Validation of Multi-Physics Coupling to Model a RbCl-RbCl-Ga Target Stack

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Introduction

• Targets at LANL’s Isotope Production Facility are irradiated with 100 MeV protons for large scale isotope production.
• The purpose of this study is to use computational tools to:
  – Obtain an accurate picture of isotope production target behavior during nominal power operating conditions.
  – Determine impact of target melting on heat transfer, transmitted energy, production rate distributions, and net yield.
• RbCl is used for the production of 82Sr (t1/2 = 25.4d). Its daughter, 82Rb (t1/2=1.3min), is used in diagnostic PET imaging.
• Monte-Carlo N-Particle (MCNP) – radiation transport code.[2]

Multi-Physics Coupling Approach

• FORTRAN is used for the iterative scripting between MCNP and ANSYS CFX.
• MATLAB is used to translate between the drastically different meshes used by CFX and MCNP.[3]
• A time-dependent simulation must be utilized to model fluid motion as progressive phase change in the partially molten RbCl salt target prevents the establishment of a true steady-state solution.[4]

Target Geometry

• The purpose of this study is to use computational tools to:
  – Obtain an accurate picture of isotope production target behavior during nominal power operating conditions.
  – Determine impact of target melting on heat transfer, transmitted energy, production rate distributions, and net yield.
• Because the targets melt during irradiation, the RbCl A- and B-slot targets are encapsulated in inconel and the Ga C-slot target is encapsulated in Nb.
• Understanding upstream target behavior is critical as downstream targets are highly sensitive to energy.

Meshing in ANSYS and MCNP

• MCNP – User created with surface definitions using a series of radial, axial, and angular planes to divide the domain into cells for which a unique density may be assigned. Captures density variation obtained in ANSYS CFX over target domain in MCNP.
• ANSYS – User interfaced meshing tool.
  – Meshing divides the domain into small cells in which equations used to model fluid flow and heat transfer may be solved.
• System of linearized equations.
• Problem symmetry is utilized.

Yield and Production Rate Calculations

• Net yield and production rates – Quantifiable means of comparing computational results to experimental data.
• Reaction of interest: 31MeVnRbCl→82SrGe
• Estimated energy ranges of interest:
  – Target A: 93–70 MeV
  – Target B: 65–40 MeV
• Cross-section data is taken from tabulated values given in the IAEA database.[5]
• All calculations are performed in MCNP.
  – Upstream density distributions impact particle energies streaming through the target.
  – Axial shift in production at top and bottom of the target.
  – Production Activity[6]:
    - Production activity = \( \frac{1}{\lambda} \ln(1 - e^{-\lambda t}) \)
    - Source intensity: \( I_{\text{source}} \)
  – Irradiation time: \( t \)

Results and Conclusions

Table I. Heat deposition in target bodies.

<table>
<thead>
<tr>
<th>Target Domain</th>
<th>Heat Deposition (W)</th>
</tr>
</thead>
<tbody>
<tr>
<td>In10B Window</td>
<td>0.353</td>
</tr>
<tr>
<td>RbCl Target A</td>
<td>4.7256</td>
</tr>
<tr>
<td>In625 Capsule A</td>
<td>0.7019</td>
</tr>
<tr>
<td>RbCl Target B</td>
<td>4.9137</td>
</tr>
<tr>
<td>In625 Capsule B</td>
<td>0.9582</td>
</tr>
<tr>
<td>Nibolium Capsule C</td>
<td>5.0648</td>
</tr>
</tbody>
</table>

Table II. Target incident and exiting energies and predicted yield ratios.

<table>
<thead>
<tr>
<th>Parameters</th>
<th>RbCl Target A</th>
<th>RbCl Target B</th>
</tr>
</thead>
<tbody>
<tr>
<td>Target Incident Energy (MeV)</td>
<td>90.832</td>
<td>70.389</td>
</tr>
<tr>
<td>Target Exiting Energy (MeV)</td>
<td>61.949</td>
<td>39.812</td>
</tr>
<tr>
<td>Yield Ratio</td>
<td>0.962</td>
<td>0.948</td>
</tr>
</tbody>
</table>

• The given \( E_{\text{in}} \) and \( E_{\text{out}} \) are the energies incident upon and exiting the target faces as predicted in MCNP.
• Previously predicted LANL values and present MCNP predictions are within – 4 – 5% of one another.
  – Further investigation into discrepancies will be performed.
• As the excitation function in RbCl Target A is less structured over the energy range, production rates are more similar at the top and bottom of the target.
• Peak linear production occurs deeper into RbCl Target B at the top of the target due to the transmitted energy spectrum distribution resulting from compounded effects of upstream density gradients.
• Capturing density gradients in each target is essential for determining the transmitted energy distribution and regions of highest production.

Future Work

• After axial and radial mesh resolution non-uniformly in MCNP to appropriately capture phase transition in the targets.
• Refine mesh in cooling water domain.
  – Simplify cooling water domain down to only cooling channels, with highly accurate inlet and outlet conditions.
• Perform iterative multi-physics coupling with refined MCNP target and ANSYS CFX cooling water mesh to obtain a new quasi-steady-state solution.
• Model Ni foils on front face of C-slot target to obtain a distribution of incident particle energies.
  – Compare computational results for isotopic ratios to experimental data.