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Calculation of Isotope Yields for Radioactive Beam Production at TRIUMF

F. Garcia¹, C. Andreoiu¹, P. Kunz^{1,2}, A. Laxdal²

¹ Department of Chemistry, Simon Fraser University, Burnaby, British Columbia, Canada

² TRIUMF, Canada's National Lab for Particle and Nuclear Physics, Vancouver,
British Columbia, Canada

fatimag@sfu.ca, corina_andreoiu@sfu.ca, pkunz@triumf.ca, aureliat@triumf.ca

Abstract

We are building a simulation of the targetry at TRIUMF to augment existing working knowledge and support target developments for radioactive beam production. The simulation, built in GEANT4, a Monte Carlo nuclear transport toolkit, consists of a uranium carbide target, bombarded by a 500 MeV proton beam. The simulation records the production rates of generated isotopes to experimental rates measured at the TRIUMF yield station. Results from this comparison are presented. This simulation will provide predictive powers to the experiments at TRIUMF.

Keywords: GEANT4, Monte Carlo Simulations, radioactive beams, actinide targets.

1. Introduction

Our understanding of fundamental nuclear science has improved dramatically over the last few decades. Due to the emergence of new technologies and techniques, facilities such as TRIUMF have been able to generate radioactive isotopes beams, which are studied for their properties or used as probes for other fundamental searches. These discoveries work towards a theoretical framework that will accurately predict the properties of new and exotic nuclei. To aid this work, predictions are necessary to give researches a baseline for their experiments. To this end, the aim of this project is to provide a predictive computational simulation of the isotope production mechanisms in place at TRIUMF, particularly for radioactive isotopes far from stability. Using the Monte Carlo nuclear transport code GEANT4, we have built a simulation of the experimental set up that provides exotic nuclei to the various experiments at TRIUMF, with the aim of providing a predictive tool for future developments and a test for experimental results. This framework will then be used to support discoveries in fundamental nuclear science and applications such as nuclear medicine by providing scientists the ability to predict the isotopic input to their experiments

2. Overview of TRIUMF

TRIUMF, Canada's National Laboratory for Nuclear and Particle Physics, houses the world's largest cyclotron. Producing 500 MeV protons via acceleration and cyclotron motion of H^+ ions [1], the facility produces ion beams that are used to study fundamental nuclear science, nuclear astrophysics and nuclear medicine applications.

2.1 Radioactive beam production

The radioactive ion beams (RIBs) generated at TRIUMF's **IS**otope and **AC**celerator (ISAC) facility are made via the **I**sotope **S**eparation **O**n-**L**ine (ISOL) technique, whereby a beam of incident particles is bombarded onto a stationary thick target. This collision induces fission, spallation and fragmentation reactions that produce a wide range of isotopes up to the target mass [2]. Uranium and thorium are suitable target materials for the production of heavy and neutron rich isotopes, though other materials such as silicon, titanium and tantalum are also used, depending on the required isotopes. Typical ISAC production targets are composed of thin foils of various materials that are stacked together to make an effective thick target. Actinide oxides and carbides are of particular interest as their thermal and chemical properties make them suitable target materials [3, 4]. The target material is encased in a tantalum target container, as seen in Figure 1a, and then mounted along the proton beam path. The bombardment will produce a plethora of isotopes that are then ionized and extracted from the target. The mechanisms which produce the isotope of interest may also produce contaminants; these are separated using standard mass separation techniques [5], but due to the resolution of the mass separator, it is not always possible to obtain a pure beam of the isotope of interest.

2.2 ISAC Yield Station

The yield station, shown in Figure 1b, is the first experiment along the beam line at the ISAC facility. Its main duty is to perform beam diagnostics by measuring intensity and isotope yield rates, though it is also capable of measuring half life and other beam properties. The beam is brought up from the target vault into the yield station and implanted onto an aluminized Mylar tape, that is cycled, providing a clean spot for measurement and removing long lived activity from the measurement region. This cycling is a useful technique when the beam contaminants are long lived as opposed to the short lived isotope of interest. Surrounding the tape are α -, β - and γ -detectors that are used to measure the lifetime, decay and activity of the implanted isotopes, all properties which are used to determine the yield rates [6].

2.3 Yield vs Production Rates

It is important to note that there is a significant difference between the yield rates and production rates of isotopes. The production rate refers to the rate at which a particular isotope is made, called the 'in-target' production, dictated by the cross section of the specific interaction that will generate the isotope [7]. This cross section represents the probability of a particular reaction producing a specific isotope, and is sensitive to the energy of the reactants and the frequency of the reaction. The observed yield rate, which is measured at the ISAC yield station, is effectively the number of nuclei of a certain isotope that is observed at the yield station. Though the yield rate is proportional to the production rate, there are several factors to be taken into account when measuring the isotope rates. The ionization, extraction and transport efficiencies and the isotope's half-life all reduce the total number of isotopes that will exit the target and arrive at the yield station to be recorded [2]. The ionization and extraction efficiencies are different for each isotope, such that in order to make a useful connection between theoretical calculations and experimental data we must choose isotopes that will be efficiently ionized and extracted, and thus detected in appreciable quantities at the yield station. The alkali metals are excellent candidates as their ionization and extraction efficiencies are on the order of 90% [8], ensuring that a large

portion of the long lived isotopes generated at the target will be detected. These are the isotopes of interest for this project, as they will benchmark the simulation results.

a)



b)



Figure 1 | High temperature tantalum target containers, as seen in Figure 1a, are filled with target material and then placed along the beam line, brought into the path of the protons to induce the collision reactions that generate the isotope beams studied at TRIUMF. The ISAC yield station seen in Figure 1b is used to characterize and diagnose isotope beams once they are generated and transported from the target module. The radioactive isotope beam comes in from below the experimental floor and is implanted onto an aluminized Mylar tape at the centre of the yield station. The isotope then decays and its identity is validated based on its decay curve and decay spectra [6].

3. Overview of GEANT4

Short for the fourth iteration of the software **GE**ometry **ANd** **T**racking, GEANT4 was developed at CERN as a nuclear transport toolkit. It is an open source C++, Monte Carlo simulation code that can be used for wide range of applications such as shielding and space physics [9]. Appropriate experimental geometry, desired outputs, and physics models must be implemented before a simulation can run. We chose to use GEANT4 for its flexibility. Within this transport code, the user is free to define not only their geometry, but their primary material system as well as their physical models. Despite having an exhaustive list of physical processes and models, GEANT4 allows the user to define any set of physical principles as per their requirement. If the physics available in the package does not suit our needs, we are free to change the processes within GEANT4 or generate custom ones, as needed. Other nuclear transport codes, such as FLUKA [10], exist that are used for these types of applications, but their physical processes and isotope generation mechanisms may not be as readily available for change as those in GEANT4. This physics implementation pliability along with a world-class collaboration and support network makes GEANT4 our tool of choice.

3.1 Physics Lists in GEANT4

The variable that we use for these simulations is the physics list. Within GEANT4, a physics list refers to a class that collects particle information, physics processes and production thresholds required to carry out a simulation [11]. Some physics lists obtain their cross sections from a theoretical formalism, while others use tabulated data gathered from experimental work. Each is optimized to work in a particular energy range, and it is crucial we choose the most appropriate one, so as to generate accurate results. Table 1 summarizes the key features of the three intranuclear cascade models pertinent in our energy range.

List	Energy Range	Treatment of Nucleus
Bertini-inspired cascade (BERT) [12]	0 MeV – 10 GeV	Three concentric shells with different densities
Binary cascade (BIC) [13]	1 MeV – 2 GeV	Isotropic density
Liege Cascade (INCLXX) [14]	1 MeV – 20 GeV	Fermi gas in static potential

Table 1 | GEANT4 physics lists pertinent at incident energies of 500 MeV [15], the energy of the protons generated by the TRIUMF cyclotron.

3.2 Simulation specifications

The boundary conditions of the simulation are defined by the ISOL technique used at TRIUMF. The incident beam is made up of 500 MeV protons with a spacial Gaussian profile with a 7 mm FWHM along the x - and y -planes, reflecting the input beam generated by the TRIUMF cyclotron.

The target is defined by the user, depending on the material of interest. The current simulation can support use of depleted Uranium – 99.77 % ^{238}U and 0.23% ^{235}U – as well as pure tantalum, thorium, titanium, niobium, silicon and carbon, all target materials which have been used at TRIUMF and for which we have data gathered at the yield station. The simulation uses realistic dimensions and material densities but a slightly simplified geometry. A cylindrical target consists of 5 disks, each 1 cm thick, and 9.5 mm in radius and stacked one after the other. A so-called virtual detector surrounds each disk of the target material, and records the isotopes produced by the bombardment, but does not itself interact with the production mechanisms nor the outgoing particles; it only serves to record the identity and kinetic energy of an outgoing particle. A visualization of the target and the virtual detector is shown in Figure 2.

The simulation outputs raw data containing single isotope instances, recorded as the proton number, baryon number and kinetic energy. A counter script is used to count the total instances of a particular isotope. This raw data is then passed to ROOT [16], the CERN data analysis software, which calculates the number of neutrons in each isotope and populates a histogram that charts the nuclides generated by the simulation, and from which a production rate for each isotope is extracted.

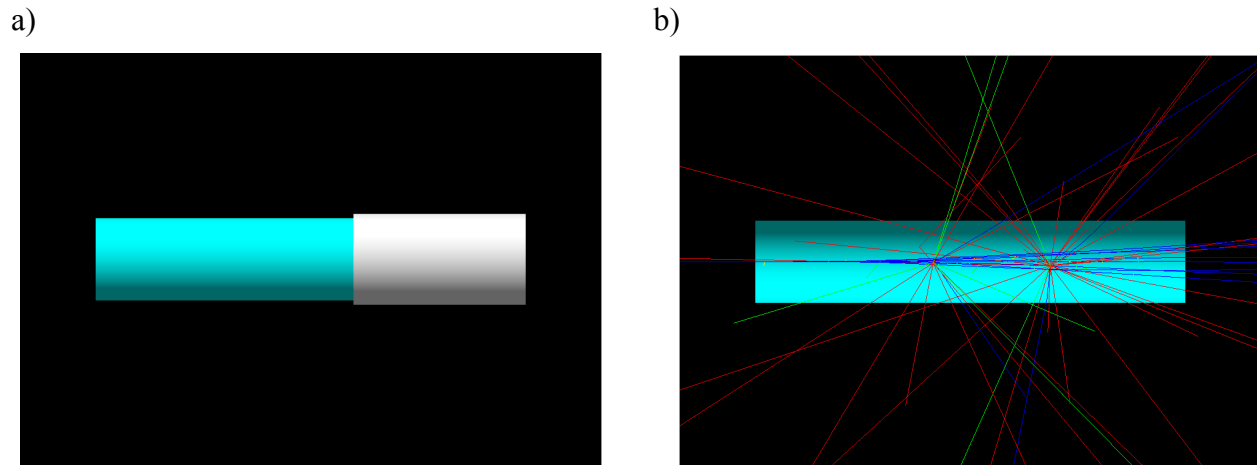


Figure 2 | Target geometry in GEANT4. In Figure 2a, the cyan disks represent the target material and the white represent the virtual detector. In Figure 2b a simulation run shows the blue lines as protons, green as photons, yellow as neutrons and red as electrons.

3.3 FLUKA

In the interest of comparison and benchmarking, an identical simulation was run in FLUKA by A. Laxdal, in order to verify that the GEANT4 geometry and simulation was built appropriately. FLUKA is another Monte Carlo based nuclear transport toolkit [10] also built at CERN. This software package has been in use at TRIUMF for some time, and is an attractive toolkit for applications such as nuclear medicine. The main difference between FLUKA and GEANT4 comes from the physics models available for implementation. While GEANT4 allows the user complete control in the definition, tuning and manipulation of the physics, FLUKA provides a rigid set of lists that are not available for user change. However, these lists in FLUKA are incredibly well maintained, supported and benchmarked, so the user need not worry about the accuracy of their results – as far as the physics is concerned; whereas with GEANT4, a great deal of work would be required to verify the validity of a user defined physics list.

Thus to verify proper implementation of adequate physics and accurate definition of the target geometry, a parallel FLUKA simulation was run. The results from this simulation are presented alongside the production rates predicted by the GEANT4 simulations, though no comment is made regarding the comparison between the two software packages.

4. Results

Direct comparison between each of the physics lists requires running each for the same number of incident particles (10^9) at the same energy (500 MeV) with the same target thickness ($0.05\text{mol}/\text{cm}^2$). The production rates are then converted to rate per incident particle values and finally extrapolated to a $1\text{ }\mu\text{A}$. The difference between the production and yield rates is evident in the comparison between the yield station data and the physics list predictions, as seen in Figure 3. The error bars included in Figure 3 are calculated using the relative standard error of the simulations, where the standard deviation of a series of parallel simulations was divided by the mean of the simulations.

A comparison of the yield curve and the theoretical production of the Lithium isotopes shows that while the INCLXX list and the BIC both follow the trend of the experimental results, the BERT list under produces the isotopes, when compared to the yields, indicating that it cannot accurately predict these elements. This under production is of concern, as the production rates are subject to ionization, transport and other efficiencies that will decrease the number of isotopes recorded as the yield rate, thus if a simulation predicts a value lower than the yield rate, then this simulation cannot be used to accurately predict the production rate of an isotope.

For the Sodium isotopes both the BERT and the BIC under produce the neutron rich Sodium isotopes, suggesting they are not adequate for handling Sodium yields. The INCLXX list, however does replicate the trend in the yield curve of the neutron rich side of the Sodium curve.

The Potassium comparison once more shows that the BERT list is not adequate, as it cannot produce Potassium isotopes at 500 MeV with 10^9 incident protons. In this instance the BIC list under produces the neutron deficient side of the yield curve. The INCLXX, in contrast, not only over produces the isotopes, as is expected, but also replicates the yield curve trend better than the BIC list.

Three different physics lists show good agreement with one another for the neutron rich Rubidium isotopes, with approximately one order of magnitude between each curve and the yield curve.

For the Cesium isotopes, the BERT physics list describes the neutron rich isotopes well, though this is not true for the neutron deficient side. Both the BIC and the INCLXX physics lists follow the same general trend, which better describes the entire yield curve. The large gap seen in the yield data at the centre of the curve is due to the half-life of these isotopes. They are either stable or very long-lived and thus cannot be identified by radiometric methods.

The BERT list results for the Francium isotopes do not follow the yield curve, particularly in the neutron deficient side, where the physics list under-produces the isotopes, but over-produces those on the neutron rich side. The BIC list fits the yield curve slightly better than the BERT, but the slow dip around mass $A = 229$ is not reflected in the yield rates. The general trend of the yield curve is best followed by the INCLXX list, where there is a peak at $A = 213$, corresponding to neutron magic number $N = 126$, and a decrease on the production rates of the neutron deficient and neutron rich isotopes on either side of this peak.

As is the case with the Cesium isotopes, the Francium isotopes are undetectable at the centre of the yield curve. In this case their very short half-lives results in very low extraction efficiencies.

5. Conclusion

The comparison between the three available physics lists and the yield station data indicates that the Liege physics list (INCLXX) is best at describing the isotopes of the alkali metals.

Though optimized for fission, the Bertini-inspired (BERT) cascade cannot accurately describe the yield curve of the Lithium, Sodium, Cesium and Francium isotopes, and is unable to predict the Potassium isotopes, thus making it an inadequate candidate for our predictive model.

While the Binary cascade can adequately describe the heavy alkali metals, it cannot do the same for their lighter counterparts, indicating it is also unsuitable for our purposes.

In contrast, the Liege model can predict, with varying degrees of accuracy, the full set of the alkali metals, suggesting that this will be the best physics list to use in the further development of the model.

Similar studies of the alkali earth metals, which also have high ionization efficiencies, may further cement the conclusion that the Liege model is the best candidate for the complete simulation.

Once the appropriate physics list has identified, and its features and predictive power have been analyzed and validated, we will have a model that can accurately predict isotope production, leading to future target developments that will help in production of exotic nuclei.

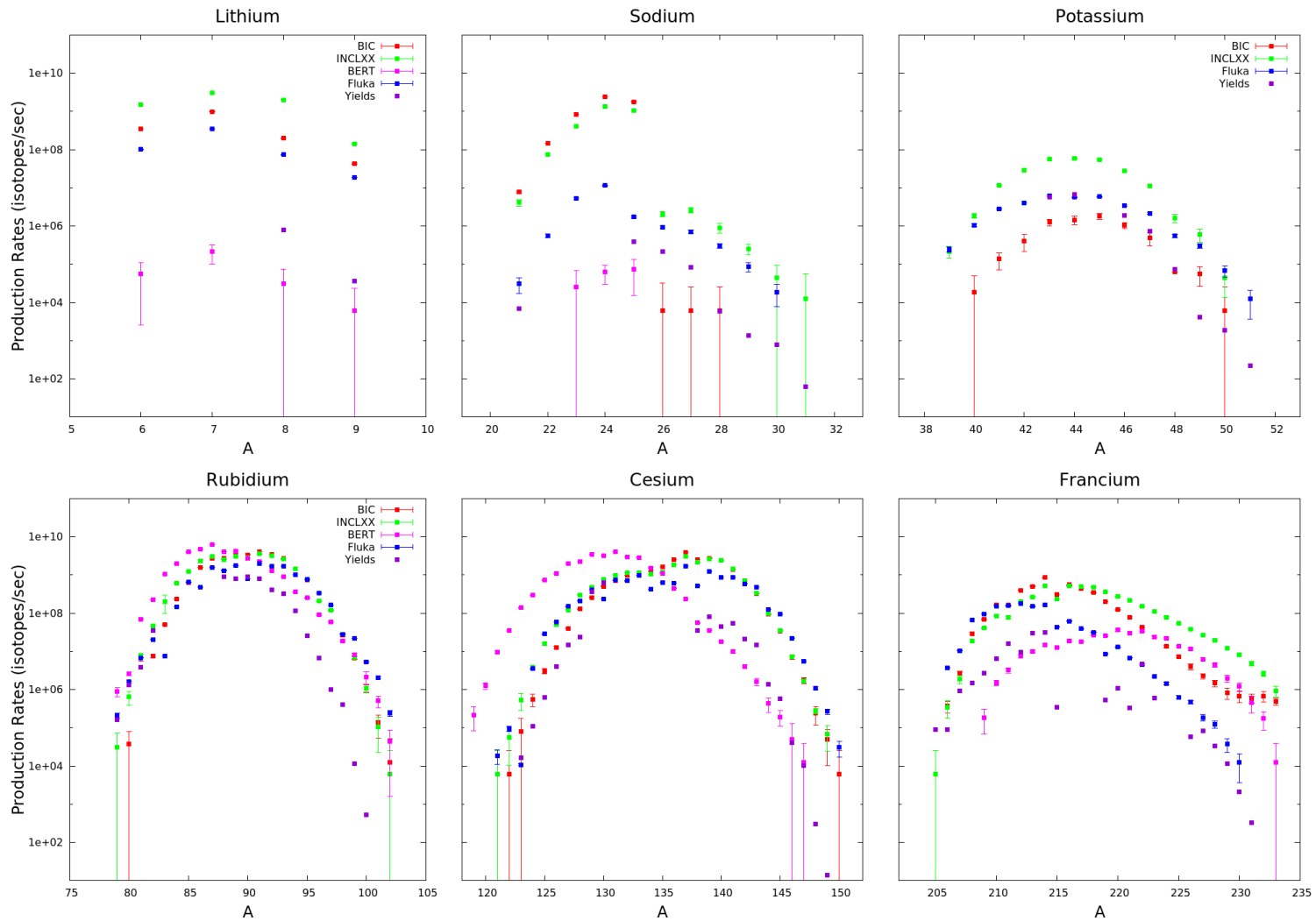


Figure 3 | Comparison plots of in-target production rates and experimental yield rates for the alkali metals. The three physics lists; the Binary cascade in red, the Liege model in green and the Bertini-inspired cascade in magenta; are plotted with their respective errors against the ISAC yield station database in pink [17]. The results from an identical simulation done in Fluka are presented in blue [18]. The Bertini-inspired cascade did not produce Potassium isotopes with the specified energy and incident proton count and is thus absent from the plot.

6. References

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