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THEORETICAL ANALYSIS AND SIMULATION OF PROTON-NUCLEAR INTERACTIONS IN LIGHT NUCLEI USING THE TALYS CODE

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A structured review is presented of the capabilities and feasibility of using the TALYS nuclear reaction code for simulation proton-nucleus interactions in light nuclei (^{12}C, ^{14}N, ^{16}O). An array of scientific publications has been analysed, covering fundamental issues of nucleosynthesis (the CNO cycle), problems in cosmochemistry, as well as applied aspects of nuclear medicine, including PET diagnostics and online monitoring of beam penetration in proton therapy. Particular attention was paid to comparing TALYS results with experimental data from the EXFOR library and the evaluated ENDF/JENDL files. The limits of the code's applicability in the resonance region and at energies above 100 MeV were determined.

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INTRODUCTION

The modern understanding of the interaction between protons and light nuclei has its origins in the fundamental work of H. Bethe, in particular his classic 1939 paper 'Energy Production in Stars' [1]. This work provided the first theoretical justification that the primary source of energy in main-sequence stars is thermonuclear fusion reactions, in which carbon and nitrogen nuclei act as catalysts. Bethe described in detail the carbon-nitrogen cycle (CNO cycle), in which four protons interact sequentially with ^{12}C and ^{14}N nuclei, ultimately producing an α- particle. It has been shown that, during proton-nucleus interactions, the fission channel predominates for nuclei with mass number $A < 12$, whilst for elements heavier than fluorine, (p, γ) radiation capture without subsequent emission of an α-particle prevails. Consequently, the CNO cycle represents a unique mechanism for a closed thermonuclear cycle. An important feature of this cycle is its closed nature: the initial ^{12}C nucleus is restored in the final reaction step, $^{15}N\,(p,\alpha)^{12}C$. Bethe demonstrated that the efficiency of these processes depends critically on the energy of the protons and the Coulomb barrier of the nuclei, which effectively determined the direction of development of experimental low-energy nuclear physics for the following decades. G. Bethe's seminal work laid the theoretical foundations of modern nuclear physics. Today, this field is developing rapidly thanks to the use of computer simulation, in particular the TALYS calculation code, which has become the standard for the further analysis of nuclear reaction mechanisms and is widely used in current research. In particular, the paper [2] investigated the role of the (p, γ) proton capture reaction in the *p-p* chain and the CNO cycle in the energy range up to 8 MeV. The TALYS code was used to theoretically calculate the reaction cross-sections for $^{7}Be\,(p, \gamma)^{8}B$, $^{12}C(p,\gamma)^{13}N$, $^{15}N(p,\gamma)^{12}C$, and $^{13}C(p,\gamma)^{14}N$. Understanding these processes is critical for modelling the evolution of main-sequence stars and estimating star formation rates in spiral and elliptical galaxies. The results obtained using TALYS were compared with data from the ENDF/B-VII library of evaluated nuclear data and the CSC-GM theoretical model. It was shown that, for the $^{12}C\,(p, \gamma)^{13}N$ reaction, the theoretical prediction from TALYS is in good agreement with the ENDF data. For the $^{15}N\,(p, \gamma)^{12}C$ reaction, the TALYS code demonstrated satisfactory agreement with other models, indicating an increase in the cross-section up to 7 MeV followed by stabilisation. However, for the $^{13}C\,(p, \gamma)^{14}N$ reaction, discrepancies were found in the low-energy region. TALYS did not reproduce the resonant peak in the 1 MeV region predicted by the CSC-GM model. For the $^{7}Be\,(p, \gamma)^{8}B$ reaction, TALYS shows a less pronounced increase in the cross-section compared with ENDF and CSC-GM, limiting the cross-section to below 5 MeV; however, the general upward trend is maintained in the 6.5...8 MeV range. In [2], it is shown that TALYS 1.6 is a powerful tool for estimating proton capture cross-sections in an astrophysical context. The discrepancies observed at low energies (E_r < 2.5 MeV) indicate that the default TALYS settings require further adjustment to accurately model the intensity of star formation. Paper [3] examines the problem of uncertainty regarding the range of protons in human tissues during radiotherapy, which limits the full realisation of this method's clinical potential. For direct (*in vivo*) verification of proton range, the detection of secondary γ-radiation arising from nuclear reactions is proposed. In this study, a comparative analysis was carried out of the predictive capability of Monte Carlo-based codes (GEANT4, MCNP6) and specialised programmes, such as TALYS 1.4 and EMPIRE 3.1, for describing proton scattering on ^{12}C, ^{14}N, and ^{16}O) in the energy range from 1 to 200 MeV. For calculations in the TALYS code, a careful selection of models was carried out: Young's optical models were used in the energy range up to 50 MeV, whilst the Madland global potential was used for higher energies. Furthermore, given the limitations of the ECIS module, the cross-sections for the ^{12}C nucleus at energies above 10 MeV were scaled according to the Tripathi parameterisation. To accurately describe the interaction mechanisms in the high-energy region, the authors have modified the deformation parameter in the TALYS nuclear structure database and have also taken into ac-

count the fact that certain low-lying levels of the nuclei under study decay exclusively via α-emission. The superiority of the TALYS and EMPIRE codes over the Monte Carlo approach in reproducing the experimental excitation cross-sections of discrete γ-lines has been demonstrated. For the 4.44 MeV line of the ^{12}C nucleus, TALYS demonstrated better agreement with experiments using high-energy protons. In proton scattering on ^{16}O, the TALYS and EMPIRE codes produced consistent spectral characteristics for the 6.13 MeV line, although they exhibited a systematic overestimation of cross-sections for very low proton energies. Furthermore, the TALYS code described the 4.44 MeV line emission for the ^{12}C residual nucleus quite accurately. For the 2.31, 1.64, and 5.11 MeV lines, TALYS reproduced the characteristics of the experimental measurements satisfactorily, in contrast to the GEANT4 and MCNP6 programmes. It was shown that the presence of modelling differences leads to a doubling of the fluctuation in the predicted proton yield towards the end of the proton run, whilst TALYS is an accurate tool for estimating cross-sections when the input parameters are appropriately configured. The evaluation of nuclear data is another area in which the TALYS computer code is used. The paper [3] addresses the problem of the shortage of evaluated nuclear data required for the production of medical and technical isotopes, particularly in the energy range 35…200 MeV. In contrast to neutron-induced reactions, which are described in detail for a wide range of targets, ENDF libraries for proton beams remain incomplete and cover only a limited number of nuclides. To address this imbalance, the authors use the TALYS code to simulate isotope production channels and to calculate reaction cross-sections, angular distributions and energy spectra of secondary particles, which is critical for the optimisation and design of target devices. The TALYS code is an effective tool for evaluating nuclear data, as it is used to calculate theoretical cross-section values, which are employed when EXFOR data are unavailable. This code is an effective scientific tool for creating up-to-date nuclear libraries for proton-induced reactions. However, it is noted in [3] that the nuclear models incorporated in TALYS require constant verification using new experimental data, as there may be significant discrepancies between TALYS predictions and experimental results in the high-energy region.

1. PHYSICAL MODELS AND TALYS PARAMETERISATION

The energy range 100…200 MeV for proton-nucleus interactions is challenging for theoretical analysis, as it corresponds to a region where several competing reaction mechanisms overlap. In [4], the TALYS code was used as a tool for analysing excitation functions and applying the exciton model. This study demonstrated that, for proton energies $E > 100$ MeV, the simulation results depend heavily on the parameters of the exciton model, in particular on the matrix element for intranuclear transitions and the level density. Using default settings can lead to serious errors when describing multinucleon systems. The study also highlights the need to account for isospin conservation in statistical decay models, which has been implemented in TALYS. As a result of this, the cross-sections of nuclei located far from the line of stability are calculated with greater accuracy. The data obtained using TALYS were compared with the results obtained by the TREND collaboration. It was shown that, for greater efficiency, the TALYS code must be used following careful tuning of the input parameters. Study [4] demonstrates the relevance of using the TALYS code for this energy range in the context of radioisotopes, but the exciton model requires certain parametric modifications.

The paper [5] investigates the mechanisms of γ-ray generation during the interaction of protons and α-particles with the nuclei of ^{12}C, ^{16}O, ^{24}Mg, and iron nuclides (*Fe*) in the energy range 5…25 MeV. The nuclear data obtained are of great importance for astrophysical applications, in particular for the interpretation of γ-spectra of solar flares, which requires a detailed description of the processes of excitation of discrete nuclear levels. The authors have carried out a detailed comparative analysis of experimental cross-sections with calculations performed using the TALYS 1.0 code (the latest version at the time of these studies). It is shown that using TALYS with its default settings satisfactorily reproduces the shape of the excitation function, but does not ensure the correct determination of absolute cross-sections for light nuclei. In particular, the use of the Koning–Delaroche global optical potential leads to a systematic underestimation of the inelastic scattering cross-sections for the ^{12}C and ^{16}O nuclei. This is because the phenomenological potentials developed for medium and heavy nuclides do not take into account the cluster structure of light nuclei. The authors emphasise that a correct quantitative assessment of the intensity of γ-lines requires consideration of strong channel coupling (the coupled-channel method), which by default plays a secondary role in calculations of such systems. The paper [5] was one of the first to highlight the systematic limitations of the TALYS code when applied to light nuclei and to demonstrate that the use of averaged potentials is unsuitable for obtaining accurate astrophysical data. The authors emphasise the inadequacy of the experimental data on the cross-sections for the formation of discrete γ-lines involved in modelling the radiation of astrophysical objects (in particular, in reactions induced by protons and α-particles). It is shown that the default settings lead to a tenfold overestimation of the cross-section for the $^{14}N\,(p, n)^{14}O$ reaction compared with experimental data. To overcome this discrepancy, the authors have modified the TALYS nuclear structure database by adding new levels to the rotational collective bands and optimising the β deformation parameters. It has been shown that modifying the coupling schemes of collective levels and a number of deformation parameters significantly improves TALYS's ability to calculate the energy dependence of interaction cross-sections. It is concluded that, for obtaining reliable results in the modelling of proton-nucleus interactions on ^{14}N and ^{16}O nuclei, the TALYS code is a suitable tool; however, further fine-tuning of parameters and interaction potentials is required.

2. NUCLEAR ASTROPHYSICS AND COSMOCHEMISTRY

Recently, the TALYS code has become one of the key tools for calculating thermonuclear processes in the interiors of stars. In particular, work [6] investigated the excitation functions of the (p, γ) and (p, α) channels for the nuclides ^{12}C, ^{13}C, ^{14}N, and ^{15}N. These reactions determine the dynamics of energy release and matter transformation in the p-p chain and the CNO cycle. Precise values of the reaction cross-sections involving these nuclei, in the energy range up to 10 MeV, allow for a more detailed study of the evolution of main-sequence stars and nucleosynthesis processes. Given the extreme complexity or physical impossibility of directly measuring such cross-sections experimentally near the astrophysical threshold, numerical modelling remains the primary source for obtaining the necessary nuclear data. In this work, the TALYS code, together with the EMPIRE programme, was used to derive the excitation function. The results were compared with data from EXFOR, TENDL-2014 and ENDF/B-VII. For the reactions $^{12}C\ (p, \gamma)^{13}N$ and $^{14}N\ (p, \gamma)^{15}O$, the TALYS calculations and existing data show a correlation within the energy range under investigation. Reactions such as $^{13}C\ (p, \gamma)^{14}N$ have a clearly pronounced resonant structure and are poorly described by the standard TALYS settings, which generate cross-section curves without resonances. The authors emphasise that standard TALYS statistical models should not be applied to the light nuclei mentioned above. They also stress the need to take resonant effects into account. Study [2] is also devoted to the radiation capture of protons in stellar nucleosynthesis processes. As astrophysical reactions generally take place at relatively low temperatures, the analysis focuses on the energy range up to 8 MeV. In this work, the TALYS 1.6 computer code was used to simulate the reactions $^{7}Be\ (p, \gamma)^{8}B$, $^{12}C\ (p, \gamma)^{13}N$, $^{15}N\ (p, \gamma)^{12}C$ and $^{13}C\ (p, \gamma)^{14}N$ and to obtain the corresponding cross-sections. The simulation results were compared with the ENDF/B-VII libraries and the CSC-GM model. For the main CNO cycle reaction in spiral galaxies, $^{12}C\ (p, \gamma)^{13}N$, the calculations obtained using the TALYS code correlate with the ENDF library data. The computer calculation of the cross-section begins at an energy of ~0.004 MeV, indicating the continuity of nuclear fusion processes. A satisfactory correlation is observed between the simulation results and the model for the $^{15}N\ (p, \gamma)^{12}C$ channel, with a steady increase in the cross-section up to an energy of 7 MeV, followed by stabilisation. However, for the $^{13}C\ (p, \gamma)^{14}N$ reaction, significant discrepancies were found in the low-energy region: the TALYS code failed to reproduce the resonance near 1 MeV predicted by the CSC-GM model and the ENDF library. The agreement between ENDF and TALYS is restored in the 3 MeV region. For the $^{7}Be\ (p, \gamma)^{8}B$ channel, the TALYS calculation showed a very slow increase in the cross-section compared with ENDF and CSC-GM, capping it in the 5 MeV region, whilst the upward trend persists in the 6.5…8 MeV energy range. Study [2] demonstrated that TALYS 1.6 is an effective tool for the theoretical estimation of proton capture cross-sections for research in the field of astrophysics. The discrepancies observed for proton energies E < 2.5 MeV indicate the need to fine-tune the resonance parameters in order to obtain accurate results.

In study [7], a detailed comparison was carried out between experimental excitation functions and calculations performed using the TALYS v.1.0/1.2 code. Targets consisting of nitrogen, oxygen, neon and silicon were irradiated with protons and α-particles in the energy range from the threshold up to 31 MeV. The aim of the experiment was to expand the database for nuclear gamma-astronomy, which will enable a better analysis of the composition of objects within which nuclear interactions occur. In the case of light nuclei, such as ^{14}N and ^{16}O, the use of standard optical and deformation parameters leads to a twofold discrepancy. With its default settings, TALYS does not reproduce the contribution from direct reactions leading to the filling of the first excited states. To ensure consistency with the experimental data, the input parameters in the TALYS command file were adjusted. Deformation parameters $\beta 2$, $\beta 3$, and $\beta 4$ were added for the low-lying levels. To account for the contribution of the direct interaction mechanism, the coupled-channel method was applied, and the parameters of the exciton model were further adjusted to accurately describe the intermediate energy region. The tuning carried out yielded acceptable results for the main gamma lines – 1.635 and 2.313 MeV for nitrogen, and 6.129 MeV for oxygen. However, some channels, in particular those leading to the emission of several nucleons, remain difficult to model. This study emphasises that, for light nuclei, the TALYS computer code should only be used with additional tuning of the input parameters.

The paper [8] investigates the formation of cosmogenic nuclides and the rate at which they accumulate in meteorites and lunar soil. In particular, this concerns nuclides such as ^{10}Be, ^{14}C, and ^{26}Al. The main objective of the study is to determine the cross-sections of nuclear reactions induced by cosmic radiation. The TALYS code was utilised to build a computational database. Using TALYS, the excitation functions of the radionuclide formation channels (in particular ^{14}C) were modelled, which is critical for the precise dating of meteorites and the reconstruction of their radiation exposure history. The use of the TALYS code made it possible to correctly account for the contribution of α-particles to the process of cosmogenic nuclide nucleosynthesis, which had been neglected in previous calculations or estimated with insufficient accuracy. Taking this factor into account has significantly improved the accuracy of modelling for systems containing light nuclides, which are characterised by relatively large cross-sections for interactions with α-particles. The results of this work demonstrate the usefulness of the TALYS code, as it allows for a fairly accurate description of the entire set of nuclear interactions in complex multi-element targets in planetary science research.

In [9], the TALYS code was used to obtain refined data on the cross-sections for the formation of discrete γ-lines, in particular the intense 6.129 MeV line of the ^{16}O nucleus, in the energy range up to 17 MeV. The study investigates inelastic proton scattering on the ^{16}O nucleus, as well as on the ^{28}Si nucleus, which is accom-

panied by the emission of gamma rays. Such data are important both for fundamental nuclear physics (in particular, in the analysis of isospin symmetry for the calculation of cross-sections of neutron-induced processes) and for addressing problems in nuclear astrophysics and reactor physics. In this work, a comparative analysis is carried out of the experimental values of the cross-section for the $^{16}O\ (p, p'\gamma)^{16}O$ reaction (the 6.129 MeV line) with the results of theoretical modelling using the TALYS 1.6 and EMPIRE 3.2.2 codes. The TALYS model prediction correctly reproduces the absolute order of magnitude of the cross-section and the general trend of the excitation function within the energy range under investigation. However, whilst maintaining the standard settings, TALYS generates a smooth excitation function curve, whereas the experimental data exhibit a resonant structure for the ^{16}O nucleus up to 17 MeV. The results of this work confirm the limitations of applying TALYS statistical models to light nuclides: by default, the code adequately describes only the average cross-section, but does not reproduce resonances in the low- and medium-energy range. To improve the accuracy of cross-section calculations for the specified reactions on the ^{16}O nucleus, it is necessary to apply the R-matrix formalism or to directly integrate the resonance parameters into the calculation model.

3. MEDICINE AND RADIATION SAFETY

The paper [10] investigates the emission of gamma radiation arising from proton-nuclear interactions on a range of targets, in particular carbon and oxygen nuclei. These reactions occur in various astrophysical environments, such as solar flares or in the atmospheres of compact celestial objects. The cross-sections for the formation of de-excitation γ-lines were measured upon irradiation of targets made of natural carbon and Mylar (which contains carbon and oxygen) in the proton energy range of 30…200 MeV. The experimental data obtained for the emission cross-sections of ten γ-lines were compared with predictions from the TALYS calculation code. Standard models of optical potentials proved inadequate for describing interaction mechanisms in light nuclei in the region of relatively high energies. To achieve sufficient accuracy in the calculations, the authors applied modified optical potential parameters and deformation parameters for nuclear states. By correcting the level deformation parameters in the TALYS database, excitation functions were obtained for the γ-lines at 4.439 and 6.129 MeV, which showed satisfactory agreement with experimental measurements. The results of [10] once again demonstrate the inadequacy of the standard TALYS settings for describing proton reactions on light nuclei such as ^{12}C and ^{16}O, particularly in the region of proton energies above 30 MeV. The authors emphasise the necessity of careful (manual) tuning of the phenomenological optical potential and correction of the collective-state deformation scheme. Only such an approach ensures the accurate determination of the excitation function for γ-transitions, which is essential for a correct spectral analysis of astrophysical sources of γ-radiation.

In [11], the cross-sections of proton-nucleus reactions on the ^{12}C, ^{14}N, and ^{16}O nuclei, leading to the formation of the ^{10}C and ^{11}C isotopes, were determined. This study was motivated by the need for accurate dose monitoring during proton therapy. Since the formation of positron-emitting nuclides occurs directly within biological tissues during irradiation, reliable cross-section values are critically important for the reconstruction of the absorbed dose profile from PET tomography data. The authors used the TALYS code, version 1.96. Simulations were carried out using the code's default parameters, and the results were compared with experimental data from the EXFOR database and the JENDL-5 and ENDF/B-VIII.0 evaluated data libraries. For the dominant $^{12}C\ (p, x)^{11}C$ channel, the TALYS code demonstrated high accuracy in reproducing experimental data over a wide energy range, confirming the reliability of the statistical models used to describe this reaction. However, in the case of the ^{10}C nucleus formation channel, a systematic discrepancy with the experimental data is observed: the theoretical values significantly overestimate the cross-sections in the sub-threshold region compared with the EXFOR data. It has been established that the TALYS code is well suited to the rapid generation of data, but evaluated data libraries such as JENDL-5 provide a better fit to experimental data for non-principal channels in light nuclei. In [11], it is shown that the TALYS code is well suited to tasks involving the estimation of major PET isotopes; however, its calculations for channels involving the emission of multiple nucleons from light nuclei require detailed analysis and comparison with evaluated data.

The article [12] analyses the (p, x) cross-sections for reactions on ^{14}N and ^{16}O nuclei, which lead to the formation of short-lived positron-active isotopes – ^{14}O and ^{15}O. These data are important for monitoring the delivered dose in vivo during proton therapy using PET. A key aspect of this study is its focus on advanced multiphoton PET techniques, in particular the use of J-PET-type scanners and positron imaging. Using such technologies, it is possible not only to determine the beam path but also to assess the level of tumour tissue hypoxia. The successful implementation of these advanced techniques requires knowledge of precise data regarding the cross-sections for the formation of the relevant PET isotopes and the associated photon yield. Estimating the cross-sections for proton-induced reactions leading to the formation of ^{14}O and ^{15}O on light elements requires a comparison of theoretical models with available experimental data. In reactions of the type $^{16}O\ (p, pn)\ ^{15}O$ or $^{14}N\ (p, n)\ ^{14}O$, a typical problem arises: the standard statistical and pre-equilibrium models built into TALYS require detailed verification, as any discrepancies in the calculation of the cross-section, particularly in the region of resonances or threshold energies, distort the reconstruction of PET images. Reliable theoretical modelling of cross-sections for ^{14}N and ^{16}O forms the basis for the further implementation of modern diagnostic methods in proton therapy. It should be noted that the specific nature of light nuclei requires a thorough analysis of the modelling results and a mandatory comparison with the data available in scientific databases.

The Master's thesis [13] is devoted to the investigation and comparison of various methods for producing the ^{15}O isotope, which plays an important role in PET.

As this nucleus has an extremely short half-life ($T_{1/2}$ ~ *122 s*), this radiopharmaceutical must be produced directly in or near medical centres. The thesis analyses nuclear reaction cross-sections as a function of the energy of incident particles in order to optimise the isotope yield and minimise associated impurities. The TALYS code was used to theoretically calculate excitation functions and subsequently compare them with experimental data from the EXFOR database. It was found that TALYS generally adequately describes the energy dependence of the cross-section for the reaction channel under investigation. However, the simulation results show sensitivity to the energy step size and input parameters. Using the theoretical TALYS curves, it was possible to evaluate the efficiency of various production channels, in particular the photonuclear reaction $^{16}O\ (\gamma, n)^{15}O$. The simulations confirm that proton-induced reactions on ^{16}O are the most promising for hospital cyclotrons. The paper presents detailed examples of TALYS input files, demonstrating the reproducibility of the modelling methodology for medical isotopes. This highlights the role of TALYS as an accessible and reliable tool for engineering calculations in nuclear medicine. Research [13] demonstrates that TALYS is an indispensable tool for evaluating alternative routes for the production of medical radionuclides. Although discrepancies with EXFOR data are observed for certain energies, the code enables the rapid comparative analysis of various reactions, which is a critical factor in the design of targets and the selection of accelerator operating modes.

The current global situation regarding cancer indicates a rise in the number of fatalities. At present, there are a number of radiotherapy methods that can halt tumour growth. In view of the subject matter of this section, it should be noted that the NSC KIPT also conducts research in the field of nuclear medicine. Study [14] outlines a plan to develop a new technology for generating neutron beams for neutron capture therapy. The authors of the paper believe that the scientific and technical infrastructure of the NSC KIPT will enable this plan to be realised and will allow the production of beams with a neutron density exceeding current radiosurgical specifications.

In [15], the cross-section of the $^{12}C\ (p, n)^{12}N$ reaction was investigated at energies up to 150 MeV. A characteristic feature of this reaction is the formation of the short-lived β^+-emitting isotope ^{12}N with a half-life of ~11 ms. Due to its very short half-life, this nuclide is the optimal choice for real-time PET imaging (beam-on PET), which allows the position of the final section of the proton trajectory to be determined almost instantaneously during the therapy session. The main problem in this case is the lack of reliable experimental data for this reaction at energies above 60 MeV, which significantly complicates the validation of theoretical models. The authors compared the results obtained on the AGOR cyclotron with calculations using the TALYS 1.96 code. It has been shown that using TALYS with standard settings does not accurately describe the $^{12}C\ (p, n)^{12}N$ reaction cross-section. This is because this reaction is 'exclusive', and its description at energies above 40 MeV is critically dependent on the parameterisation of the exciton decay model. In its default mode, TALYS overestimates cross-sections in the range from 40 to 100 MeV. It is emphasized that the preequilibrium parameters of the code are optimised for heavy nuclei and do not take into account the specific features of the carbon nucleus structure, which leads to an incorrect distribution of energy amongst the nucleons in the initial stages of the cascade. The article emphasises that the formation of ^{12}N has a threshold of approximately 20 MeV, and that the accuracy of the simulation in the sub-threshold region is critical for the precise reconstruction of the Bragg peak shape. Study [15] points to serious limitations of TALYS 1.96 when modelling specific formation channels for nuclides with extremely short half-lives in light nuclei. This work demonstrates that the successful application of the code for PET monitoring requires correction of the parameters of the exciton model for light nuclear systems, as standard calculations do not provide the necessary clinical accuracy.

The report [16] examines the production of secondary neutrons and protons during the interaction of protons with an energy of E_p = 50 MeV with the nuclei of ^{12}C, ^{14}N, and ^{16}O. An accurate estimation of the yield of secondary nucleons is a critical factor for fundamental research, dosimetry and radiation safety, particularly in calculations of biological protection and the assessment of the associated (subcritical) dose in proton beam therapy. To model total and differential cross-sections, as well as the yield of secondary particles per incident proton, the TALYS 1.96 calculation code was used with default parameters. Numerical analysis using TALYS made it possible to clearly determine the energy thresholds for neutron production, which differ significantly for each of the nuclides studied: for the ^{12}C nucleus, the threshold is approximately 20 MeV; for ^{14}N, up to 10 MeV; and for ^{16}O, in the range of 17…18 MeV. The highest neutron yield per proton in the primary beam was recorded for the oxygen nucleus. Similarly, to the neutron channel, the ^{16}O nuclide has the highest yield of secondary protons – 1.47 per proton. At the same time, an analysis of the differential cross-sections showed that the highest average energy of secondary protons is observed for the ^{14}N target – 12.72 MeV – whilst for the ^{12}C and ^{16}O nuclei it is approximately 10 MeV. This work confirms that the TALYS 1.96 code is an effective tool for evaluating the spectra and yield of secondary nucleon emission at proton energies E_p = 50 MeV. The total and differential cross-sections obtained using TALYS 1.96 allow for a detailed analysis of the kinematics of secondary particles, providing the reliable data required for the optimisation of radiation protection and clinical dosimetry applications.

The paper [17] investigates ways of improving the accuracy of dosimetric planning in proton radiotherapy. A significant problem with Monte Carlo transport codes, such as MCNPX, is the presence of errors in the calculation of depth-dose distributions due to an insufficiently accurate description of the nuclear interactions of protons with water and the body's biological tissues. The authors sought to ensure dose prediction accuracy better than 2% (the clinical error tolerance), which requires the use of up-to-date evaluated nuclear data. Although the article focuses on the MCNPX transport

code, it demonstrates the important role of TALYS in generating high-precision nuclear data for libraries. To improve the accuracy of the simulation results, evaluated data files for the ^{16}O nucleus (in the energy range up to 200 MeV) were additionally incorporated; these were obtained using TALYS, which was employed as a generator of initial cross-sections. Simulation in the MCNPX code, using estimated data calculated in the TALYS code and processed by the NJOY module, made it possible to account more accurately for the contribution of nuclear reactions to the total absorbed dose. This is particularly important when determining the energy release from secondary particles (neutrons, α-particles and kick-off nuclei) beyond the Bragg peak. From a methodological point of view, the TALYS code formed the basis of a multi-stage calculation scheme, in which it serves as the source of primary information on process cross-sections. Report [17] demonstrates the great significance of TALYS as a reliable tool for creating nuclear data libraries used in medical physics, as the radiation safety of patients undergoing radiotherapy depends directly on the accuracy of its calculations.

4. SPECTROSCOPY AND DIFFERENTIAL CHARACTERISTICS

The study [18] investigates the shape of the spectral line and the angular distribution of secondary γ-radiation with an energy of 4.44 MeV, arising from the inelastic scattering of protons on ^{12}C nuclei. The proton beam energies were 70.54 and 88.97 MeV. The relevance of this work stems from the need for a detailed understanding of the physical nature of the Doppler broadening of γ-lines, on which the accuracy of online monitoring of the Bragg peak position in proton beam therapy depends. To determine the differential cross-sections, angular distributions and to calculate the angular p–γ correlations between the scattered proton and the emitted γ-photon, the authors used the TALYS 1.8 code. The differential cross-sections for inelastic scattering calculated using TALYS served as input data for a model describing the anisotropy of the emission and explaining the shape of the spectral lines. It has been established that TALYS correctly describes the kinematics of the recoil nuclei, which directly determines the Doppler broadening of the 4.44 MeV line. Simulations carried out using TALYS data have demonstrated good agreement with the experimental spectra in the 90…150° angle range. This confirms the reliability, suitability and adequacy of the code for describing the differential cross-sections of the interaction of intermediate-energy protons with carbon nuclei. Study [18] shows that the use of TALYS plays an important role not only in calculating integral cross-sections, but also in the detailed modelling of microscopic reaction characteristics, such as angular distributions. This fact is of fundamental importance for the development of precision detector systems in medical physics, where the shape of γ-lines serves as a marker of proton energy directly within biological tissues.

The article [19] presents the results of a detailed study of inelastic scattering of protons and neutrons on ^{16}O and ^{28}Si nuclei. The aim of the work is to measure the cross-sections for the production of discrete γ-lines, in particular the 6.129 MeV line for the ^{16}O nucleus, and to verify the concept of isospin symmetry in order to derive neutron cross-sections from proton data. This work is of significant importance for reactor physics and astrophysics. The work presents a detailed comparison of experimental data with calculations using the TALYS 1.9 code.

Calculations performed using TALYS have shown that, for light nuclei (in particular ^{16}O), inelastic scattering at low energies (E < 20 MeV) is governed by competition between direct excitation and compound nucleus formation. It was shown that the use of the Koning–Delaroche global optical potential does not allow for a detailed description of the experimental data on oxygen. For correct modelling using TALYS, the need to take into account deformation parameters for the first excited states using the coupled-channel method is emphasised. Unlike heavy nuclei, for which TALYS provides a satisfactory agreement with experiment, for the ^{16}O nucleus the Hauser–Feshbach model provides only an average description, completely ignoring the resonant structure that dominates the cross-section at E < 15…20 MeV. This study shows that TALYS is an effective tool for describing general energy dependencies and macroscopic cross-sections, but has fundamental limitations when modelling the microscopic resonance picture of light nuclei. This once again highlights the need to apply individual settings for the code's input parameters for each nucleus, rather than using their default values.

5. DISCUSSION

As can be seen from the previous sections, the application of the TALYS code is not limited to classical studies in nuclear physics. It is an important scientific tool that allows for the modification of input parameter settings and the conduct of in-depth analysis. In [10], modifications to the standard settings – in particular the deformation parameters – helped to achieve a high degree of agreement between the theoretical prediction and the experimental data. In the study [7], an additional correction to the default settings of the TALYS code was also carried out: optimal agreement between the experimental data and the calculation was achieved after modifying the model implemented in the code. Furthermore, the TALYS code can be used to review previously obtained experimental data.

The essay [20] examines a re-evaluation of experimental data on the interaction of protons with an energy of E_p = 50 MeV with the nuclei ^{12}C, ^{14}N, and ^{16}O, which were obtained using the nuclear photogelatin method. Using the TALYS 1.96 code, a comprehensive theoretical analysis of these interactions was carried out, and it was shown that the statistical models incorporated into the code generally describe the reaction channels under investigation satisfactorily. In particular, calculations using the TALYS code made it possible to identify the contribution of the ^{8}B and ^{9}B intermediate resonances to the reactions. It should be noted that this code can serve as a theoretical basis for experimental studies, as demonstrated in publication [4], where TALYS was used for the theoretical analysis of excitation functions. At the same time, the TALYS code can be considered the optimal tool for problems in medical physics. In the

article [21], in addition to TALYS, the EMPIRE v3.2.2, INCL++ v5.2.9 and ALICE/ASH programmes were used. The aim of this work is to assess the secondary radioactive background and the yield of secondary particles (in particular protons) arising during proton therapy from the interaction of the beam with equipment components, air and the patient's biological tissues. It is shown that TALYS demonstrates better agreement with experimental cross-sections for light nuclei compared with EMPIRE and ALICE, particularly in the low- and intermediate-energy ranges.

CONCLUSIONS

A comprehensive analysis of the body of scientific literature on the use of TALYS for light nuclei allows the following main conclusions to be drawn.

Predictive capability and validation: TALYS demonstrates a significant advantage over standard hadron interaction modules in Monte Carlo transport codes (GEANT4, MCNP6). It provides an accurate reproduction of cross-sections for the dominant isotope production channels (e.g. ^{11}C), which reduces the uncertainty in clinical dosimetry to < 2%. However, for specific 'exclusive' reactions (such as $^{12}C\,(p,\,n)^{12}N$), the code requires careful calibration of pre-equilibrium parameters.

Limitations of the default settings: The global phenomenological models (in particular, the Koning–Delaroche optical potential) incorporated in TALYS by default are optimised for medium and heavy nuclei. For light systems ($A \leq 16$), they systematically underestimate the direct mechanism of collective state excitation. This leads to discrepancies of a factor of 2–3 when calculating the γ-line yield without manual correction of the deformation parameters (β_L).

Resonance structure and low energies: The statistical approach (the Hauser–Feshbach formalism) in TALYS, by its very nature, ignores the individual resonance structure of light nuclei, which dominates at energies E_p < 20 MeV. For astrophysical problems involving the CNO cycle, this limits TALYS to being a tool for assessing general trends only, whereas a combination of TALYS with the R-matrix method or resonance parameters is required for the precise calculation of reaction rates.

Revision and generative role: The code has proved critically effective in re-evaluating outdated experimental data (for example, photochemical measurements from the 1950s), enabling the quantitative account of 'invisible' neutron channels, which account for up to 46% of the inelastic cross-section. TALYS also remains the primary source of estimated data for new radioisotopes in the 100…200 MeV range.

Methodological recommendation: To achieve the required accuracy when working with ^{12}C, ^{14}N, and ^{16}O, it is necessary to use a modified version of the TALYS code ('Modified TALYS'), which allows global potentials to be replaced with local, specific ones (e.g. Young/ Medland), the activation of the bound-channel method for low-lying levels, and the incorporation of phenomenological deformation parameters from the RIPL-3 database.

The examples of work given above demonstrate that the TALYS computational code is currently an effective tool in research into nuclear physics and its practical applications, capable of meeting modern scientific requirements.

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ТЕОРЕТИЧНИЙ АНАЛІЗ ТА МОДЕЛЮВАННЯ ПРОТОН-ЯДЕРНИХ ВЗАЄМОДІЙ НА ЛЕГКИХ ЯДРАХ ЗА ДОПОМОГОЮ КОДУ TALYS

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Представлено структурований огляд можливостей та доцільності використання коду ядерних реакцій TALYS для моделювання протон-ядерних взаємодій на легких ядрах (^{12}C, ^{14}N, ^{16}O). Проаналізовано масив наукових публікацій, що охоплюють фундаментальні питання нуклеосинтезу (CNO-цикл), задачі космохімії, а також прикладні аспекти ядерної медицини, включаючи ПЕТ-діагностику та онлайн-моніторинг пробігу пучка в протонній терапії. Особливу увагу приділено порівнянню результатів TALYS з експериментальними даними бібліотеки EXFOR та оціненими файлами ENDF/JENDL. Встановлено, що TALYS є потужним інструментом для розрахунку повних перерізів та спектрів вторинних частинок, проте його ефективність для легких ядер критично залежить від ручної модифікації параметрів деформації та оптичних потенціалів. Визначено межі застосування коду в резонансній області та при енергіях понад 100 МеВ.