

# Optical Model Tuning Studies for Optimized Medical Isotope Production

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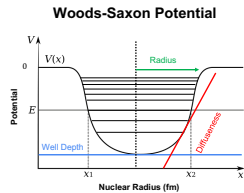
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## Motivation

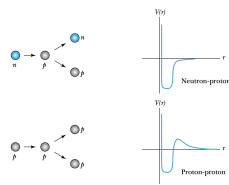
The demand for medical radionuclides has increased significantly over the past decade, primarily due to their success in targeted theranostic cancer applications<sup>12</sup>. Therefore, knowledge regarding the methods to produce such isotopes is vital to aid in the success of the fight against cancer. Cross section data is a key component for informed production choices. However, this data is usually limited or non-existent for novel isotopes. Nuclear reaction modeling codes can predict cross section information but tend to break down for complex reactions involving heavy nuclei targets or light ion incident particles. For this reason, improvement of nuclear reaction model parameters are required to determine the most effective manner in which to produce medical isotopes. To this end we have explored the effect of optical model parameter tuning on cross section prediction using the EMPIRE<sup>1</sup> nuclear modeling program.

## What is an Optical Model?

- Due to the attractive nuclear strong force, each proton or neutron existing in the nucleus acts on all surrounding nucleons with an individual potential<sup>7</sup>
- The optical model (OM) simplifies this complicated many body problem by modeling the nucleus as a **mean potential** of all nucleons<sup>6</sup>
- This mean potential describes how an incident particle will interact with the nucleus and ultimately how nucleons will be scattered out of the nucleus
- The most generalized OM is the Woods-Saxon potential<sup>9</sup>
- Nuclear reaction codes use parameterizations of the Woods-Saxon potential based on available experimental data<sup>11</sup>
- When little or no data exists, these parameters must be tuned to result in accurate cross section predictions



$$V(r) = -\frac{V_0}{1 + \exp((r - R)/D)}$$



## Methods

- Modeled proton and <sup>4</sup>He induced reactions with EMPIRE<sup>1</sup>
- Chose reactions with limited or no experimental data and high disagreement with other codes (TALYS<sup>2</sup>, PACE<sup>3</sup>)
- Investigated effects of manual OM parameter tuning
- Adjusted three separate parameters of real and imaginary Woods-Saxon OM:
  1. **Radius**
  2. **Diffuseness**
  3. **Depth**
- Created custom python script for rapid output of OM change effect on cross sections
- Goal: minimize disagreement with experimental data or PACE predicted cross sections where no data existed

### Reactions Modeled (EMPIRE):

<sup>156</sup>Gd(p, 2n)<sup>155</sup>Tb  
<sup>157</sup>Gd(p, 3n)<sup>155</sup>Tb  
<sup>111</sup>Cd(p, n)<sup>111</sup>In  
<sup>44</sup>Ca(p, 2n)<sup>43</sup>Sc  
<sup>153</sup>Eu(<sup>4</sup>He, 2n)<sup>155</sup>Tb  
<sup>209</sup>Bi(<sup>4</sup>He, 2n)<sup>211</sup>At

### OM Parameterization:

A.J. Koning, J.P. Delaroche<sup>4</sup> – RIPL OMP Index: 5405

- The parameterization equations for the real and imaginary depths are given below:

$$V_V(E) = v_1[1 - v_2(E - E_f) + v_3(E - E_f)^2 - v_4(E - E_f)^3]$$

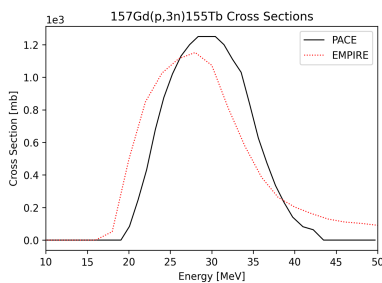
$$W_V(E) = w_1 \frac{(E - E_f)^2}{(E - E_f)^2 + (w_2)^2}$$

$$E_f^p = -\frac{1}{2}[S_p(Z, N) + S_p(Z + 1, N)],$$

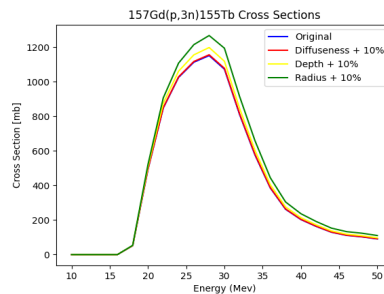
- $S_p$  = proton separation energy
- Radius and Diffuseness are constants determined during their study

## Results

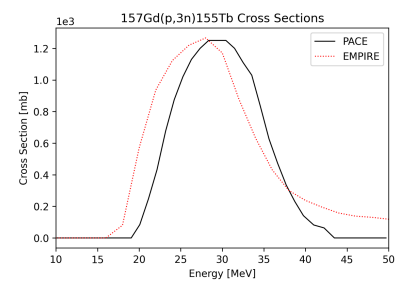
Case Study: <sup>157</sup>Gd(p, 3n)<sup>155</sup>Tb



### Individual Parameter Tuning Effects



### Example of Manually Optimized Parameters



## Conclusions

### For proton induced reactions studied:

- OM diffuseness produces the least effect on cross section prediction
- OM radius has greatest impact on cross section prediction
- OM depth has low effect at lower energy but becomes more effective at high incident energy

### For <sup>4</sup>He induced reactions studied:

- Inconclusive results due to added complexity of heavier incident nucleus
- More methodical testing protocol needed

### Future work

- Extend manual optimization method to automatic chi-squared regression fitting protocol to achieve better cross section fits
- Explore optimization methods for level density, gamma strength functions in addition to OM
- More experimental cross section data needed to validate OM parameters and increase accuracy of cross section predictions

## References

1. M. Herman, R. Capote, B. Carlson, P. Obložinský, M. Sin, A. Trkov, H. Wienke, and V. Zerkin. EMPIRE: nuclear reaction model code system for data evaluation. Nuclear data sheets, 108(12):2655–2715, 2007.
2. A. J. Koning, S. Hilaire, and M. C. Duivestijn. TALYS: Comprehensive nuclear reaction modelling. In AIP Conference Proceedings, volume 769, pages 1154–1159. American Institute of Physics, 2005.
3. O. Tarasov and D. Bazin. Development of the program LISE: application to fusion–evaporation. Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms, 204:174–178, 2003.
4. A. Koning and J. Delaroche. Local and global nucleon optical models from 1 keV to 200 MeV. Nuclear Physics A, 713(3):231–310, 2003.
5. R. Capote, M. Herman, et al. RIPL – reference input parameter library for calculation of nuclear reactions and nuclear data evaluations. Nuclear Data Sheets, 110(12):3107–3214, 2009.
6. K. S. Krane. Introductory nuclear physics. John Wiley & Sons, 1991.
7. R. D. Evans and R. Evans. The atomic nucleus, volume 562. McGraw-Hill New York, 1955.
8. Thornton, Stephen T., and Andrew Rex. Modern physics for scientists and engineers. Cengage Learning, 2012.
9. P. E. Hodgson. The nuclear optical model. Reports on Progress in Physics, 34(2):765, 1971.
10. P. E. Hodgson. Compound nucleus reactions. Reports on Progress in Physics, 50:1171, 1987.
11. S. Hilaire. Statistical nuclear reactions. IAEA: N. p., 2001.
12. L. A. Bernstein, D. A. Brown, A. J. Koning, et al. Our future nuclear data needs. Annual Review of Nuclear and Particle Science, 69:109–136, 2019.