first-order linear differential equation, known as the Bateman equation [1].In this equation the fission source term (production of fission products and fission neutrons) is neglected because this codes is tailored for fusion activation problems. In a homogeneous, infinite and infinitely dilute material, the time evolution rate of nuclides 'i' can be written as[2] :

$$\frac{dx}{dy} = \frac{dx}{dy} \tag{1}$$

The first term on the R.H.S is the loss term for nuclide i. λ_{ii} is the total decay coefficient of nuclide i (sum of all the decay constant/decay modes of nuclide i, through which i could be converted into other nuclides) and $\hat{\sigma}_{ii}$ is the total reaction cross-section of nuclide i. N_i is the initial number of atoms of isotope i and N_j is the initial number of atoms of nuclide j. The second term on the R.H.S is the gain term, the production of nuclide i from various other nuclides j. λ_{ii} is the decay constant of isotope j to isotope i and $\hat{\sigma}_{ij}$ is the reaction cross-section of isotope j to produce isotope 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 λ_{ij} and $\hat{\sigma}_{ij}$ are independent of N_j, these can be written in a matrix form [3]:

$$\frac{dx}{dy} = \frac{dx}{dy} \tag{2}$$

where N is the vector containing the concentration of all isotopes at time t and Λ is the matrix of coefficients given as

$$\Lambda_{ij} = \lambda_{ij} + \sigma_{ij}\Phi \tag{3}$$

In case of i = j, the ij and ij are negative. The solution of the above equation is:

$$N(t) = etN(0) \tag{4}$$

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 time independent 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, decay gamma spectrum, radwaste index, gas production and pathways for radioactive isotopes present in the activated material.

2 Getting ACTYS

The ACTYS [4] code is hosted on github and can be clone or downloaded from https://github.com/aktyagi-iterindia/ACTYS. Alternatively, the executable file and DATA folder of ACTYS can be obtained by

emailing at actys@iterindia.in. 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 clone ACTYS from github repository,

1. go to home folder in linux and do cd
2. git clone https://github.com/aktyagi-iterindia/ACTYS
3. you will have ACTYS folder in $HOME area

To run ACTYS following are the prerequisite.

1. Create a folder to keep ACTYS executable file and the license file and data folder.
2. Run sample input files and compare the outputs generated with the sample output given. If the test fails, user should report the error to actys@iter- india.org. or to anil.tyagi@iterindia.in or subhash.puthanveetil@iterindia.in

3 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 main- tained 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 reac- tions such as (n,Xp), (n,Xd), (n,Xt), (n,Xh) and (n,Xα), 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.

4 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	Number of neutron energy groups
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
DEBUG	=0, Will not print any warning messages =1, Will print some important warning messages for debugging =2, Will print some messages and values from the linear chain solver for debugging and checking numerical errors (only recommended for developers
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.
FLUX	total flux value for the particular irradiation step.
DOSE	0 or 1, any other value will show error. Switch to calculate dose in air assuming point source =0, Will produce results treating gammas from point source for estimating dose at given distance in air. =1, Will not produce any results for dose in air.
DOSE_DIST	Distance in cm at which dose to be calculated. Only active if DOSE switch is already defined.
INTR	time step given in intervals. For example to simulate 1 year irradiation and another 1 year shutdown for the syntax should be **INTR 2** **TIME 1 Y FLUX 1.0E15** **TIME 1 Y FLUX 0.0**
CONT	time steps given in continuous fashion. For example to simulate 1 year irradiation and another 1 year shutdown for the syntax should be **CONT 2** **TIME 1 Y FLUX 1.0E15** **TIME 2 Y FLUX 0.0**
PULSE	To start the irradiation in pulsed format
ON	to specify the ON time (or time during which reactor is switched on) during a pulsed irradiation.
OFF	to specify the OFF time (or time during which reactor is switched off) during a pulsed irradiation.
STOP	to end the pulsed type irradiation

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.

Structure of input file

1 ACTYS	Header for the input file (Can be anything)

2	**/home/ACTYS/Data**	Address and name of DATA folder and license file
3		Empty Line before material description
4	**ELE 1.0 KG**	ELE for elemental composition and quantity in Kg
4	**ISO -1 AD**	ISO for isotopic composition and AD for Atomic density
5	**1**	1 Number of Elements or isotopes in the input material
6	**Cr 100**	Cr 100 Element name and its weight fraction
6	**Cr50 1.0E25**	Cr50 1.0E25 Isotope name and its number of atoms
7		Empty Line before keywords
8	**CROP 0**	CROP 1: isotopic inventory and related radiological quantities not printed
9	**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 (in next line)
13	**Cr51**	
14	**PPATH 2**	Pathways for the daughter of given isotopes, 2 is for number of isotopes (in the following lines)
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. Two pulse of following,
22	**OFF 4.54E-02 D FLUX 0.00E+00**	OFF- cooling for given time with zero flux,
23	**ON 4.63E-03 D FLUX 7.00E+18**	ON-Irradiation for given time with given flux.
24	**STOP**	to stop the pulse analysis
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 conatins groupwise neutron spectrum. First column contains the average energy of the neutron group and the second column contains the neutron flux in n/cm2 s1 . The spectrum is given in the order of lowest to highest energy. General Structure of the file is given in Figure-1. First column is energy bind edge and second column is flux value. Number of rows are as per the energy group structure.

5 Howe to Run

5.1 For Windows System

(A) **Option-1**

(a) The actys_license file is to be kept in Data folder.

(b) Use folder explorer to go to the folder where actyswindows.exe executable is located.

(c) Create new input file or copy paste modified older input file in the same folder

(d) Check the address of data folder and flux file given in input file is correct.

(e) Double click on actyswindows.exe executable file

(f) The program will ask for the name of the input file. If the location of

```
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
1.37E-05  1.30E+12
1.76E-05  1.37E+12
2.26E-05  1.43E+12
2.90E-05  1.50E+12
3.73E-05  1.58E+12
4.79E-05  1.66E+12
6.14E-05  1.74E+12
7.89E-05  1.83E+12
1.01E-04  1.92E+12
1.30E-04  2.02E+12
1.67E-04  2.12E+12
2.14E-04  2.22E+12
2.75E-04  2.33E+12
3.54E-04  2.45E+12
4.54E-04  2.57E+12
```

Figure 1: sample neutron spectrum

(g) Input file and executable is same, write the name of the input file only. If input file is not in the folder then write the complete address where the input file is located.

(h) Wait for the activation run to finish

(i) Two files with same name as input file but with extension inputfilename.out and inputfilename.path will be created. The location of these two files is the same as of the input file.

(B) **Option-2**

(a) Open Command window

(b) Go to the folder location where actyswindows.exe is kept.

(c) Create new input file or copy paste modified older input file in the same folder

(d) Check the address of data folder and flux file given in input file is correct.

(e) Run actyswindows.exe by typing actyswindows.exe in the command window.

(f) 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 input file is not in the folder then write the complete address where the input file is located.

(g) Wait for the activation run to finish

(h) Two files with same name as input file but with extension inputfilename.out and inputfilename.path will be created. The location of these two files is the same as of the input file.

5.2 For Linux System

(a) The actys_license file is to be kept in Data folder.

(b) Open Terminal

(c) Go to the folder where output files are to be generated.

(d) Create new input file or copy paste modified older input file in the same folder.

(e) Check the address of data folder and flux file given in input file is correct.

(f) Type the path of the linux executable e.g. /home/ACTYS/actyslinux or ../../actyslinux or ./actyslinux if the executable is in the same folder.

(g) The program will ask for the name of the input file. If the input file not in the same folder, write the fullpath with the name of the input file e.g. /home/ACTYS/ex-1/input.

(h) Wait for the activation run to finish

(i) Two files inputfilename.out and inputfilename.path will be created in the run folder.

6 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.

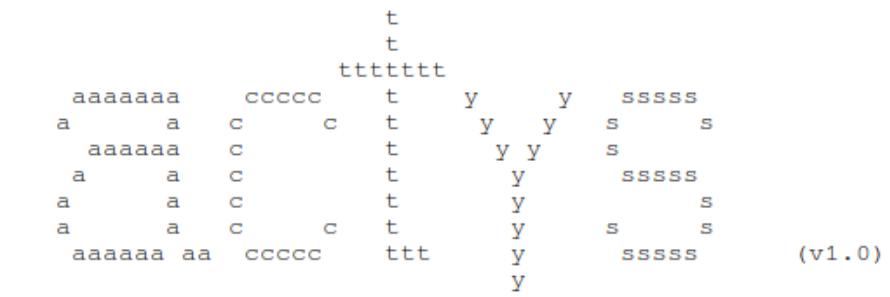
Error Message	**Solution**
Wrong MATERIAL FORM identifier. Either ELE or ISO	Check the entry at line number 4 in input file
Wrong MAT description. Only AD/KG accepted	Check the entry at line number 4 in input file
Number of isotopes/elements cannot be negative	Check the entery on line number 5 in input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

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

7 Output File

If the input file name is **example** then the output files created by ACTYS will be **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. Following are the different sections of example.out file (refer: Figure-2).



Welcome to "ACTYS" - ACTIVATION ANALYSIS CODE

NEUTRONICS GROUP, ITER-INDIA (IPR)
SEPTEMBER 2020

Wed Jun 26 16:25:45 2024

****

CROSS SECTION DATA RETRIEVED FROM => /home/solps/mcnp_tools/ACTYS/Data
DECAY DATA => JEFF3.1.1RDD

****

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

```
 ***************************
 ---------------MATERIAL DESCRIPTION-------------    1.0000000000000000      KG
      Cr  1.000000E+02

 ----------INPUT TIME SCENARIO-------------
 INTR              1
TIME   1.00000E+02 S FLUX 1.30000E+16


------Isotopic concentartion post material processing
 Cr50       5.03234E+23
 Cr52       9.70436E+24
 Cr53       1.10040E+24
 Cr54       2.73912E+23

 ------Initial Material Mass composition (grams)---------
Cr   1000.00000

 Pathways to be generated and saved
 Dominant nuclides will be printed
 Primary parent contribution will be listed
Total neutron flux from the "Flux file" :       2.00025E+14
```

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

```
  #          1
**********FINAL CONCENTRATION after DELTA TIME STEP  1.0000E+02  seconds********

      FLUX   1.30000E+16 --- Irradiation
```

NUCLIDE	HALF LIFE seconds	ATOMS	MASS g	ACTIVITY Bq	DOSE Sv/hr	a-HEATING KW	b-HEATING KW	g-HEATING KW
H1	Stable	6.01095E+17	1.00595E-06	0	0	0	0	0
H2	Stable	1.78036E+16	5.95439E-08	0	0	0	0	0
H3	3.89105E+08	3.77668E+13	1.89146E-10	6.72774E+04	0.00000E+00	0.00000E+00	6.15202E-14	0.00000E+00
He3	Stable	3.13000E+11	1.56758E-12	0	0	0	0	0
He4	Stable	1.20871E+17	8.03365E-07	0	0	0	0	0
Ar40	Stable	5.81704E+00	3.86013E-22	0	0	0	0	0
K43	7.99200E+04	4.14223E+00	2.95498E-22	3.59256E-05	7.27979E-15	0.00000E+00	1.78179E-21	5.56114E-21
Ca42	Stable	5.24302E+04	3.65302E-18	0	0	0	0	0
Ca43	Stable	2.29359E+06	1.63613E-16	0	0	0	0	0
Ca44	Stable	8.46828E+07	6.18099E-15	0	0	0	0	0
Ca45	1.40832E+07	1.68669E+06	1.25914E-16	8.30156E-02	1.57533E-19	0.00000E+00	1.02683E-18	1.26930E-25
Ca46	Stable	2.11051E+08	1.61049E-14	0	0	0	0	0
Ca47	3.92083E+05	1.90662E+07	1.48659E-15	3.37063E+01	1.04435E-08	0.00000E+00	1.86102E-15	5.72657E-15
Ca48	1.67255E+27	2.37173E+04	1.88854E-18	9.82905E-24	9.40754E-35	0.00000E+00	3.43910E-39	7.40155E-41
Sc44	1.42920E+04	2.30427E+00	1.68203E-22	1.11755E-04	5.91013E-14	0.00000E+00	1.06720E-20	3.82411E-20
Sc44m	2.10960E+05	1.07001E+00	7.81066E-23	3.51570E-06	1.50561E-16	0.00000E+00	1.84868E-23	1.55054E-22
Sc45	Stable	4.12912E+06	3.08243E-16	0	0	0	0	0
Sc45m	3.16000E-01	1.22547E+04	9.14825E-19	2.68807E+04	3.34002E-09	0.00000E+00	3.70382E-14	2.63272E-15
Sc46	7.23928E+06	8.60638E+08	6.56756E-14	8.24044E+01	4.52327E-08	0.00000E+00	1.47958E-15	2.65307E-14
Sc46m	1.87000E+01	4.60140E+07	3.51135E-15	1.70559E+06	1.14171E-05	0.00000E+00	1.60953E-11	2.26698E-11
Sc47	2.89526E+05	4.86402E+08	3.79230E-14	1.16448E+03	1.01272E-08	0.00000E+00	3.03310E-14	2.02221E-14
Sc48	1.57212E+05	6.97493E+08	5.55389E-14	3.07524E+03	2.89642E-06	0.00000E+00	1.08192E-13	1.65038E-12
Sc49	3.43200E+03	5.10657E+08	4.15080E-14	1.03135E+05	3.45273E-08	0.00000E+00	1.35478E-11	5.51953E-14
Sc50	1.02500E+02	2.43346E+07	2.01850E-15	1.64561E+05	1.49377E-04	0.00000E+00	4.28210E-11	8.43195E-11
Sc50m	3.50000E-01	3.95935E+04	3.28419E-18	7.84118E+04	3.04117E-06	0.00000E+00	5.11130E-13	3.32170E-12
T145	1.10880E+04	3.23677E+05	2.41640E-17	2.02341E+01	3.64011E-09	0.00000E+00	1.21033E-15	2.82640E-15
T146	Stable	6.65147E+13	5.07548E-09	0	0	0	0	0

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

```
Number of isotopes for which inventory is listed  53  out of  376 considered


Net activity of the material is   7.365525E+14  Bq  or   1.990682E+04 Curie
Total Contact Dose is   3.071564E+05 Sv/hr
    Total Decay heat    2.921914E-01    KW

Total material mass :  1.00000E+03 g
    Specific activity :   7.36552E+14 Bq/Kg
 ------Material Mass composition (grams)---------
V5      0.00005
Cr    999.99990
```

	NUCLIDE	Bq	% Activity	NUCLIDE	Sv/hr	% Dose	NUCLIDE	KW	% Decay heat
1	V52	6.26923E+14	85.116	V52	2.68882E+05	87.539	V52	2.52386E-01	86.377
2	V53	7.89178E+13	10.714	V53	2.31463E+04	7.536	V53	2.58785E-02	8.857
3	Cr55	1.56572E+13	2.126	V54	1.48738E+04	4.842	V54	1.06273E-02	3.637
4	V54	1.21594E+13	1.651	T151	1.26989E+02	0.041	Cr55	2.76130E-03	0.945
5	T151	1.89627E+12	0.257	Cr49	1.22069E+02	0.040	T151	3.74754E-04	0.128
6	Cr49	6.12152E+11	0.083	Cr55	3.26948E+00	0.001	Cr49	1.61214E-04	0.055
7	Cr51	3.85627E+11	0.052	Cr51	2.16145E+00	0.001	Cr51	2.24742E-06	0.001
8	V49	8.35751E+08	0.000						

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

```
 ------------------------------------------------------------
  TYPE    Isotope          Bq/kg
     A    H3          6.72774E+04
     A    V49         8.35751E+08
Material is TYPE A (a/c to ANDRA Classification)     8.36E+05
 ------------------------------------------------------------

 *----------Gamma Spectrum-----------------*
 1     5.37021E+08     8.54938E+08
 2     5.17052E+02     2.74382E+02
 3     8.82288E-05     2.00658E-05
 4     3.64363E+10     3.86711E+09
 5     2.89563E+10     1.53662E+09
 6     2.05220E+11     6.53419E+09
 7     6.03915E+11     1.37348E+10
 8     1.24069E+12     1.97517E+10
 9     6.31568E+11     7.18183E+09
```

(e) After the list of dominating isotopes, group-wise gamma spectrum is listed.

```
 *----Isotope wise Gamma Source (MeV/s)-----*
K43          3.47075E-05
Ca47         3.57285E+01
Sc44         2.38682E-04
Sc45m        1.59136E+01
Sc46         1.65592E+02
Sc46m        1.41494E+05
Sc47         1.26216E+02
Sc48         1.03008E+04
Sc49         1.07592E+02
Sc50         5.25275E+05
Sc50m        2.07217E+04
Ti45         1.76298E+01
Ti51         6.86518E+11
Ti52         2.15058E+04
V47          3.69369E-01
V48          6.55659E+04
V49          7.45980E+05
V52          9.05871E+14
V53          8.19524E+13
V54          4.97651E+13
Cr49         6.40233E+11
Cr51         1.26141E+10
Cr55         1.05408E+10
Mn54         1.43961E+00
Mn56         3.01083E+04
 *------------------------------------------*
```

(f) Isotopic total gamma emission.

```
********************END OF TIME STEP**************************

                                                Total CPU Time =      0.141 sec



 #            2
**********FINAL CONCENTRATION after DELTA TIME STEP  6.3115E+07  seconds*********
```

(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.

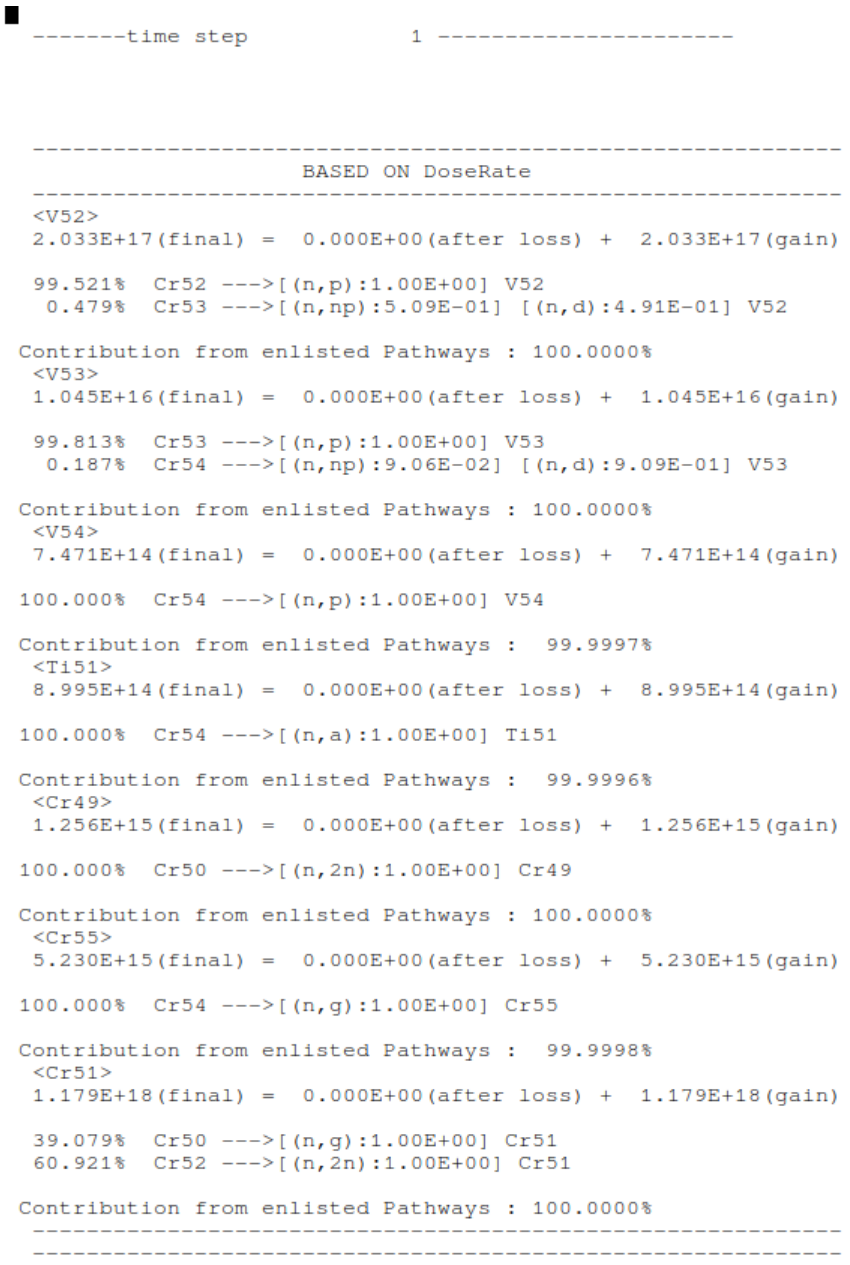
```
********************END OF TIME STEP************************

                                        Total CPU Time =     17.328 sec


-----------------------------------PROBLEM SOLUTION TABLE-----------------------------------------
  #      TIME(s)     CUMLTVE      FLUX       ACTIVITY      Dose     Heating(KW)      H3       Activity
                     TIME(y)    (n/cm2/s)     (bq/Kg)     (mSv/h)
--------------------------------------------------------------------------------------------------
  1   1.000E+02   3.171E-06   1.300E+16   7.316E+14   3.037E+08   2.894E-01   3.646E+04     A
  2   6.312E+07   2.001E+00   2.680E+16   2.596E+16   5.062E+09   4.816E+00   6.819E+10     B
  3   3.923E+03   2.001E+00   0.000E+00   1.425E+16   2.947E+08   2.338E-01   6.819E+10     B
  4   4.000E+02   2.002E+00   7.000E+18   2.176E+18   8.899E+11   8.526E+02   6.834E+10     B
  5   3.923E+03   2.002E+00   0.000E+00   1.635E+16   1.055E+09   8.726E-01   6.834E+10     B
  6   4.000E+02   2.002E+00   7.000E+18   2.178E+18   8.905E+11   8.531E+02   6.849E+10     B
  7   8.640E+04   2.004E+00   0.000E+00   1.453E+16   2.390E+08   1.817E-01   6.848E+10     B
  8   1.000E+11   3.173E+03   0.000E+00   2.115E+05   2.896E-04   3.267E-13   0.000E+00     A


Total Irradiation Time =   1.000632E+11  s
Total Fluence          =   1.404867E+30  n/cm2
Neutrons produced      =    11637
```

(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: structure of *.out file

8 Path File

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



```
-------time step            1 ----------------------


 ------------------------------------------------------------
                     BASED ON DoseRate
 ------------------------------------------------------------
 <V52>
 2.033E+17(final) =  0.000E+00(after loss) +  2.033E+17(gain)

 99.521%  Cr52 --->[(n,p):1.00E+00] V52
  0.479%  Cr53 --->[(n,np):5.09E-01] [(n,d):4.91E-01] V52

Contribution from enlisted Pathways : 100.0000%
 <V53>
 1.045E+16(final) =  0.000E+00(after loss) +  1.045E+16(gain)

 99.813%  Cr53 --->[(n,p):1.00E+00] V53
  0.187%  Cr54 --->[(n,np):9.06E-02] [(n,d):9.09E-01] V53

Contribution from enlisted Pathways : 100.0000%
 <V54>
 7.471E+14(final) =  0.000E+00(after loss) +  7.471E+14(gain)

100.000%  Cr54 --->[(n,p):1.00E+00] V54

Contribution from enlisted Pathways :  99.9997%
 <Ti51>
 8.995E+14(final) =  0.000E+00(after loss) +  8.995E+14(gain)

100.000%  Cr54 --->[(n,a):1.00E+00] Ti51

Contribution from enlisted Pathways :  99.9996%
 <Cr49>
 1.256E+15(final) =  0.000E+00(after loss) +  1.256E+15(gain)

100.000%  Cr50 --->[(n,2n):1.00E+00] Cr49

Contribution from enlisted Pathways : 100.0000%
 <Cr55>
 5.230E+15(final) =  0.000E+00(after loss) +  5.230E+15(gain)

100.000%  Cr54 --->[(n,g):1.00E+00] Cr55

Contribution from enlisted Pathways :  99.9998%
 <Cr51>
 1.179E+18(final) =  0.000E+00(after loss) +  1.179E+18(gain)

 39.079%  Cr50 --->[(n,g):1.00E+00] Cr51
 60.921%  Cr52 --->[(n,2n):1.00E+00] Cr51

Contribution from enlisted Pathways : 100.0000%
 ------------------------------------------------------------
 ------------------------------------------------------------
```

(a) Pathways for dominating isotopes

```
------------------------------------------------------------
               PATHWAYS FOR REQUESTED NUCLIDES
------------------------------------------------------------
<Cr51>
1.179E+18(final) =  0.000E+00(after loss) +  1.179E+18(gain)

39.079%  Cr50 --->[(n,g):1.00E+00] Cr51
60.921%  Cr52 --->[(n,2n):1.00E+00] Cr51

Contribution from enlisted Pathways : 100.0000%

------------------------------------------------------------
------------------------------------------------------------
```

(b) Pathways for isotopes requested through keyword PATH

```
------------------------------------------------------------
            PATHWAYS FOR DAUGHTERS OF Cr50
------------------------------------------------------------


   H1 ------> 5.53E+17
1.01E+17  Cr50 --->[(n,np):2.90E-01] [(n,p):7.06E-01] H1

   H2 ------> 1.47E+16
1.54E+15  Cr50 --->[(n,d):1.00E+00] [(n,pd):2.76E-13] H2

   H3 ------> 2.05E+13
3.70E+09  Cr50 --->[(n,t):1.00E+00] H3

  He3 ------> 1.10E+11
1.08E+11  Cr50 --->[(n,h):1.00E+00] He3

  He4 ------> 1.11E+17
1.06E+16  Cr50 --->[(n,na):2.65E-03] [(n,a):9.97E-01] He4
1.32E+11  Cr50 --->[(n,g):1.00E+00] Cr51 --->[(n,na):5.64E-05] [(n,a):1.00E+00] He4

 Ti46 ------> 2.82E+13
2.82E+13  Cr50 --->[(n,na):1.00E+00] Ti46
9.90E+08  Cr50 --->[(n,a):1.00E+00] Ti47 --->[(n,2n):1.00E+00] Ti46

 Ti47 ------> 1.06E+16
1.06E+16  Cr50 --->[(n,a):1.00E+00] Ti47
```

(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: Structure of *.path file

9 Test Case

The second international Activation calculation benchmark comparison study, carried out by IAEA in 1994 [5] is used as sample test case for ACTYS.

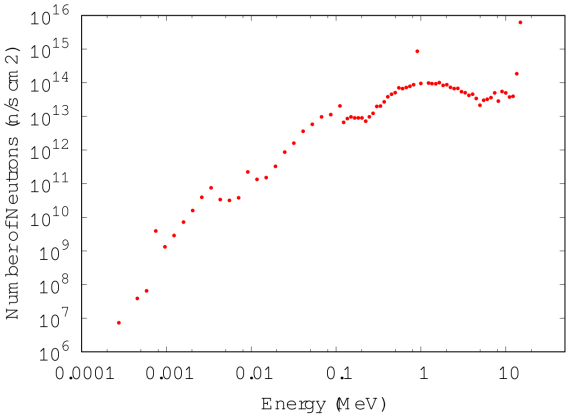


Figure 4: Neutron spectrum in 100 group structure (Normalized to 5 M W/m2 Wall loading

(a) 1kg of natural iron irradiated for 1 year using the GAM-II 100 group neutron spectrum, as given in figure 4.

(b) 1.0 x 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, 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. The input files are available in example folders for linux and windows. An example file is shown below with the Keywords in blue color and user inputs shown in pink color. The entries in pink can be edited by the user. Also, more keywords can be added that are given in the Section 4 above.

example-1 input file witho isotope composition

```
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
```

example-2 input file with Element composition

```
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
```

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 λ_{AB} and initial concentration $N_B(0) = 0.0$, the Bateman equation is given as:

$$\frac{dA}{dt} = -\lambda_{AB}A \tag{5}$$

The solution of the above equation is :

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

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

$$\frac{dB}{dt} = \lambda_{AB}A - \lambda_{BC}B \tag{7}$$

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

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

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

$$\frac{dN_i}{dt} = \lambda_{i-1}N_{k-1} - \lambda_i N_i \tag{9}$$

where, λ_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:

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

where

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

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 $\sigma_i j * \phi$ is added to the decay constant λ_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 .

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

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

$$P_n < (\text{cutoff} * N_o + ll) \tag{13}$$

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

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

The term $(1 - e^{-d_1 t})$ can be used to define an appropriate cutoff. More details can be found in [6]

APPENDIX-B

Radiological quantities calculated by ACTYS

The radioactive nuclides generated in a material after neutron irradiation,would emit ionizing radiations like α, β and γ 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 Bq = 1 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:

$$\gamma_i = \sum_j P_i E_i A_j \tag{15}$$

Where, γ_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'.

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:

$$D_i = C\frac{B}{2}\sum_g \frac{\mu_a}{\mu_m} E_g \frac{A_i}{M} \qquad \text{where} \qquad \mu_m = \sum \frac{m_i}{M}\mu_i \tag{16}$$

Where $C = 5.767^{-10}$ is the conversion factor from Mev/s to Sv/hr, $B = 2$ is the buildup factor, μ_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.

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 i.e. Très Faible Activité in French)

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

$$IRAS = \sum \frac{A_i}{10^{C_i}} \tag{17}$$

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.

APPENDIX-C

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	

References

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[6] Sai Chaitanya Tadepalli, Priti Kanth, Gunjan Indauliya, Ishwita Saikia, Shishir P. Deshpande, and Subhash P.V. Development and validation of actys, an activation analysis code. *Annals of Nuclear Energy*, 107:71–81, 2017.