Radionuclide Yield Calculator (version 2.0) MANUAL

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About

Radionuclide Yield Calculator is a program dedicated to radioisotope production with the use of the cyclotron. It calculates the yield, activity and number of nuclei of any isotope for different production conditions. It was written in python programming language (version 2.7) using the TKinter module and compiled with PyInstaller (version 3.4). RYC uses SRIM module by J. F. Ziegler.

Main features

- fit different functions to the cross-section data
- import the TENDL cross-sections
- calculate TTY (production yield)
- calculate the activity at EOB (end of bombardment)
- calculate the number of produced nuclei
- search the radioactive impurities

System requirements

- Windows 64-bit
- it is NOT necessary to install SRIM software separately

RYC files

- *RYC.exe*: launches main program window
- *Manual.pdf* and *Manual_short.pdf*
- *LICENSE.txt*: license for this program
- *SRModule.exe*, *SCOEF03.dat*, *SNUC03.dat*, *VERSION* and *SR.IN*: SRIM files, needed for the calculation of the stopping-power [http://www.srim.org/]
- *SRoutput.txt*: file that stores SRModule output
- *TENDL-lib* (optional): stores the cross-section from TENDL-2015 on the stable isotopes [https://tendl.web.psi.ch/tendl_2015/tendl2015.html]

RYC layout and use

Save/Load project

Under the *File* top menu, you can find *Save project* option that saves the current state of program in the separate file (in txt format). After reopening RYC, you can choose *File*, *Load project* and select earlier saved file to load all saved data into the current session.

TENDL settings

Select this entry under the *File* top menu to decide whether RYC should connect with TENDL-2017 website or use files in the TENDL-lib directory. In the first case, RYC must be able to connect with the internet. In the latter, the TENDL-lib directory must be downloaded and placed among the other RYC files.

Example

Under *Edit* top menu, you can select *Example* option which will overwrite the current session with exemplary inputs used in this manual. The example is ^{44}Sc production via ^{44}Ca(p,n)^{44}Sc on ^{44}CaCO$_3$ target (^{44}Ca enriched to 97.1%).

Clear all

Clear all option under *Edit* top menu will remove all inputs and outputs in the current session.
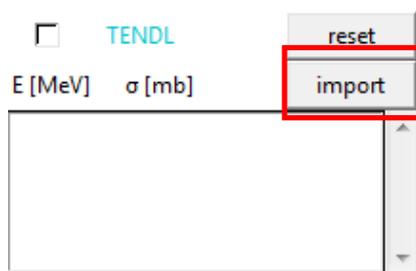
Cross-section inputs

There are three fields dedicated for user-defined cross-section and one more for TENDL. You can select which data-sets are to be considered in further analysis by checking the corresponding check-boxes.

For user-defined data, enter or modify the cross-section data by typing one energy value [MeV] and corresponding cross-section value [mb] (separated by space or tabulator) per row in text-box. You can use scientific notation. Use point "." as the decimal separator. Do not use any other symbols and do not add empty rows.

You can also paste data-sets into the text-boxes. In this case, first two columns will be interpreted as energy and cross-section while the other columns will be ignored.

You can name each data-set above the text-box (the name will serve as the label on plot).

Import TENDL

This command imports the cross-section from TENDL (TALYS-based evaluated nuclear data library) and insert it in the text-box. For that, you need to specify *Projectile*, *Target nuclide*, *Product nuclide* and its *State* (in *Parameters inputs*).

By default, RYC will try to connect with the TENDL-2017 website. If it fails, you can download TENDL-lib directory which contains TENDL-2015 cross-sections for the nuclear reactions on the stable isotopes. Then, change the *TENDL settings* to use TENDL-lib.

State "all" corresponds to TENDL's "tot"; most of the used nuclear reactions have only this cross-section, unless there is a clear distinction between ground and metastable states. Only in the latter case, use "g" or "m" states to import corresponding cross-section from TENDL.

For more information, see https://tendl.web.psi.ch/tendl_2017/tendl2017.html.

You can modify or add new entries to the TENDL-lib directory or create empty TENDL-lib and put there only the cross-section interesting for you (without downloading TENDL-lib and all its content from the website). To do that, follow this file notation (from TENDL-2015):
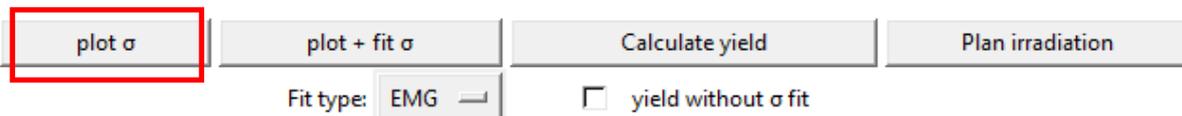
tendl_2015-<projectile>_file-<target symbol>-<target A>_residual_rp<product Z, 3 digits><product A, 3 digits>-<state>.txt

For example, for ^{107}Ag(α,x)^{72tot}Rb reaction the file path would be:

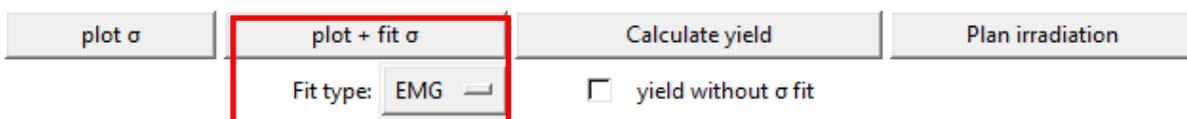*tendl_2015-alpha_file-Ag-107_residual_rp037072-tot.txt*

The file must have two columns that correspond to E [MeV] and σ [mb].

plot σ

This command plots the cross-section data on the *cross-section plot*. Only the selected data-sets will be used. Don't select empty data-sets. Deselecting all cross-section data and using this function will clear the plots.

plot + fit σ

This command works in the same way as *plot σ* but additionally it also fits the function to the data using the least-square method. You can select the fitting function from the *Fit type* list:

- EMG (Experimentally Modified Gaussian distribution)
- GGD (Generalized Gaussian Distribution, generalized error version)
- q-W (modified q-Weibull distribution)
- pol-*n* (polynomial of degree *n*)

Consider removing zero-values from the cross-section data-sets to improve the fit. Deselecting all cross-section data and using this function will clear the plots.

Parameters inputs

Projectile impaling on the target: choose p (proton), d (deuteron) or α (alpha particle).

Target nuclide: atomic mass followed by the symbol of the element on which the nuclear reaction of interest occurs. If only the symbol of the element is given, e.g. "Ca", the program will assume the mass of natural element.

Chemical form: select metal or compound target (and mark if it's gaseous). In the latter case, list all the elements in the text-box: symbol of each element and its stoichiometry per row (separated by space or tab; don't use empty rows). The atom specified in *Target nuclide* must be present. See also *Mixed target*.

Density of the target chemical form will be used to calculate stopping-power.

Enrichment: abundance of the target nuclide in target material. Put 100 if you use the cross-section values on natural target.

Product nuclide: atomic mass followed by the symbol of the element, e.g. "44Sc", which is the desired product of nuclear reaction.

State of the product nuclide: g (ground), m (metastable), all (sum of all states).

Half-life of the product nuclide: the value in hours [h] or days [d]. See also *Stable product case*.

Calculate yield

This command performs the following operations:

1. refreshes the *cross-section plot* and *fit* (if needed),
2. launches the SRIM module (*SRModule.exe*) in the background to calculate stopping-power in the target (the SRIM software doesn't have to be installed separately for this),
3. integrates cross-section and stopping-power with the use of Simpson's algorithm to calculate the Thick Target Yield (TTY), in other words, production yield,
4. plots the yield on the *yield plot*.

You can also perform this procedure without the cross-section fit. To do it, select the check-box *yield without σ fit* and select only one data set to be used. The selected data-set must consist of at least three non-zero unique values.

Please wait up to 2 seconds for this command to execute.

Deselecting all cross-section data and using this command will clear the plots.

The following formula is used for TTY calculation:

$$TTY(E) = \frac{H\,N_A\,\lambda}{Z\,e\,M} \int_{0}^{E_{max}} \frac{\sigma(E)}{\mathrm{d}E/\mathrm{d}x(E)}\,\mathrm{d}E \quad \left[\frac{\text{MBq}}{\mu\text{Ah}}\right]$$

where: H − enrichment and purity, N_A − Avogadro's number, λ − decay constant of the radioisotope, Z − charge of the fully ionized projectile, e − elementary charge, M − atomic mass

of the target, E_{max} – maximal energy of the projectile penetrating the target, dE/dx – stopping-power of the projectile in the irradiated target.

Plan Irradiation

plot σ	plot + fit σ	Calculate yield	Plan irradiation

Fit type: EMG ⎯ ☐ yield without σ fit
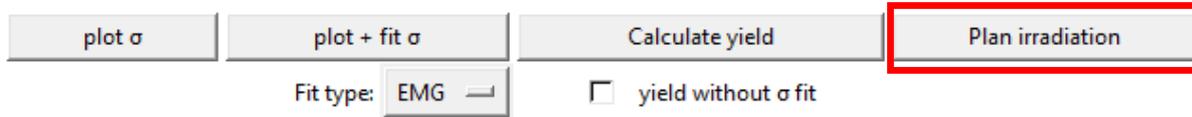
Plan irradiation creates a separate window to specify the conditions of the irradiation:
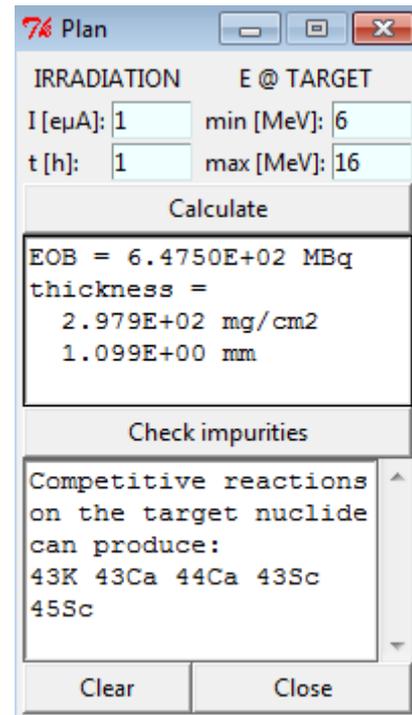
- beam current *I* [eµA],
- irradiation time *t* [h],
- the energy range of the projectile inside the target (from E_{max} [MeV] to E_{min} [MeV]).

The *Calculate* command prints the outcome of such irradiation, based also on the current yield (it must be calculated earlier for the selected energy range with *Calculate yield* command). It prints the activity at the end of bombardment (*EOB*) and the required target thickness. The selected energy range will be visible on *cross-section plot*.

The following formula is used for *EOB* calculation:

$$EOB = TTY^{Emax \rightarrow Emin} \cdot \frac{I}{\lambda} \cdot \left(1 - e^{-\lambda t}\right) \text{ [MBq]}$$

The *Check impurities* command uses E_{max} [MeV] input and compares it with energy thresholds of other nuclear reactions from TENDL to estimate the potential radioactive contaminants produced on the element specified in Target nuclide. This command requires to define a mass of the target nuclide in *Parameters inputs* and will use the specified *TENDL settings* thus it requires either the internet connection or the TENDL-lib directory (the first case might take more time, depending on the E_{max} input).

```
7⅙ Plan                    ▢ ▫ ✕

IRRADIATION        E @ TARGET
I [eµA]: 1         min [MeV]: 6
t [h]:   1         max [MeV]: 16
        Calculate
┌─────────────────────────────┐
│EOB = 6.4750E+02 MBq         │
│thickness =                  │
│   2.979E+02 mg/cm2          │
│   1.099E+00 mm              │
└─────────────────────────────┘
        Check impurities
┌─────────────────────────────┐
│Competitive reactions    ▲   │
│on the target nuclide        │
│can produce:                 │
│43K 43Ca 44Ca 43Sc          │
│45Sc                     ▼   │
└─────────────────────────────┘
     Clear            Close
```

Stable product case

It is possible to calculate the production of stable isotopes. To do that, proceed exactly as in radioactive product case described above but use 0 as half-life in *Parameters inputs*. All outputs will be then given in number of produced nuclei instead of activity. *Calculate yield* will utilize the following formula:

$$TTY_{stable}(E) = \frac{H\,N_A}{Z\,e\,M} \int_{E_{thr}}^{E_{max}} \frac{\sigma(E)}{\mathrm{d}E/\mathrm{d}x(E)} \mathrm{d}E \left[\frac{\text{nuclei}}{\mu Ah}\right]$$

and *Calculate* in *Plan Irradiation* will assume no decay of the product during the irradiation, estimating the number *N* of produced nuclei as:

$$N = TTY^{Emax \rightarrow Emin}_{stable} \cdot t \cdot I \text{ [nuclei]}$$
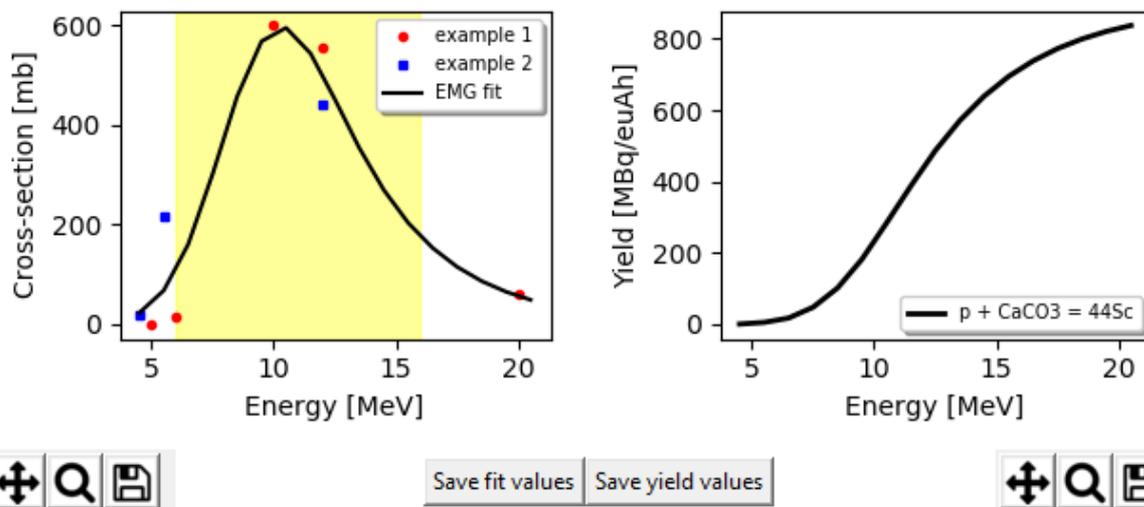
Graphs

Two graphs, *cross-section plot* and *yield plot*, are updated automatically by the program. Each has its own command panel in which you can select a tool to edit the graph with:

- *panning tool* allows to move the graph by clicking and holding left mouse button on it, or change the scale with the right mouse button,
- *zooming tool* allows to create a rectangle on the graph by clicking, holding and moving left/right mouse button and zoom in/out the graph upon the release,
- *disc tool* creates a "png" image of the corresponding graph on your computer.

Save fit/yield values create a "txt" file with the values of the fit/yield from the graph.

Mixed target

If you want to calculate the yield of nuclear reaction on the element that is just the contaminant in the whole target, you have to include the target chemical composition it in the compound target *Chemical form* (in *Parameters inputs*).

Let's say you want to calculate the yield of ^{43}Sc production via ^{40}Ca(α,p) on ^{nat}CaCO$_3$ that is mixed with graphite in mass proportions 20:80.

Stoichiometry of CaCO$_3$ is 1 : 1 : 3 for Ca : C : O respectively.

This translates to masses of 40 : 12 : 48 and the respective molecular mass of 100 g/mol.

To keep the ratio 20:80, you need to add 400 g of graphite.

Overall, the compound mass would be 40 : 412 : 48 which is 500 g total.

Therefore the stoichiometry for the mixed target (^{nat}CaCO$_3$ mixed with graphite in 20:80 ratio) is 1 : 34.3 : 3 (and this stoichiometry should be used in the compound list in RYC).

You also have to provide the *Density* of the mixed target. In *Enrichment* section, you still use the abundance of ^{40}Ca in ^{nat}CaCO$_3$ which is 97%.

Troubleshooting

Cross-platform

The program is designed for Windows 64-bit but you can try to launch it on macOS or Linux with the use of the emulator (for example *Wine*, https://www.winehq.org/). In this case, make sure that files with the extension "exe" are launched by default by the emulator and the emulator has the Microsoft Visual Basic 5.0 run-time files installed (this is required to run *SRModule.exe*).

Yield calculations

On certain computers, *Calculate yield* command might calculate no TTY and leave the *yield plot* empty, preventing the calculation of *EOB* in *Plan Irradiation*. This happens due to lack of Microsoft Visual Basic 5.0 run-time files without which SRModule cannot run hence RYC has no stopping-power values to calculate TTY. To fix this, run *Msvbvm50.exe* available at the Microsoft website [https://support.microsoft.com/en-us/help/180071/file-msvbvm50-exe-installs-visual-basic-5-0-run-time-files] that will install necessary DLL files.

False positive malware

Some operating systems or antivirus software might consider RYC a malware thus preventing RYC to launch at all. This is most likely because they consider RYC as from Unknown Publisher. If the antivirus is not providing any solutions, you can try to run RYC as the administrator or unblock RYC under its file properties (right click on *RYC.exe* file).

No connection error

In certain cases, RYC will not communicate with TENDL website even though the computer has the internet connection. This might happen due to many individual factors. Consider checking your OS firewall or using TENDL-lib directory (see: *Import TENDL*) to solve this.

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The files *SRModule.exe*, *SCOEF03.dat*, *SNUC03.dat*, *VERSION* and *SR.IN* are distributed under the same conditions as SRIM program. They may be freely copied and used for any non-commercial application. Their inclusion in any commercial software requires a license from SRIM.org. See the legal notice "/Data/Legal.rtf" in the www.SRIM.org directory for full details.