University of Birmingham Tool for Isotope Production (UoB-TIP)

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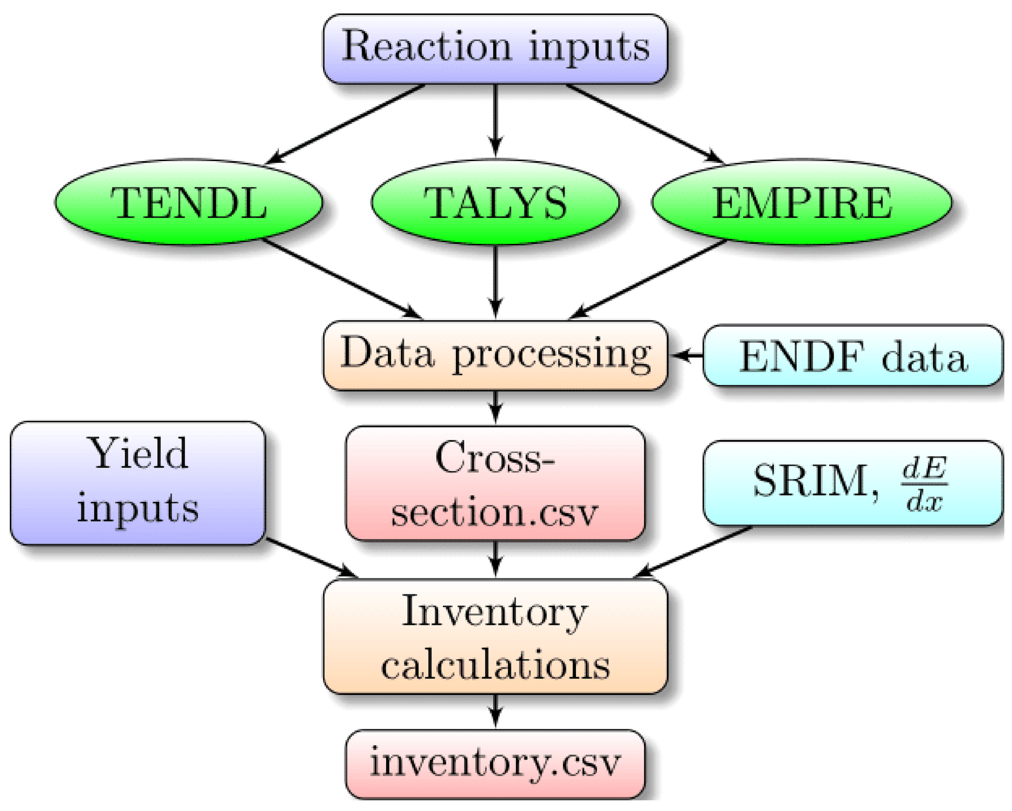
Introduction

- University of Birmingham - Tool for Isotope Production aims to utilise the benefits of nuclear reaction codes such as **EMPIRE**[1], **TALYS**[2] and precompiled **TENDL**[2] data
- automating execution and data processing
- Calculating production **cross-section** and production **yield**
- While leveraging the benefits of existing infrastructure this package aims to **streamline calculations**
- Output data in a clear and concise **machine and human readable format**
- Provide intuitive **data visualisations**
- Utilise nuclear decay data from **ENDF** and stopping power from **SRIM** by default.
- Enable calculations with **complex targets including molecular or compound** and accounting for impurities in the target



Aims

- Automate reaction calculations
- Allow complex targets (molecules and compounds)
- Run a large number of reactions easily
- Clear and concise data outputs
- Intuitive data visualisations
- Run yield calculations with user data
- Easy to use interface

Installation and usage

UoB-TIP is available through a variety of routes

- **Python** package (pip, conda)
- **Docker** container
- Executable with a **GUI** interface
- **Released later this year**
- For be kept up to date with release details **register interest with: r.allen.4@pgr.bham.ac.uk**

UoB-TIP Data Structures

UoB-TIP outputs data in a **nested directory** for reactions and sub-reactions as shown in the figure below.

```
UoB-TIP
└ Project Title
  ├ Cross-Section
  │ └ Reaction_i
  │   ├ XS-datafile.csv
  │   ├ visualisation.png
  │   └ Sub reaction_j
  │     ├ XS-datafile.csv
  │     └ visualisation.png
  ├ Stopping Power
  └ Production Yield
```

- **.csv output** file containing all data
- A row for each product
- Each product contains product name, excitation energy, half-life and cross-section data

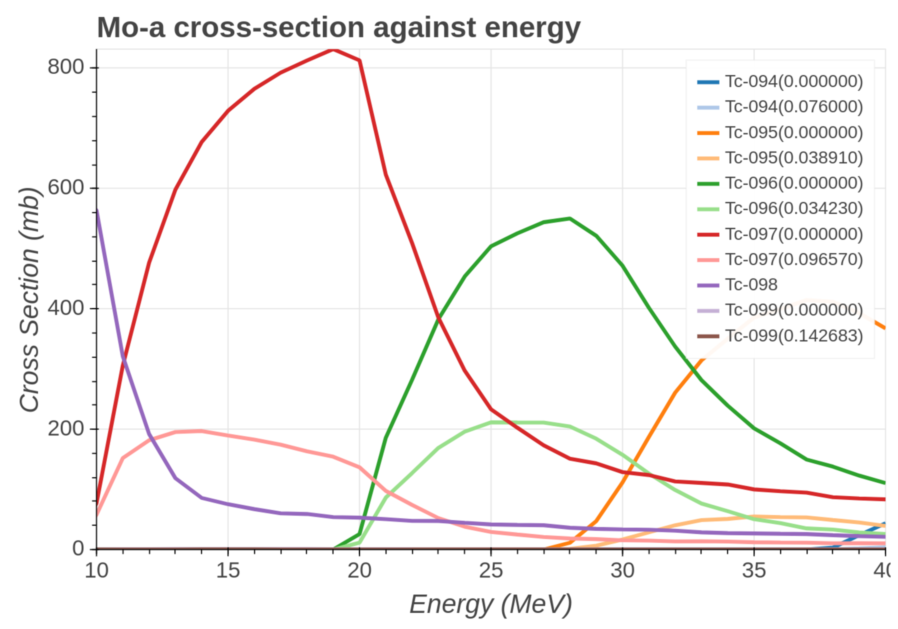
Product	Half-life	decay types	E_1	E_2	E_3	E_4	...	E_n

User Inputs

- Two input categories, reaction and yield inputs
- **Reaction inputs** include: target, projectile, and optional nuclear models.
- **Yield inputs** include: beam current, irradiation time, beam energy and target thickness

Cross-Section

- Calculated using TALYS or EMPIRE (user specified)
  - Large amount of **optional nuclear parameterisation**
- Alternatively cross-seciton data can be extracted from TENDL data files.



Reaction Rate

- Reaction rate is the number of **reactions per second** for a given reaction channel
- Determined by cross-section, target thickness, beam current and irradiation time

$$R_{A\to B} = \frac{I_{beam}}{z_p q_e}\frac{1}{V_{tar}}\int_{E_f}^{E_i}\left(\frac{dE}{dx}\right)^{-1}\sigma_i(E)dE \quad (1)$$

Stopping Power

- Contains **pre-calculated stopping power** from SRIM
  - For ^1H, ^2H, ^3He and ^4He projectiles
  - For all elements Z=1 to Z=115
  - For energies 0→100MeV
- Users **may define their own stopping power** using a .csv (for comlpex targets and higher energies)

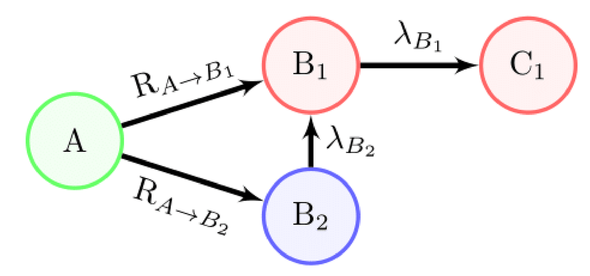
Inventory Calculations

- Inventory calculations cover the quantity of products (in terms of **mass and activity**) with respect to time during irradiation and subsequent cooling.
- For the simple case where $A \to B_1 \to C_1$. A is the target isotope, which produces B upon irradiation. B_1 is unstable and decays into B_2. The number of particles of B_1 with respect to time during irradiation is:

$$N_{B_1}(t) = \frac{R_{A\to B_1}}{\lambda_{B_1}}(1-e^{-\lambda_{B_1}t_{irrad}})e^{-\lambda_{B_1}t_{cool}} \quad (2)$$

- The scenario becomes more complex with some produced **produced both directly by the beam** and through the **decay of other isotopes**, as well as the decay of other products
- Several reasonable assumptions are made:
  1. Only the target isotopes are present at t=0
  2. The beam only interacts with target isotopes

- A product, B_1 which is produced both through the beam interacting with the target, A, as well as the decay of isotopes, B_2.



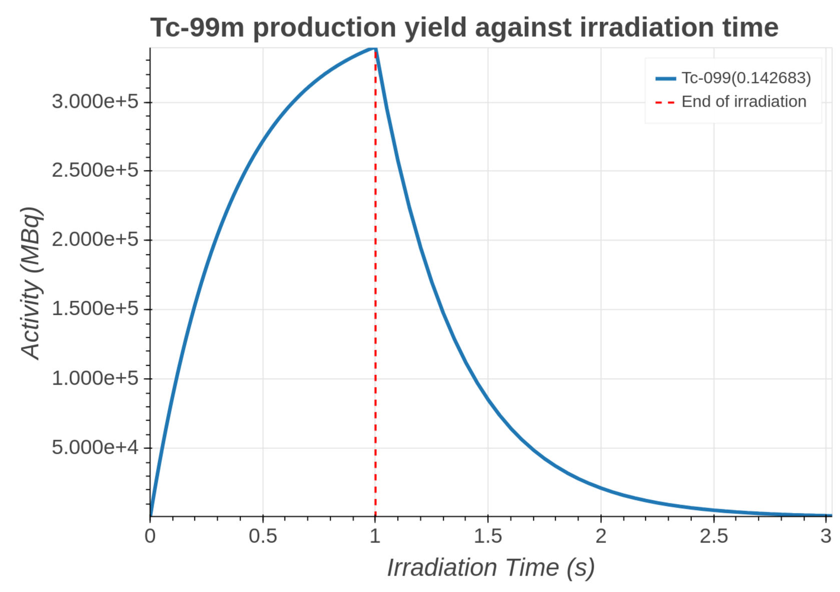
The number of B_2 with respect to time is given as:

$$N_{B_2}(t) = N_A(0)\frac{R_{A\to B_2}}{\lambda_{B_2}-R_A}\left[e^{-R_At}-e^{-\lambda_{B_2}t}\right]$$
$$+N_A(0)\frac{R_{A\to B_1}\lambda_{B_1\to i}}{\lambda_{B_1}-R_A}\left[\frac{e^{-R_At}-e^{-\lambda_{B_2}t}}{\lambda_i-R_A}-\frac{e^{-\lambda_{B_1}t}-e^{-\lambda_{B_2}t}}{\lambda_{B_2}-\lambda_{B_1}}\right] \quad (3)$$

- **Activity** may be calculate from the number of radioactive nuclei:

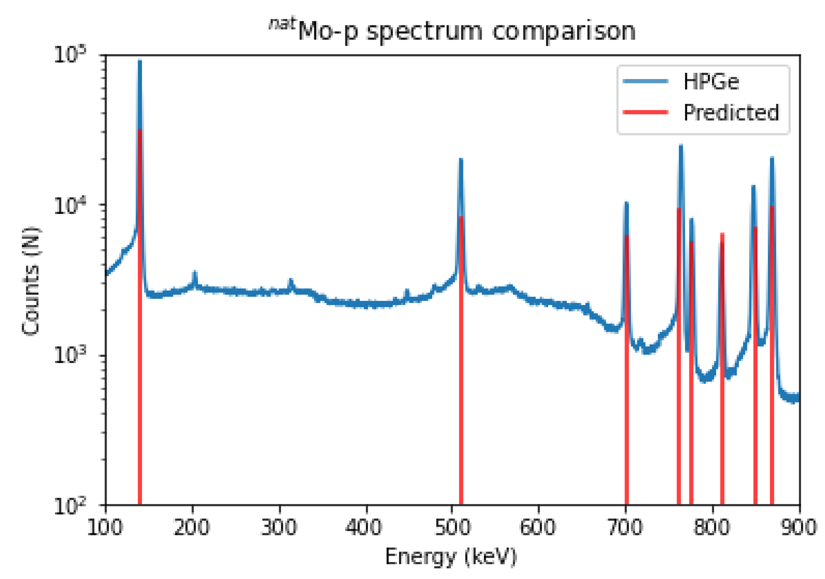
$$A_i = N_i\lambda_i \quad (4)$$

- A .csv file is produced containing the activity or number of **quantity of products against irradiation and cooling time**.
- This may also be plotted, showing any number of products, as below for ^{99}Mo(p,n)^{99m}Tc.



Decay Energies

- **Gamma and alpha spectra may be predicted** at any time, t, during or following irradiation using activities calculated from ENDF decay data
- This is **shown below for ^{nat}Mo-p** predicted overlaid with a spectrum taken using a HPGe detector.



- **Future implementations** include gaussian energy broadening, background and efficiency.
- These data may be used as **initial paramaterisation for automatic peak fitting**

References

[1] "M. Herman, R. Capote, B.V. Carlson, P. Oblozinsky, M. Sin, A. Trkov, H. Wienke, V. Zerkin "EMPIRE: Nuclear Reaction Model Code System for Data Evaluation", Nucl. Data Sheets, 108 (2007) 2655-2715.".

[2] A.J. Koning and D. Rochman "Modern Nuclear Data Evaluation with the TALYS Code System", Nuclear Data Sheets, Volume 113, Issue 12, Pages 2841-2934. (2012) https://doi.org/10.1016/j.nds".

[3] Ziegler, James F.; Ziegler, M. D.; Biersack, J. P. "Nuclear Instruments and Methods in Physics Research Section B, Volume 268, Issue 11-12, p. 1818-1823."

[4] A.J. Koning, D. Rochman, J. Sublet, N. Dzysiuk, M. Fleming and S. van der Marck, "TENDL: Complete Nuclear Data Library for Innovative Nuclear Science and Technology", Nuclear Data Sheets 155 (2019) 1,

[5] A.G. Young, ENDF/B-VI MAT 7925, January 1984

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