Theoretical Investigation of ⁶⁴Cu Production in a *p*- induced reaction: Medical and Industrial Perspectives*

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Copper-64 (⁶⁴Cu) is an emerging theranostic radionuclide, valued for its dual decay pathways $(\beta^+: 17.4\%, \beta^-: 38.5\%, \text{ and } e^-\text{-capture: } 44.1\%)$ and a half-life of 12.7 hours, making it suitable for both positron emission tomography (PET) imaging and targeted radiotherapy. This study presents a theoretical evaluation of ⁶⁴Cu production using three nuclear reaction simulation codes, PACE4 [1], EMPIRE-3.2.2 [2,3], and TALYS-1.96 [4], focusing primarily on the 64 Ni $(p, n)^{64}$ Cu [5,6] reaction channel. These have been employed to decipher the reaction mechanism and check the predictive ability of underlying theoretical models. EMPIRE-3.2.2, a modular code system incorporating various nuclear reaction models, including the optical model, pre-equilibrium exciton model, and Hauser-Feshbach statistical approach with width fluctuation corrections, was employed to evaluate proton-induced reaction channels on enriched ⁶⁴Ni. TALYS-1.96, a versatile code based on the Hauser-Feshbach statistical model, was used to compute excitation functions, reaction cross-sections, and yield predictions across a wide range of proton energies. PACE4, employing a Monte Carlo approach within the framework of the compound nucleus formation and de-excitation, provided corroborative data on reaction dynamics and residual nucleus formation. The modeling outcomes identified the optimal proton energy window (10-15 MeV) for maximizing ⁶⁴Cu yield while minimizing co-production of contaminants such as ⁶¹Cu and ⁶⁷Cu. The yield of ⁶⁴Cu at different projectile energies and the thick-target yield in the optimum energy range have also been determined through theoretical modeling. Results from all three codes were benchmarked against available experimental datasets to validate model reliability. These theoretical insights are crucial for guiding experimental production using medium-energy medical cyclotrons and for improving target design and recovery strategies.

In terms of application, ⁶⁴Cu-labeled radiopharmaceuticals such as ⁶⁴Cu-DOTATATE [7] and ⁶⁴Cu-ATSM [8] have demonstrated significant clinical value in oncology for imaging neuroendocrine tumors, hypoxic tissues, and for theranostic use in personalized treatment planning. Industrially, ⁶⁴Cu serves as a reliable radiotracer in metallurgical process monitoring, corrosion studies, and fluid dynamic modeling due to its manageable half-life and detectability. The integration of advanced nuclear reaction modeling with practical radiochemical applications underscores the interdisciplinary importance of ⁶⁴Cu and supports its broader adoption in both healthcare and industry. This convergence of theoretical nuclear physics, radiochemistry, and applied science underscores the growing importance of ⁶⁴Cu and supports its continued expansion as a cornerstone radionuclide in the evolving landscape of theranostics and radiotracing technologies.

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