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From Simulation to Experiment: Multi-Code Modelling and Validation of Carbon-11 Production Using Natural Boron Targets

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ABSTRACT

Background: Carbon-11 is an essential radioisotope used in positron emission tomography (PET) for various applications in neurology, oncology and cardiology. Although a method for cyclotron production, based on the $^{14}\text{N}(\text{p},\alpha)^{11}\text{C}$ reaction and using gaseous targets, is well established, alternative production methods using high-power lasers are sought. The $^{11}\text{B}(\text{p},\text{n})^{11}\text{C}$ reaction with laser-driven accelerated protons is considered within the “Dr. Laser” project at Extreme Light Infrastructure–Nuclear Physics (ELI-NP). This study prepares the laser-driven production route by evaluation of the production of ^{11}C on three types of target materials: amorphous metallic boron (purity 95%), crystalline metallic boron (purity 98%) and boron nitride (purity 98%). The proposed approach integrates modelling of the excitation functions using the TALYS code with the evaluation of experimental irradiations performed at the TR-19 cyclotron at Horia Hulubei National Institute for Physics and Nuclear Engineering (IFIN-HH). The goal of this study is to assess the optimal target material and to investigate the dependence of produced activity on the incident energy of the $^{11}\text{B}(\text{p},\text{n})^{11}\text{C}$ reaction.

Results: At an extracted proton beam energy of 15 MeV from the cyclotron, an effective incident energy on the target surface of 14 MeV was determined by evaluation of the proton transport through the experimental components, i.e. an aluminium window, a helium cooling layer and a sealing foil, using the SRIM/TRIM (Stopping and Range of Ions in Matter/Transport of Ions in Matter) code. By correlating this value with the simulated effective cross-sections, it is demonstrated that the energy fits into the optimal region of the excitation function for obtaining the maximum reaction yield. The experimental activities, corrected to EOB (end of bombardment), were found to be 7.77 GBq, 10.87 GBq, and 12.37 GBq for targets of amorphous metallic boron with purity 95%, crystalline metallic boron with purity 98%, and boron nitride with purity 98%, respectively. Experimental yields of 3.11 GBq/μAh, 4.35 GBq/μAh and 4.95 GBq/μAh were obtained for the three different targets, respectively. Although the measured values were 11.90% to 14.54% lower than the theoretical predictions, they demonstrated a strong correlation with the mathematical model. Sample quality analysis

by gamma spectrometry confirmed an excellent radionuclide purity of over 99.9% for all three targets.

Conclusions: The $^{11}\text{B}(\text{p},\text{n})^{11}\text{C}$ nuclear reaction at a proton energy on target of 14 MeV is optimal for ^{11}C production using solid natural boron targets. The boron nitride target provided the highest activity and yield values, a performance attributed to its higher apparent density and the contribution of additional nuclear reactions induced on nitrogen atoms, also resulting in ^{11}C . The radionuclide purity of the ^{11}C isotope obtained complies with the requirements of the European Pharmacopoeia, while the small but expected differences between the experimental results and the theoretical model validate the efficiency of irradiation on solid targets for the synthesis of high-purity radiopharmaceuticals. These results are to be implemented in the laser-driven nuclear reaction simulations and experiments.

Introduction

Carbon-11 ($T_{1/2} = 20.361$ min) decays by β^+ (960.5 MeV; 99.75%) and by electron capture (1982.5 MeV; 0.25%), as seen in Figure 1 [1], and is used in positron emission tomography under various radiopharmaceutical forms in neurology, oncology and cardiology [2,3]. Due to its short half-life, clinical utility is constrained by the availability of medical cyclotrons in or near nuclear medicine facilities. Because its stable isotope, ^{12}C , is present in all organic molecules, ^{11}C is a very versatile radionuclide for labelling of virtually any bioactive molecule [4].

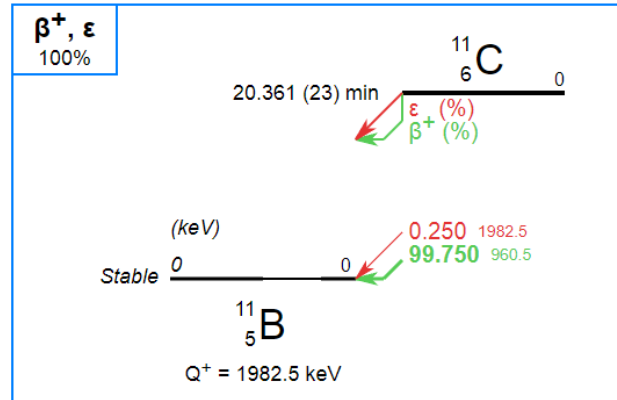


Figure 1. Decay scheme of ^{11}C . Figure taken from ref. [1].

The following nuclear reactions can be employed in cyclotron production of ^{11}C : $^{11}\text{B}(\text{p},\text{n})^{11}\text{C}$, $^{14}\text{N}(\text{p},\alpha)^{11}\text{C}$ and $^{10}\text{B}(\text{d},\text{n})^{11}\text{C}$. Among them, one is particularly useful in practice, the $^{14}\text{N}(\text{p},\alpha)^{11}\text{C}$ reaction, which is the established production route with cyclotrons nowadays. While the most popular method for regular cyclotron production of ^{11}C is via the $^{14}\text{N}(\text{p},\alpha)^{11}\text{C}$ reaction, other production routes based on boron targets have also been studied [3]. Specifically, the $^{11}\text{B}(\text{p},\text{n})^{11}\text{C}$ reaction is a practical way to use solid targets to produce carbon-11. This reaction has a relatively low threshold energy, approximately 3 MeV, and can be induced with proton beams available at many medical cyclotrons, making it technically accessible for this radioisotope production [5,6].

The excitation function and the yield for thick targets of the $^{11}\text{B}(\text{p},\text{n})^{11}\text{C}$ reaction have been evaluated experimentally throughout a broad proton energy range, showing that significant activities of ^{11}C can be obtained under appropriate irradiation conditions. Thus, research on ^{11}B -based solid targets is still important for the advancement and improvement of carbon-11 cyclotron production methods [7].

The motivation for performing experiments using ^{11}B targets of different isotopic purities came as a challenge, to compare the activity amount and yield of ^{11}C production using the (p,n) nuclear reaction that will be studied at the high-power laser system at the ELI-NP facility in Măgurele, Romania. We tested boron-based solid targets as they are considered a possible ^{11}C production route with high-power lasers. This possibility will be investigated within the Dr. Laser project at ELI-NP, which addresses medical applications of high-power lasers.

Methods

The TR-19 Cyclotron

The ACSI (Advanced Cyclotron Systems, Inc.) TR-19 cyclotron is a variable-energy cyclotron installed at the Radiopharmaceutical Research Centre (CCR) of the Horia Hulubei National Institute for Research and Development in Physics and Nuclear Engineering (IFIN-HH), Măgurele, Romania (Figure 2) [8].

The cyclotron accelerates negative hydrogen ions (H^-) and delivers proton beams with variable extraction energies between 14 and 19 MeV, with a 100 keV energy step, and beam currents up to 300 μA . It is equipped with two extraction ports, allowing for dual beam operation and flexible use of beam lines for different experimental and production setups. On one of the extraction ports of TR-19, 2 extension lines are installed, one 6m long which ensures, among other applications, radiobiology experiments using proton-beam irradiation, and the short one, at 26 degrees, which has an automated solid target irradiation station mounted. The other extraction port can support the installation of up to 4 reaction chambers. One of installed reaction chambers is dedicated to solid targets irradiation [9].



Figure 2. TR-19 cyclotron, @CCR, IFIN-HH, Romania

Comparison of the ^{11}C Production Routes

The database and standardized format for experimental nuclear reaction data, Experimental Nuclear Reaction Data (EXFOR), allows for the collection, storage, exchange and retrieval of detailed experimental measurements from laboratories around the world. It is coordinated by the Network of Nuclear Reaction Data Centres (NRDC), under the auspices of the International

Atomic Energy Agency (IAEA) [10]. The experimental cross-section for $^{11}\text{B}(p,n)^{11}\text{C}$ reaction data were obtained from the EXFOR database.

A comparative analysis of the excitation functions of $^{11}\text{B}(p,n)^{11}\text{C}$ and $^{14}\text{N}(p,\alpha)^{11}\text{C}$ was carried out using experimental data from the EXFOR database to support the choice of the best reaction route.

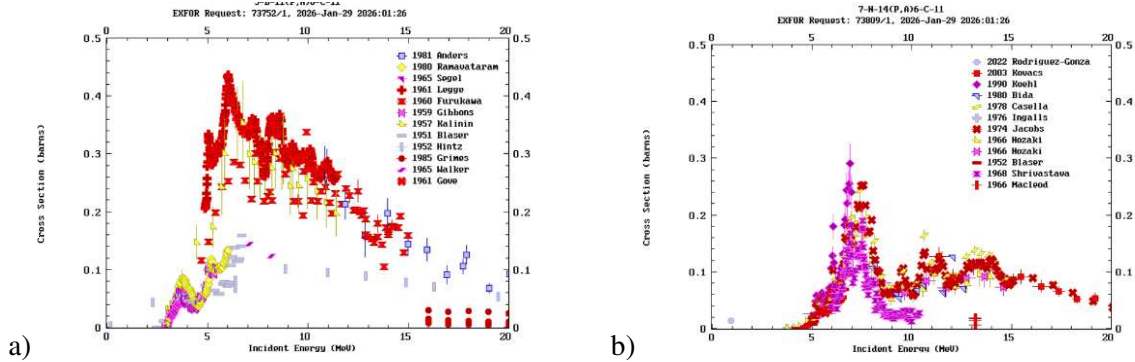


Figure 3. Comparative cross-sections of the $^{11}\text{B}(p,n)^{11}\text{C}$ and $^{14}\text{N}(p,\alpha)^{11}\text{C}$ reactions as a function of incident proton energy. Data taken from Ref.[11]

The $^{11}\text{B}(p,n)^{11}\text{C}$ reaction has substantially larger cross-section values in the proton energy range that is relevant to medical cyclotrons (up to 20 MeV), according to experimental cross-section data. Depending on the dataset, the reaction often achieves maximal cross-section values in the range of several hundred millibarns (approx. 400-500 mb), with a threshold at about 2.8 MeV (Figure 3. a)).

The $^{14}\text{N}(p,\alpha)^{11}\text{C}$ reaction, on the other hand, has significantly lower maximum cross-section values, typically around 300 mb in the same energy domain, despite being exoenergetic and having a reasonably large excitation function (Figure 3. b)).

The significantly greater cross-section values of the $^{11}\text{B}(p,n)^{11}\text{C}$ reaction offer a definite advantage in terms of possible activity, as the production yield is proportional to the integral of the reaction cross-section over the effective proton energy interval within the target. Based on this comparison, the $^{11}\text{B}(p,n)^{11}\text{C}$ reaction was selected for further optimization and analysis.

Excitation Function Simulations (TALYS)

Following the reaction selection, the excitation functions of the $^{11}\text{B}(p,n)^{11}\text{C}$ reaction were calculated using the TALYS nuclear reaction code, accessed via the online platform. TALYS is a program that simulates nuclear reactions up to energies of 200 MeV. It is used in nuclear physics to indicate how accurate experimental data is, but also as a tool for applications that need nuclear data. Simulations were performed for a proton energy range of 0–20 MeV, covering the entire range relevant to the cyclotron operating conditions, including the reaction threshold as well as the region of maximum cross-section [12,13].

TALYS was also used to obtain the theoretical cross-sections as a function of incident proton energy and to identify the energy domain corresponding to optimal production yield. In addition to the primary $^{11}\text{B}(p,n)^{11}\text{C}$ production channel, TALYS calculations were also carried out for competing nuclear reactions, namely $^{11}\text{B}(p,d)^{10}\text{B}$, $^{11}\text{B}(p,np\alpha)^6\text{Li}$, and $^{11}\text{B}(p,n\alpha)^7\text{Be}$. The inclusion of these channels, presented in Figure 4, allowed evaluation of possible competitive

reactions that may influence radionuclidic purity or affect the overall reaction yield at higher proton energies.

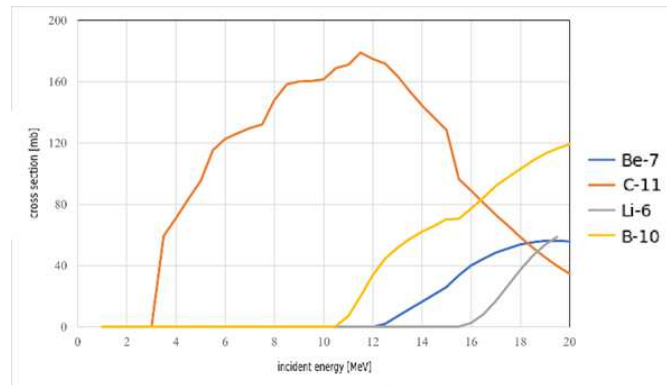


Figure 4. Excitation functions of the $^{11}\text{B}(p,n)^{11}\text{C}$ reaction obtained with TALYS code and the relevant contaminants (^7Be , ^6Li , ^{10}B) [14].

The excitation functions were used to identify the energy region corresponding to optimal ^{11}C production while minimizing contributions from competing reactions. The calculated excitation function served as the basis for irradiation optimization. To confirm that the chosen irradiation parameters allow operation in the most advantageous energy range for optimizing ^{11}C production, the cross-section curve was then correlated with the effective proton energy range inside the target, as shown by SRIM simulations.

Experimental Data Retrieval and Theoretical–Experimental Comparison (EXFOR)

A comparison was made between the theoretical cross-sections calculated using TALYS covering the proton energy range of 0–20 MeV and the experimental excitation functions that were taken from the database. In this comparison, the general energy dependency between the theoretical calculations and the experimental results was examined for consistency. The comparison is illustrated in Figure 5.

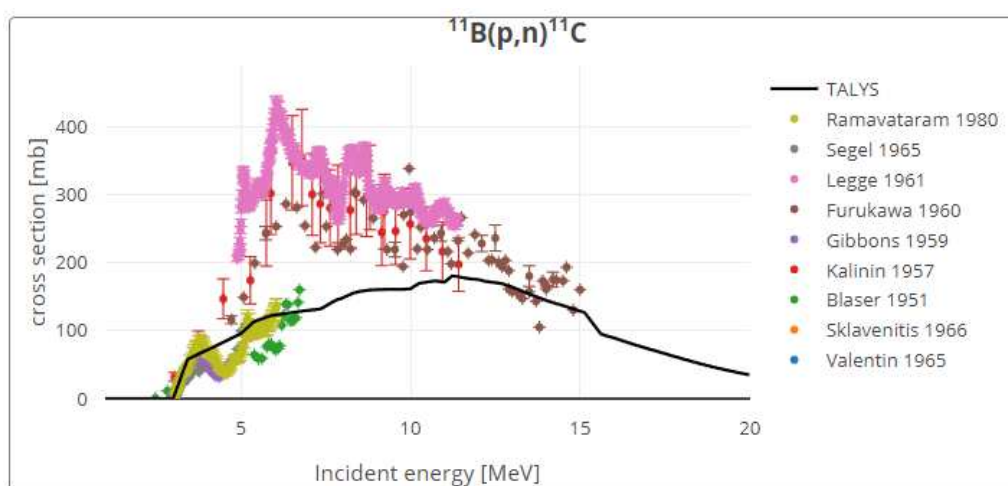


Figure 5. Excitation function of $^{11}\text{B}(p,n)^{11}\text{C}$ nuclear reaction with TALYS simulation (curved line) and EXFOR database [11,14].

Discrepancies are observed between the experimental data from the EXFOR databases and the TALYS simulation. Although the TALYS simulation initially appears to understate the experimental data, some factors need to be considered. The available EXFOR datasets were mostly published between 1950 and 1985 and exhibit significant dispersion, limited energy coverage and varying experimental conditions (beam energy resolution, target characterization and activity determination techniques). In several cases, measurements were limited to narrow low-energy intervals and did not cover the entire 0–20 MeV range that is relevant to modern medical cyclotrons.

TALYS provides a self-consistent theoretical framework covering the entire energy domain of interest, allowing continuous excitation function modelling and direct implementation in thick-target yield calculations [13]. Even though there are discrepancies between TALYS predictions and some experimental datasets, the theoretical model was thought to be more suitable for predictive optimization because of its reproducibility and internal consistency. Therefore, the EXFOR data were not the only foundation for selecting the irradiation parameters, but were mainly used to confirm the worldwide trend of the excitation function.

SRIM/TRIM simulations

SRIM (Stopping and Range of Ions in Matter) is a widely used Monte Carlo simulation software package designed to model the interaction of energetic ions with matter. It allows calculations for ion stopping powers, projected ranges, energy loss, and radiation damage in target materials over a broad energy range (from a few eV up to several GeV). TRIM (Transport of Ions in Matter) is designed for the detailed simulation of ion transport in condensed matter. The code is capable of simulating complex target geometries composed of multilayered structures, allowing the characterization of each material separately, with different elemental compositions and physical properties [15].

While TALYS provides theoretical excitation functions for the nuclear reactions, allowing identification of the energy region where the cross-section reaches its maximum, SRIM simulations are necessary to determine how the proton beam actually acts inside the boron target.

The SRIM/TRIM code (v2013) was used to run energy loss simulations in order to identify the effective proton energy range inside the target. Proton energy degradation was calculated through the thickness of the boron target as well as through components of the irradiation experimental setup configuration, such as the aluminium window for the proton beam exit from the cyclotron and the aluminium foil sealing the target itself at the irradiation position.

By correlating the proton beam extraction energy from the cyclotron with the calculated energy losses through the 2 aluminium layers, the beam energies at target entry and the beam energies at target exit were determined. The resulting effective energy window was then overlapped on the excitation function derived from TALYS to verify that the irradiation occurs in the region of the optimal cross-section for maximizing ^{14}C production.

Theoretical calculation

Analytical formulas based on nuclear reaction theory were used to determine the theoretical ^{14}C production characteristics, such as the production rate, activity at the end of bombardment (EOB), and theoretical yield. These calculations consider the number of nuclei in the target,

the incident particle flux, the energy-dependent reaction cross-section, and the radioactive decay occurring during irradiation [16].

The atomic mass (A) of ^{11}B , the isotopic abundance (H_i), the mass of the target (m), the purity of the target (p) and the Avogadro's number (N_A) were used to calculate the total number of nuclei in the target. The total number of ^{11}B nuclei in the target accessible for the (p,n) nuclear reaction is given by the expression:

$$N_{B \text{ target}} = \frac{m \cdot p \cdot H_i}{A} N_A \quad (1).$$

Production rate of ^{11}C nuclei (s^{-1}) is:

$$R = \Phi N_{B \text{ target}} \langle \sigma \rangle \quad (2),$$

$$\langle \sigma \rangle = \frac{1}{\Delta E} \int_{E_{in}}^{E_{out}} \sigma(E) dE \quad (3),$$

where Φ is the flux of incident particles ($\text{cm}^{-2} \cdot \text{s}^{-1}$), $\langle \sigma \rangle$ is energy-averaged reaction cross-section (mb), ΔE – energy loss of the beam throughout the target thickness, E_{in} is the energy of the proton when entering the target (MeV), E_{out} the energy of the proton when exiting the target (MeV) and $\sigma(E)$ is energy-dependent microscopic reaction cross-section (mb).

Theoretical activity at the EOB (in GBq):

$$\Lambda_{theo.} = R (1 - e^{-\lambda t}) \quad (4),$$

where t is time of irradiation (s), and λ is decay constant (s^{-1}).

Theoretical yield $Y_{theo.}$ ($\text{GBq} \cdot \mu\text{A}^{-1} \text{h}^{-1}$) and average specific activity ($\text{MBq}/\text{mg}_{\text{target}}$) are calculated:

$$Y_{theo.} = \frac{\Lambda_{theo.}}{I \cdot t} \quad (5),$$

$$\Lambda_m = \frac{\Lambda_{theo.}}{m_{\text{target}}} \quad (6),$$

where I is beam current (μA) and m_{target} is the mass of the target (mg).

In the case of the BN target, both nuclear reactions should be taken into account: $^{11}\text{B}(\text{p},\text{n})^{11}\text{C}$ and $^{14}\text{N}(\text{p},\alpha)^{11}\text{C}$. The total number of ^{14}N nuclei in the target and the total number of nuclei in the BN target employed in ^{11}C production are calculated as:

$$N_{BN \text{ total}} = N_B + N_N = \frac{m \cdot p \cdot w_B \cdot H_B}{A_B} \cdot N_A + \frac{m \cdot p \cdot w_N \cdot H_N}{A_N} \cdot N_A \quad (7),$$

where w_B and w_N is mass fraction of boron and nitrogen.

Similarly, in the case of BN target, eq. (2) and (4) become:

$$R_{BN} = \Phi (N_B \langle \sigma_B \rangle + N_N \langle \sigma_N \rangle) \quad (8),$$

$$\Lambda_{theo.} = R_{BN} (1 - e^{-\lambda t}) \quad (9).$$

Experimental production of ^{11}C via (p,n) nuclear reaction using solid targets at the TR-19 cyclotron

Two metallic boron targets with different purity levels (95% and 98%) and one boron nitride (BN) target, were successively irradiated in the ACSI standard solid target holder (Figure 6.a). The holder allows irradiation at beam currents up to 80 μA , with an effective target diameter of 10 mm. The system is employed in the production of radionuclides such as ^{64}Cu , ^{89}Zr , ^{68}Ga , ^{67}Ga , $^{99\text{m}}\text{Tc}$ and ^{124}I [17, 18].

In Figure 6, the solid target holder used for the irradiations and the prepared boron target are shown. Figure 6.a) presents the ACSI standard solid target holder, while Figure 6.b) illustrates the boron target mechanically pressed onto the tantalum support prior to insertion into the holder. An aluminium sealing foil was employed to ensure mechanical fixation of the pressed target material into the tantalum support during irradiation in the cyclotron. The target disk is manually inserted into the dedicated slot of the target holder and positioned to ensure precise beam centring onto the boron target.

After irradiation, the target is pneumatically transferred into a tungsten-shielded container for safe handling.

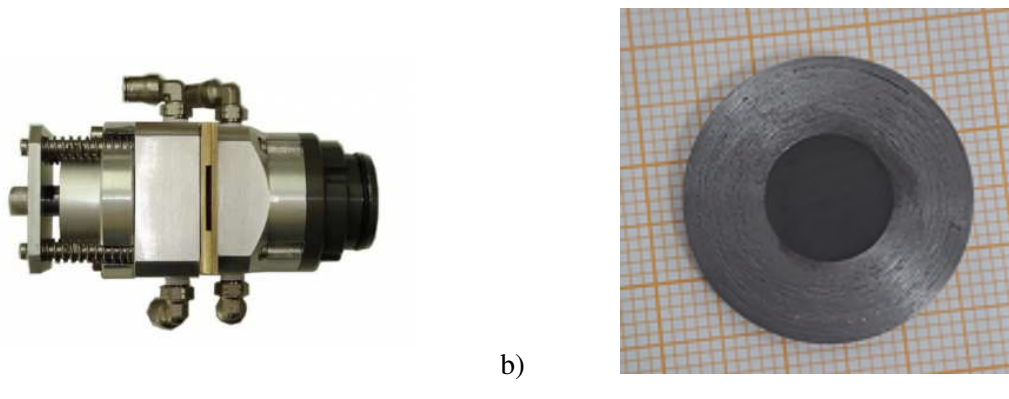


Figure 6. *a) Solid target holder-ACSI [20]; b) tantalum support with boron target pressed inside*

The geometrical configuration considered in both the experimental procedure and the TRIM simulations is illustrated in Figure 7. The extracted proton beam first passes through the aluminium entrance window, propagates through the helium cooling layer and the aluminium sealing foil, and finally interacts with the boron target, placed into the tantalum support. The arrangement ensures efficient heat dissipation under high beam currents while maintaining the structural integrity of the target during irradiation.

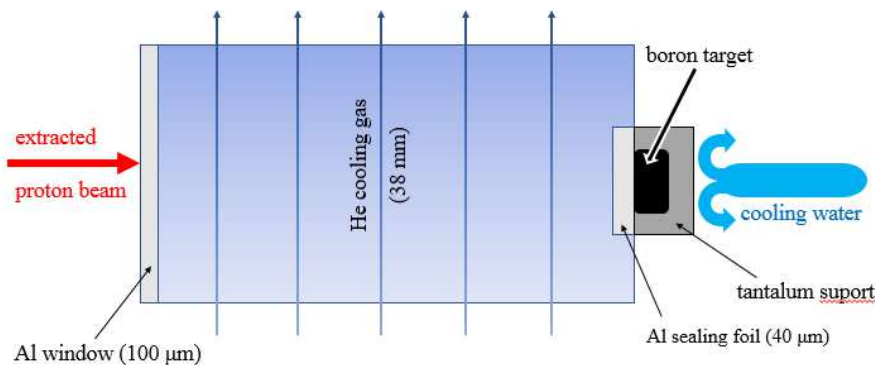


Figure 7. *Experimental configuration of the solid target holder*

The physico-chemical parameters relevant for irradiation and energy loss calculations are presented in Table 1. These include information regarding the target material, structural form, chemical purity, particle size, mass, and target thickness. The apparent density was calculated from the measured mass and geometrical volume. The boron targets were prepared by the Target Laboratory of IFIN-HH [19,20].

Table 1. *Physicochemical characteristics of boron targets*

No.	Target material	Structural form	Chemical purity (%)	Particle size (μm)	Mass (mg)	Target thickness (mm)	Apparent density (g/cm^3)
1.	Metallic boron (B)	amorphous	95	0.9	103	1	1.31
2.	Metallic boron (B)	crystalline	98	45	144.3	1.35	1.356
3.	Boron nitride (BN)	crystalline	98	1	184.7	1.35	1.7

Results

We determined the input energy on the 3 types of targets using TRIM, taking into account the aluminium window (100 μm), He cooling channel (38 mm) and the aluminium sealing foil (40 μm). Variations in the energy at the target exit occur due to differences in the physicochemical properties of the targets, including chemical composition, chemical purity, thickness, and apparent density (presented in Table 1). The calculated density provides a realistic representation of the effective material density under irradiation conditions and ensures improved accuracy of the simulation results. The results are presented in Table 2.

Table 2. *TRIM/SRIM simulation results*

No.	Target material	Chemical purity of target material	Proton beam extracted	Proton energy on target	Proton energy out of target
1.	Metallic boron (B)	95 %	15 MeV	14 MeV	9.87 MeV
2.	Metallic boron (B)	98 %			7.11 MeV
3.	Boron nitride (BN)	98 %			4.38 MeV

The energy of the incident protons extracted from the cyclotron was set to 15 MeV. Following the simulations performed, we obtained an input energy on the target of 14 MeV (Figure 8). The proton extraction energy from the cyclotron and the effective proton energy at the target surface is indicated by two vertical lines.

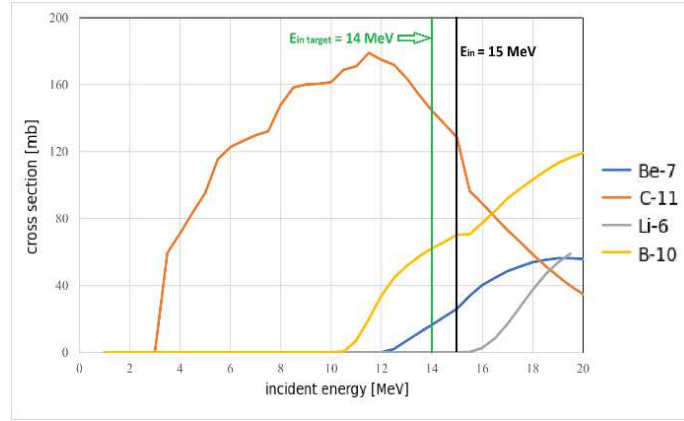


Figure 8. Incident proton energy (vertical black line) and incident energy on target (vertical green line) obtained with TRIM, depending on the effective cross-sections obtained with TALYS.

Considering the competing reactions induced by proton irradiation of boron targets, three reaction channels were simulated using TALYS. Among the resulting products, only ^7Be ($T_{1/2} = 53.22$ days) contributes to radionuclide purity calculations, whereas ^{10}B and ^6Li are stable isotopes. At the 14 MeV incident energy at the target entrance (determined with TRIM), the effective production cross-section of ^7Be is below 20 mb, indicating a negligible contribution to the radionuclide purity (RNP).

To model proton transport under realistic irradiation conditions, three TRIM simulations were performed, corresponding to the 95% metallic boron, 98% metallic boron, and boron nitride targets. The experimental assembly includes, in addition to the aluminium window and aluminium sealing foil, a helium cooling layer (38 mm) positioned in front of the target. However, due to the significantly larger geometrical thickness and comparatively low stopping power of helium, its inclusion in a single cumulative TRIM simulation masks the energy loss contributions of the thinner solid layers. Its contribution to the total energy loss was verified to be insignificant compared to that of the solid layers.

Thus, in Figure 9 the energy losses according to the experimental setup, through the 2 aluminium layers and each boron target are represented.

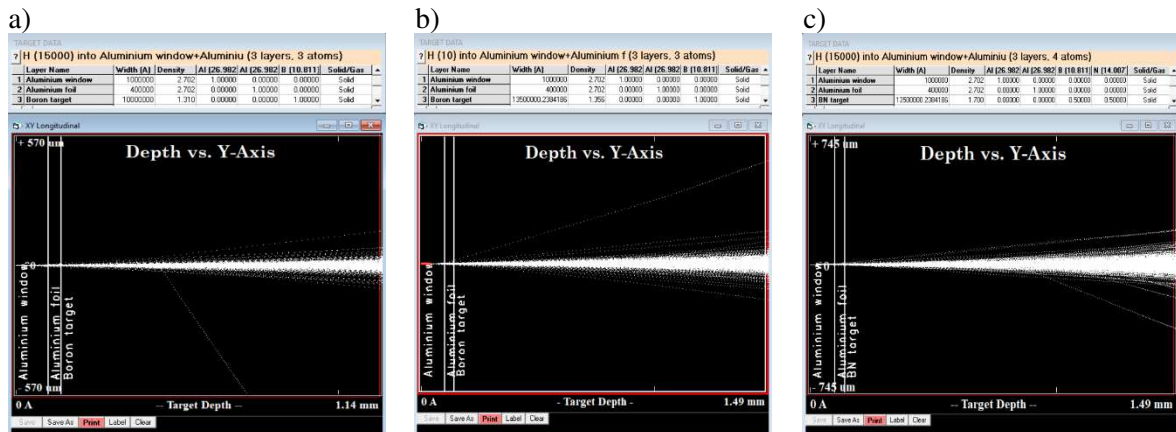


Figure 9. TRIM simulation of proton beam transport through aluminium window, aluminium foil and three different boron targets for C-11 production: a) B metallic (purity 95%); b) B metallic (purity 98%) and c) BN- (purity 98%)

Table 3 presents the irradiation parameters, experimental results and theoretical calculations.

Table 3. *Comparison of theoretical and experimental activities and production yield (all calculations are reported for EOB)*

No.	Extracted proton energy (MeV)	Beam current (μA)	Irradiation time (min)	Target material	Activity corrected for EOB (GBq)	Activity theo. (GBq)	Yield (GBq /μAh)	Yield theo. (GBq /μAh)	Average specific activity (MBq/mg _{target})	Average specific activity theo. (MBq/mg _{target})
1.	15	5	30	Metallic boron (B) 95%	7.77±0.76	8.82±0.61	3.11±0.30	3.53±0.24	75.43	85.63
2.				Metallic boron (B) 98%	10.87±0.45	12.72±0.52	4.35±0.18	5.09±0.21	75.33	88.15
3.				Boron nitride (BN) 98%	12.37±0.69	14.31±0.58	4.95±0.28	5.72±0.23	66.97	77.48

BN target contains both ^{11}B and nitrogen ^{14}N . In addition to ^{11}C produced via $^{11}\text{B}(\text{p},\text{n})$ nuclear reaction, ^{14}N can participate in concurrent reactions such as (p,α) and (p,n) , leading to the formation of radionuclides including ^{11}C and ^{14}O . As a result, the BN target can generate additional radioactive species beyond those produced by ^{11}B , contributing to an increased cumulative activity at EOB. For the 95% purity metallic ^{11}B target, the theoretical activity was 8.82 GBq, while the experimental value reached 7.77 GBq. Similarly, for the 98% purity metallic ^{11}B target, the activity decreased from a theoretical 12.72 GBq to an experimental 10.87 GBq. In the case of the BN target (purity 98%), the theoretical activity of 14.31 GBq was reduced to 12.37 GBq experimentally.

Characterization of the irradiated targets

The gamma spectrometric system used to determine the radionuclide purity of the irradiated targets was a 25% relative efficiency HPGe (high-purity germanium) detector, Baltic Scientific Instruments, Riga, Latvia with a 4096-channel multi-channel analyser (MCA) system. Spectral analysis and processing were performed with Inter Winner 7.0 software (ITECH Ltd.) [21, 22].

For the spectrometric analysis, the targets were placed at a distance of 5.5 cm from the detector, at 1h post-EOB. In all three instances, there was less than 0.25% dead time during the measurements. The acquisition time was 600 seconds for each individual sample. In the gamma-ray spectrums show the presence of ^{40}K at 1460.8 keV, originating from the natural background, and ^{11}C , which is indicated by the 511 keV annihilation peak (Figure 10). For each of the three cases, the determined radionuclidic purity exceeds 99.9% based on these measurements.

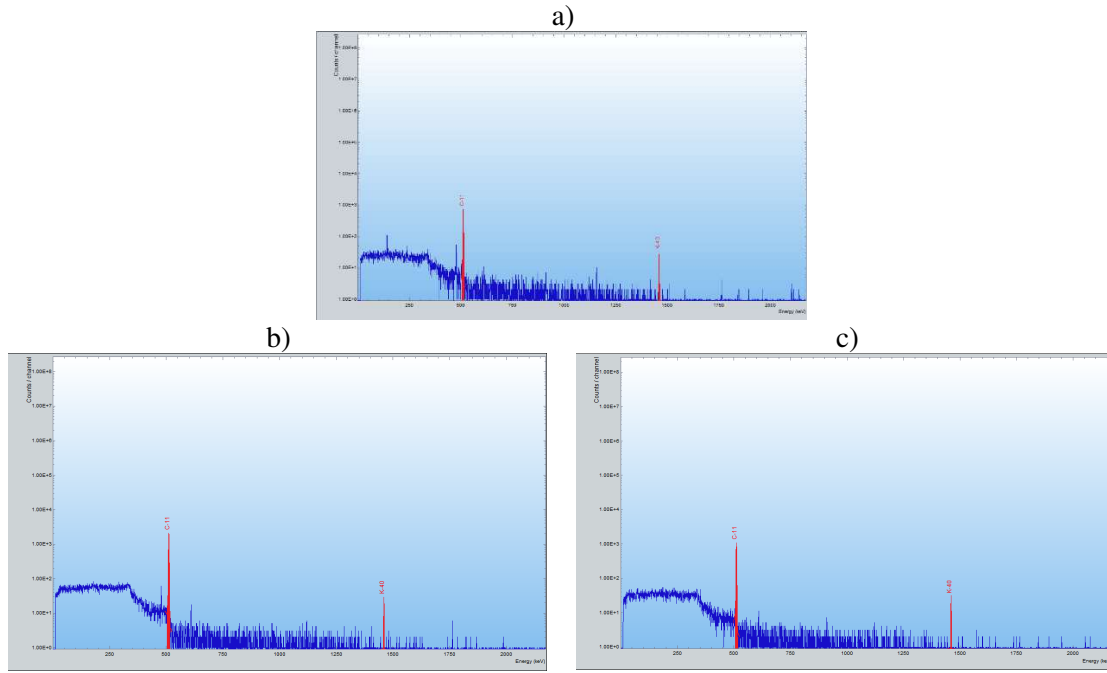


Figure 10. Gamma spectrum for: a) B-11 purity 95%, b) B-11 purity 98%, c) BN purity 98%; acquisition time: 600 sec.

In the case of the BN target, an additional acquisition of 30 minutes was performed with the target placed at 15 cm from the detector. In these conditions, the dead time was approximately 3%. The analysis of the corresponding spectrum (Figure 11) confirms an excellent RNP>99.9%, with the clear identification of the ^{11}C annihilation peaks at 511 keV and 1022 keV, along with the ^{40}K peak at 1460.8 keV associated with the natural radiation background.

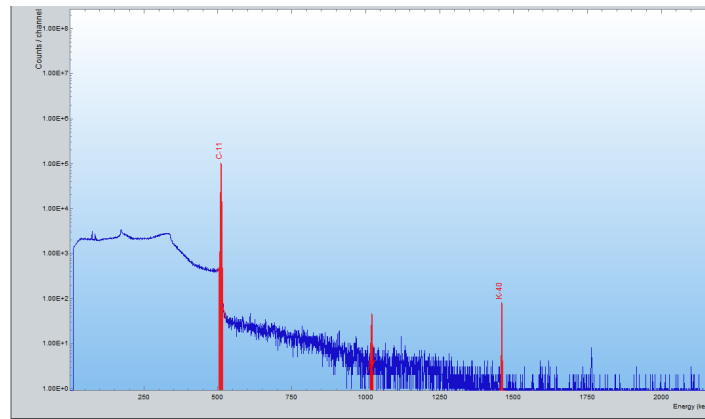


Figure 11. Gamma spectrum for BN target; acquisition time: 1800 sec

The half-life was determined using a dose calibrator and its associated software, VDC-405 (Veenstra Instruments, Netherlands). The calculated half-life values ranged between 0.33 h and 0.34 h (approximately 19.8 to 20.4 minutes), as presented in Figure 12, which aligns closely with the value of ^{11}C ($T_{1/2} = 20.361$ min), data taken from ref. [1].

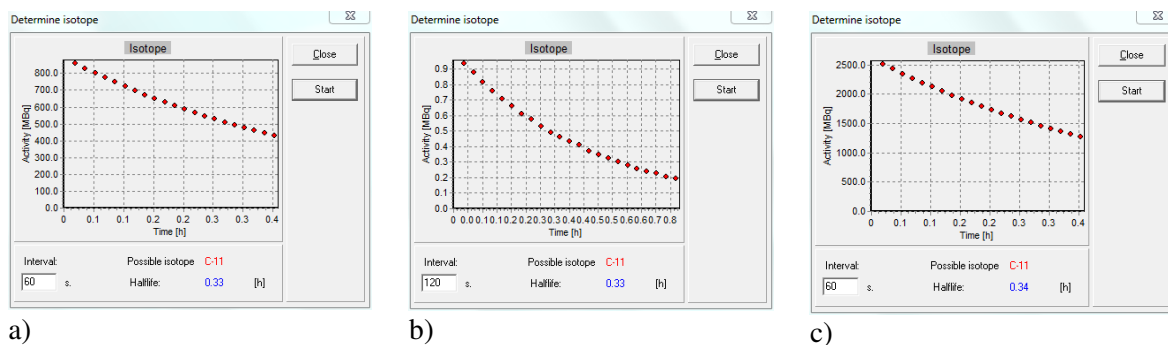


Figure 12. Half-life determination of ^{11}C for: a) ^{11}B purity 95%, b) ^{11}B purity 98%, c) BN purity 98%.

Discussion

Irradiation of boron targets with protons highlights the existence of competing reaction channels, whose contribution must be rigorously evaluated in the context of radionuclide purity. Simulations performed with the TALYS code indicate that, among the resulting products, only ^7Be is radiologically relevant, having a half-life of 53.22 days, while ^{10}B and ^6Li are stable isotopes and do not influence the radionuclide purity. The proton energy at the target entrance, estimated at 14 MeV by simulations performed with TRIM, implies the formation of ^7Be , with an effective cross section of less than 20 mb. This low value suggests a low probability of production of this radionuclide, which translates into a negligible contribution to the radionuclide impurities of the final product. Therefore, even if the nuclear reaction is possible, its impact on radionuclide purity is minimal, supporting the adequacy of the energy conditions selected for irradiation and confirming the feasibility of using boron targets in applications that require high purity standards.

The production yield is strongly influenced by the irradiation parameters, including the incident beam energy, beam current intensity, irradiation time, and target geometry. Variations in any of these factors can significantly affect the reaction rate and, consequently, the overall activity obtained at the end of bombardment.

The measured activities showed a clear dependence on both the chemical purity and the structural form of the boron target material. The lowest activity was obtained for the 95% purity metallic boron target, followed by the 98% metallic boron target, while the highest activity was measured for the 98% boron nitride target.

The increase in activity between the two metallic boron targets can be attributed to the higher effective ^{11}B content in the 98% purity material, resulting in a larger number of available target nuclei for the $^{11}\text{B}(p,n)^{11}\text{C}$ reaction.

The activity corrected for EOB measured for the BN target was consistently higher than that obtained for the metallic ^{11}B targets under identical irradiation conditions (14 MeV protons). This difference can be explained by several factors related to target composition, density, and the availability of multiple nuclear reactions.

A comparison between theoretical and experimental EOB activities shows that, for all investigated targets, the experimentally measured values are consistently lower than the calculated ones. The discrepancies between these values can be attributed to several practical factors that were not fully accounted for in theoretical calculations, such as variable shape of

the proton beam, proton energy degradation within the experimental setup, and the structural form of the targets' particles.

A similar trend is observed for the production yield values. Experimental and theoretical values of the BN target exhibit a more noticeable difference, which is probably caused by other variables such self-absorption effects, or higher uncertainty related to multi-element nuclei.

The lowest percentage difference was recorded for the amorphous metallic boron target (95% purity), showing a discrepancy of only 11.90%. In contrast, the crystalline metallic boron target (98% purity) presented the highest difference (14.54%). For the boron nitride (BN) target, despite its more complex chemical composition, the 13.56% difference confirms the validity of using mass fractions to calculate the combined C-11 production rate from both the ^{11}B and ^{14}N reaction channels. The BN target produced the highest experimental activity (12.37 GBq) due to its greater mass and the supplementary contribution from the nitrogen (p, α) channel, crystalline metallic boron (98% purity) remains the most efficient target material for achieving high specific activity. The percentage differences identified between the theoretical and experimental values present a good correlation.

Across all three configurations, the experimental data demonstrated high consistency. This strong correlation confirms that the measured radioactivity originates almost exclusively from the decay of carbon-11. Furthermore, the target material's purity (95% vs. 98%) did not significantly alter the decay profile or the linearity of the logarithmic activity curves. In all instances, the activity exhibited a mono-exponential decay, which is characteristic of a high-purity radionuclidic sample. The slight variation observed in BN target, where the software reported 0.34h, can be attributed to higher initial activity levels (exceeding 2500 MBq) and the associated statistical fluctuations or dead-time corrections within the detection electronics.

Conclusions

This work confirms the suitability of the $^{11}\text{B}(\text{p},\text{n})^{11}\text{C}$ reaction for cyclotron-based production of ^{11}C at an extracted proton energy of 15 MeV. According to simulation data, the effective beam energy on target is 14 MeV after taking into consideration energy losses in the aluminium entrance window, helium cooling layer, and aluminium sealing foil. This energy lies within the optimal region of the excitation function, ensuring efficient reaction cross-section values.

The higher EOB activity observed for the BN target comparative to the 2 metallic boron targets can be attributed to its greater apparent density, the presence of nitrogen enabling additional nuclear reaction, and its favourable physical structure. These findings underline the importance of considering both compositional and structural properties of solid targets when predicting radionuclide production yields under proton irradiation.

The experimental findings show that target composition and structural features may have an equally significant, if not dominant, impact on the effective yield. The significantly reduced yield of 95% purity ^{11}B target emphasizes how sensitive production efficiency is to isotopic abundance and presence of a significant amount (5%) of other nuclei.

Overall, although experimental activities and yields are systematically lower than theoretical predictions, the trends remain consistent across all targets. The maximum experimental activity

and production yield are provided by the BN target, which is followed by the 98% purity ^{11}B target and the 95% purity metallic ^{11}B target. It was observed that both the corrected activity at the EOB and the experimental yield exhibit a systematic deviation of approximately 12–15% below the estimated theoretical values, for all 3 types of targets.

In conclusion, the experimental data validate the theoretical model, showing a solid correlation, with low deviations (11.9% – 14.5%). The amorphous boron target (95% purity) demonstrated the best agreement with the theoretical estimates and the highest specific activity, confirming a superior activation efficiency. On the other hand, although boron nitride (BN) generated the highest total activity, due to its higher mass and the contribution of the nitrogen reaction channel, crystalline boron metal targets remain the optimal materials for maximizing the specific activity.

The radionuclidic purity (RNP>99.9%), calculated based on spectral data, for all 3 types of targets of different purities, complies with the requirements of the European Pharmacopoeia (Ph. Eur.) 11th Edition, which shows that the production of ^{11}C on the ACSI solid target system is ideal for obtaining radiopharmaceuticals with a high purity.

These findings highlight to the importance of taking into consideration the practical irradiation conditions and material-related variables when converting theoretical calculations into real production. These results confirm the efficiency of proton irradiation of boron-based targets in generating ^{11}C with radionuclidic purity suitable for subsequent radiopharmaceutical synthesis.

List of abbreviations

ACSI	Advanced Cyclotron Systems, Inc.
CCR	Radiopharmaceutical Research Centre
ELI-NP	Extreme Light Infrastructure–Nuclear Physics
EOB	end of bombardment
EXFOR	Experimental Nuclear Reaction Data
HPGe	high-purity germanium
IAEA	International Atomic Energy Agency
IFIN-HH	Horia Hulubei National Institute for Physics and Nuclear Engineering
NRDC	Network of Nuclear Reaction Data Centres
PET	positron emission tomography
RNP	radionuclidic purity
SRIM	Stopping and Range of Ions in Matter software package
TRIM	Transport of Ions in Matter software package

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Declarations

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Data availability

The data and materials are available on reasonable request to the corresponding author.

Ethics approval and consent to participate

Not applicable.

Consent for publication

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Competing interests

Authors declare no conflict of interest concerning the submitted work.

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