Validating PHITS for heavy ion fragmentation reactions

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Abstract

The performance of the Monte Carlo code system PHITS is validated for heavy-ion transport capabilities by performing simulations and comparing results against experimental data from heavy-ion reactions of benchmark quality. These data are from measurements of isotope yields produced in the fragmentation of a 140 MeV/u ^{48}Ca beam on a beryllium target and on a tantalum target. The results of this study show that PHITS performs reliably.

Introduction

The Facility for Rare Isotope Beams (FRIB) is being designed and established at Michigan State University as a DOE Office of Science national user facility for the study of nuclear structure, reactions, and astrophysics [1]. FRIB consists of a driver linac for the acceleration of stable heavy-ion beams, followed by a fragmentation separator and a stopped beam/ReAccelerating facility (ReA) [1]. Stable heavy-ion beams having >200 MeV/u at beam powers up to 400 kW will be used to produce rare isotopes by in-flight fragment separation in the fragmentation separator. Selected rare isotopes will be stopped and reaccelerated. Beginning in the Electron Beam Ion Trap (EBIT) charge state booster, beams from ReA3 will range in energy from 0.3 to 6 MeV/u. The maximum energy is 3 MeV/u for heavy nuclei such as uranium, and 6 MeV/u for ions having A<50. All rare isotope beams that can be produced by fragmentation or in-flight fission with sufficient intensity can be reaccelerated.

To support design and operations, the performance of the Monte Carlo code system PHITS [3] is validated for heavy-ion transport capabilities by performing calculations of rare isotope yields and comparing results against experimental data from heavy-ion reactions of benchmark quality [4]. The calculations have been compared to measurements of isotope production cross-sections from the fragmentation of a 140 MeV/u ^{48}Ca beam on a beryllium target and on a tantalum target [4]. The results of these comparisons can be used to suggest possible code improvements. Simulations were carried out using recent introduction of PHITS version 2.52 updated to version 2.64 of the PHITS code system, with comparisons to previous studies [7] using PHITS version 2.13.

Motivation

The first motivation of our study is that predictions of radionuclide distributions and residual radioactivity are especially important in determining inventories for facility licensing and for operational health physics and radiation protection purposes. These predictions can be obtained from Monte Carlo simulations that describe rare isotope production from the most important processes of spallation, fragmentation and fission processes, followed by activation calculations of residual radioactivity build-up and decay. For safe operations it is important that calculations are accurate.

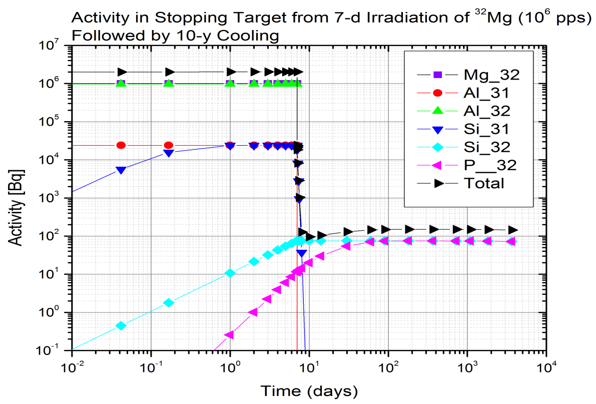
As an example, the rare isotope beam of ^{32}Mg (86 ms half-life) is possible for study at ReA. Although its half-life is very short, its decay includes beta-delayed neutron emission branches to daughters having half-lives much larger than the assumed typical irradiation time (here taken as 7 days). A summary of relevant decay properties of ^{32}Mg and its daughters are given in Table 1.

Table 1. ^{32}Mg parent, daughter half-lives and decay modes

Parent Nucleus	Parent Half Life	Decay Mode	Daughter Nucleus
$^{32}_{12}Mg$	86 ms	β- : 100.00 % β-n : 5.50 %	$^{32}_{13}Al$, $^{31}_{13}Al$
$^{32}_{13}Al$	33.0 ms	β- : 100.00 % β-n : 0.70 %	$^{32}_{14}Si$, $^{31}_{14}Si$
$^{31}_{13}Al$	644 ms	β- : 100.00 %	$^{31}_{14}Si$
$^{32}_{14}Si$	153 y	β- : 100.00 %	$^{32}_{15}P$
$^{31}_{14}Si$	157.3 m	β- : 100.00 %	$^{31}_{15}P$ stable
$^{32}_{15}P$	14.262 d	β- : 100.00 %	$^{32}_{16}S$ stable

The time evolution of a 10^6 ion/s beam of ^{32}Mg and daughter activities deposited in a stainless steel stopping target was calculated using DCHAIN-SP 2001 [8] and is shown in Figure 1. After the 7 day irradiation is stopped, the total activity is nearly constant at ~ 150 Bq for 10 years, owing to the long half-life of Si-32 that decays to ^{32}P. The extremity dose rate resulting from this activity is about 0.01 mGy/h, the level of which is important for health physics and radiological protection purposes. This result underscores that reliable calculations of rare isotope yields, in this case that of ^{32}Mg, are important for safe operations planning at a rare isotope beam facility.

Figure 1. Activity in a stopping stainless steel target as a function of time from a 7-d irradiation by a 10^6 pps ^{32}Mg beam



The total activity is the sum of activities from the decays of ^{32}Mg and its daughters.

The second motivation is to validate the default value of the "switching time" t_{sw} used in the JQMD model [9] within PHITS. The JQMD model treats dynamical processes in nucleus-nucleus collisions, e.g. direct and non-equilibrium reactions that form highly excited fragments. Later in the time evolution of these systems, the statistical model GEM [10] is used to describe statistical processes, e.g. decays of the fragments by fission and evaporation. Within PHITS simulations, the JQMD calculations of dynamical processes are stopped, excited nuclei are created, and results transferred to GEM for decay in a statistical way at the "switching time" specified by the parameter *nqtmax*. This parameter is necessary because of two-step nature of the calculations. The default value in PHITS is 150 fm/c (one fm c-1 is 3.3 x 10-24 s). Beginning with PHITS version 2.13, the parameter *nqtmax* can be set externally. We found previously [7] that calculations using 100 fm/c better described the heavy-ion fragmentation production cross-sections at 140 MeV/u (see Figure 2). Subsequently, Iwamoto et al. [11] used values for t_{sw} of 50, 100, and 150 fm c-1 to generate neutron energy spectra for comparison against experimental data [12] from 6.25 MeV amu-1 and 10 MeV amu-1 C-12 ions and 10 MeV amu-1 O-16 ions incident on a thick copper target. The shape of neutron energy spectra was compared with experimental data near the evaporation component. The slope is especially sensitive to the evaporations stage and thus to t_{sw}. Iwamoto et al. concluded that 100 fm/c is preferred over 150 fm/c to best describe the neutron energy spectra. Thus, establishing the best setting for the parameter nqtmax apparently will help serve to obtain the most reliable sets of calculated fragment production cross-sections and neutron energy spectra.

Figure 2. Comparisons of experimental fragmentation production cross-sections for sulphur isotopes from 140 MeV/u ^{48}Ca incident ion reactions with a Be target to calculations using PHITS versions 2.11 and 2.12 with the switching time parameter *nqtmax* set to 150 (default), 130, and 100 fm/c

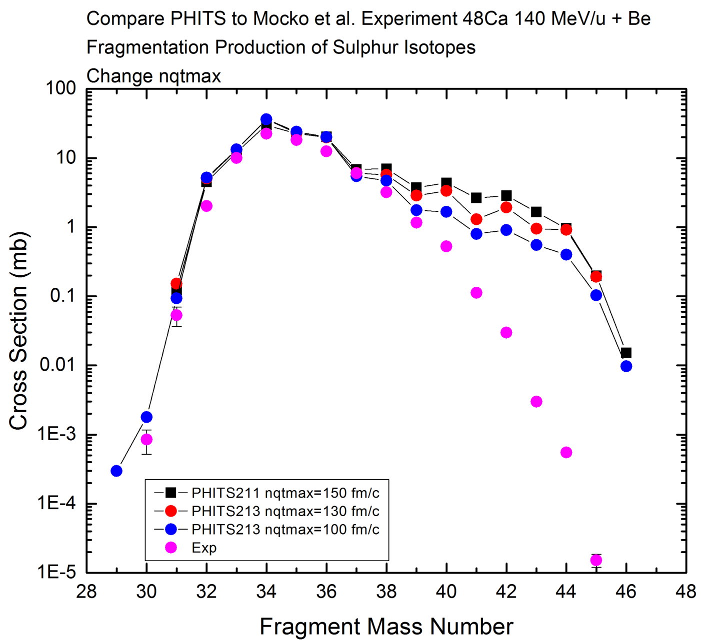
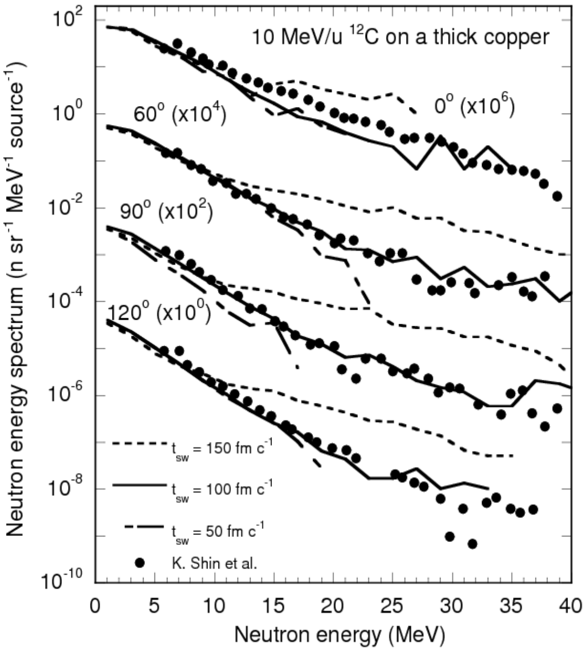


Figure 3. Neutron energy spectra using switching times 50, 100 and 150 fm/c for 10 MeV amu-1 C-12 incident ion reactions with a thick copper target



Fragment production calculations

Our studies were carried out on the isotope production cross-sections from projectile fragmentation reactions [4] using the ^{48}Ca beams at 140 MeV/u on beryllium and tantalum targets at the Coupled Cyclotron Facility at the National Superconducting Cyclotron Laboratory at Michigan State University. We performed calculations using PHITS version 2.64 to obtain fragmentation production cross-sections for those systems, and compared them with the measured values. Comparisons are made to previous calculations performed using PHITS version 2.13 [7].

The physics models used in the calculations, in addition to the JQMD model, were the INCL4.6 model [13] for light particle production and the Kuratoma model for calculating the total reaction cross-sections of nucleon–nucleus and nucleus–nucleus interactions [14]. The latter is set by parameters *icrhi* = 2 and *icxsni* = 1. The production cross-sections were obtained using the T-YIELD tally in PHITS. The *axis* = *dchain* option was used, which provides a table of isotope production sorted by element. The *unit* = 1 option was chosen, providing the production per beam particle. To convert the production to cross-section, the tally's multiplicative factor "*factor*" was set to $\frac{10^{27} mb{-}cm^{-2} \times target\ atomic\ mass}{Avogadro's Number \times target\ areal\ density}$. The target sizes and areal densities were taken from [4].

Results and discussion

Figure 4 shows the experimental measurements of cross-sections for phosphorus isotopes produced by 140 MeV/u ^{48}Ca incident ion reactions with a Be target compared to calculations by PHITS versions 2.13 and 2.64 with nqtmax = 100 fm/c and version 2.64 with nqtmax = 150 fm/c. Both versions significantly overpredict the data for the larger mass numbers. As observed previously [7], agreement between data and calculations is improved with nqtmax = 100 fm/c compared to the default value of 150 fm/c. Also, version 2.64 provides better agreement with the data than does version 2.13. The same conclusions are reached for the measurements taken with the Ta target, as shown in Figure 5.

Figure 4. Comparisons of experimental fragmentation production cross-sections for phosphorus isotopes from 140 MeV/u ^{48}Ca incident ion reactions with a Be target to calculations using PHITS versions 2.13 and 2.64 with the switching time parameter *nqtmax* set to 150 (default) and 100 fm/c

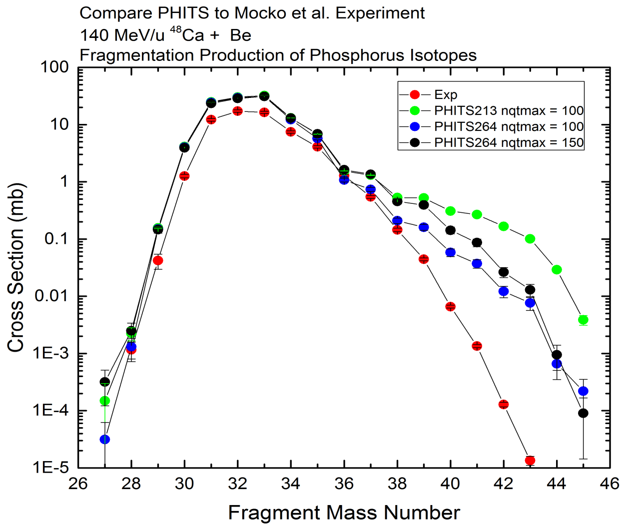
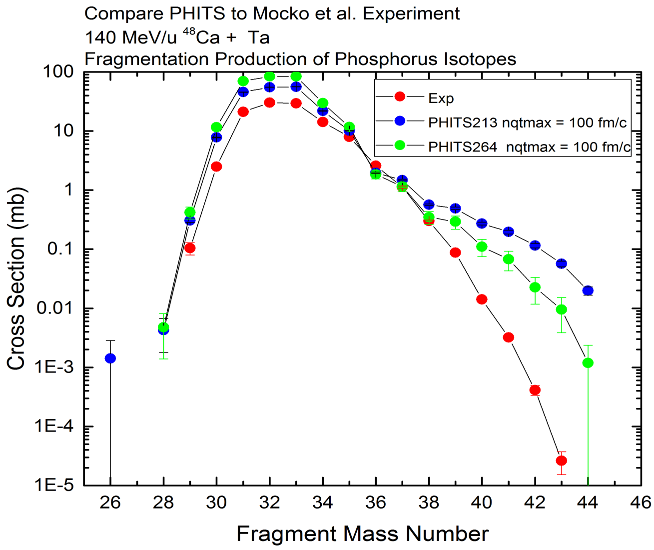


Figure 5. Comparisons of experimental fragmentation production cross-sections for phosphorus isotopes from 140 MeV/u ^{48}Ca incident ion reactions with a Ta target to calculations using PHITS versions 2.13 and 2.64 with the switching time parameter *nqtmax* set to 100 fm/c



Focusing on production of lighter fragments, comparisons were made between data and calculations for the production of carbon isotopes. Figures 6 and 7 show the results for the Be target and the Ta target, respectively. In these cases, no clear choice can be made between the code versions or between the values of *nqtmax* for the values studied. It is noted that the calculations slightly under predict the data from the Be target for the larger mass numbers and that there is good agreement with data from the Ta target for both versions.

Figure 6. Comparisons of experimental fragmentation production cross-sections for carbon isotopes from 140 MeV/u ^{48}Ca incident ion reactions with a Be target to calculations using PHITS versions 2.13 and 2.64 with the switching time parameter *nqtmax* set to 100 and 150 fm/c

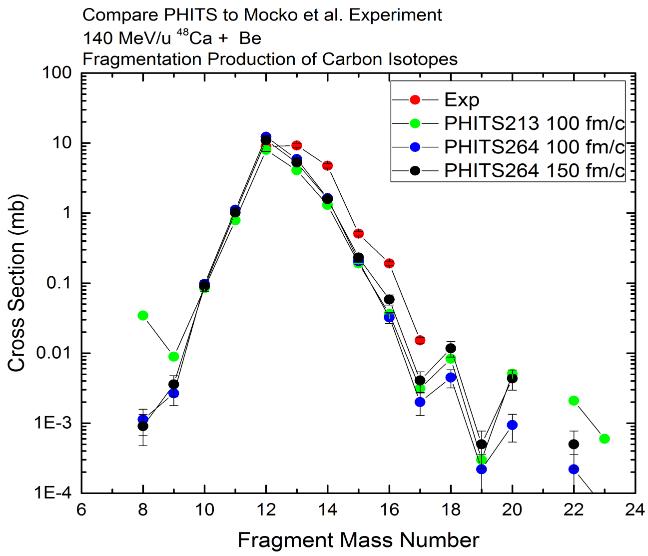
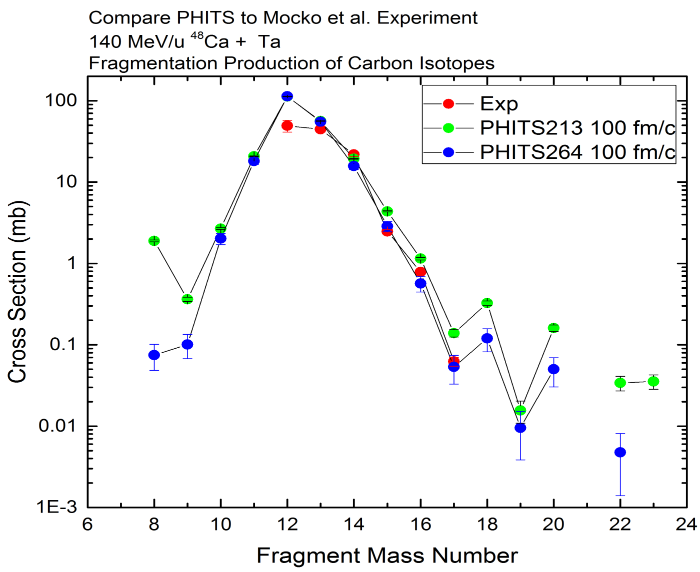


Figure 7. Comparisons of experimental fragmentation production cross-sections for carbon isotopes from 140 MeV/u ^{48}Ca incident ion reactions with a Ta target to calculations using PHITS versions 2.13 and 2.64 with the switching time parameter *nqtmax* set to 100 fm/c



Focusing on production of the heaviest measured fragments, comparisons were made between data and calculations for the production of titanium isotopes. Figures 8 and 9 show the results for the Be target and the Ta target, respectively. It is noted that the calculations underpredict the data from the Be target and overpredict the data from the Ta target, and that no clear choice can be made between the code versions or between the values of *nqtmax* for the values studied.

Figure 8. Comparisons of experimental fragmentation production cross-sections for titanium isotopes from 140 MeV/u ^{48}Ca incident ion reactions with a Be target to calculations using PHITS versions 2.13 and 2.64 with the switching time parameter *nqtmax* set to 100 and 150 fm/c

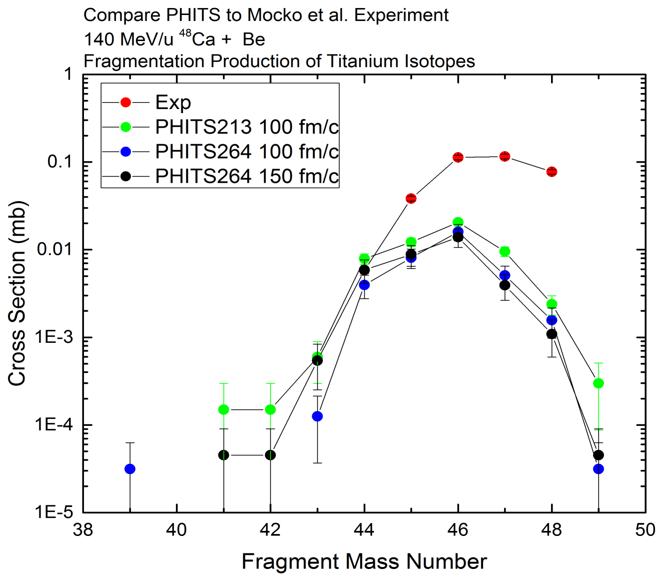
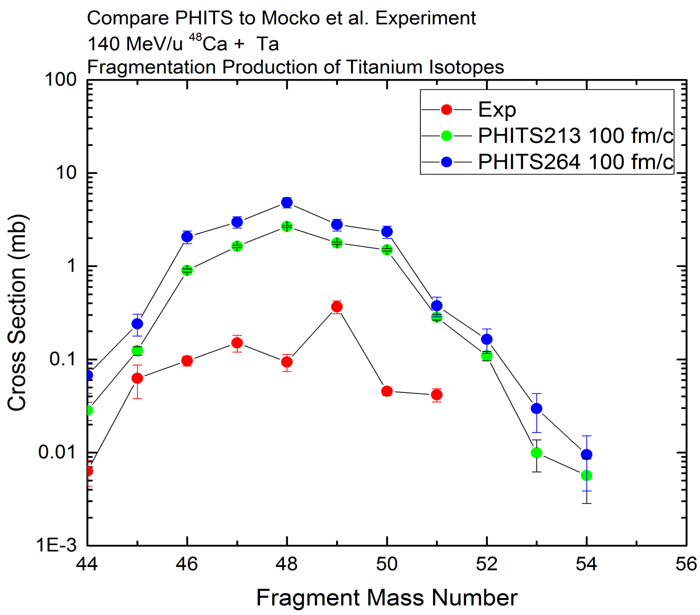


Figure 9. Comparisons of experimental fragmentation production cross-sections for titanium isotopes from 140 MeV/u ^{48}Ca incident ion reactions with a Ta target to calculations using PHITS versions 2.13 and 2.64 with the switching time parameter *nqtmax* set to 100 fm/c



Summary

Reliable calculations of rare isotope yields are important for safe operations planning at FRIB and other rare isotope beam facilities. The recent introduction of PHITS version 2.52 updated to version 2.64 contains many new models and other improvements. Our study of fragment production cross-sections is limited in scope, but the impact of those improvements is evident in that we have found that version 2.64 performs better than version 2.13. In this study, we have found that comparisons to data are improved using the switching time parameter *nqtmax* = 100 fm/c rather than the default value of 150 fm/c. We plan to continue our tests, to provide performance feedback to the PHITS authors and to solicit suggestions from them on improving our calculations.

Acknowledgements

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