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 ^{82}Sr ($t_{1/2}$ = 25.4d). Its daughter, ^{82}Rb ($t_{1/2}$=1.3min), is used in PET scans for cardiac perfusion studies.
- Gallium produces ^{68}Ge. Its daughter, ^{68}Ga ($t_{1/2}$=68min), is used in diagnostic PET imaging.
- **Simulation Tools**
  - ANSYS CFX – computational fluid dynamics (CFD) simulation software.[1]
  - Monte-Carlo N-Particle (MCNP) – radiation transport code.[2]

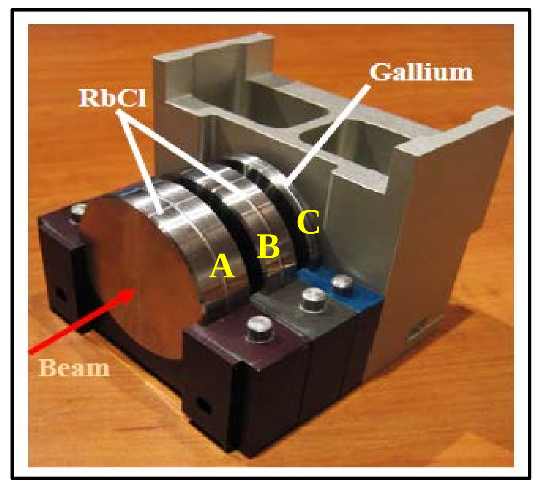
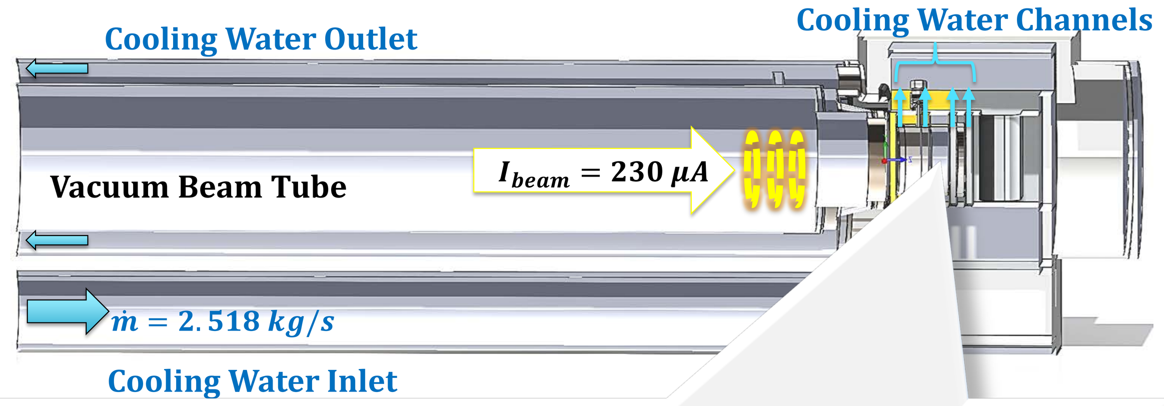


Figure 1. Routine target stack configuration at Los Alamos National Laboratory's Isotope Production Facility.

Target Geometry

Figure 2. Cross-sectional view of target geometry with appropriate boundary conditions.



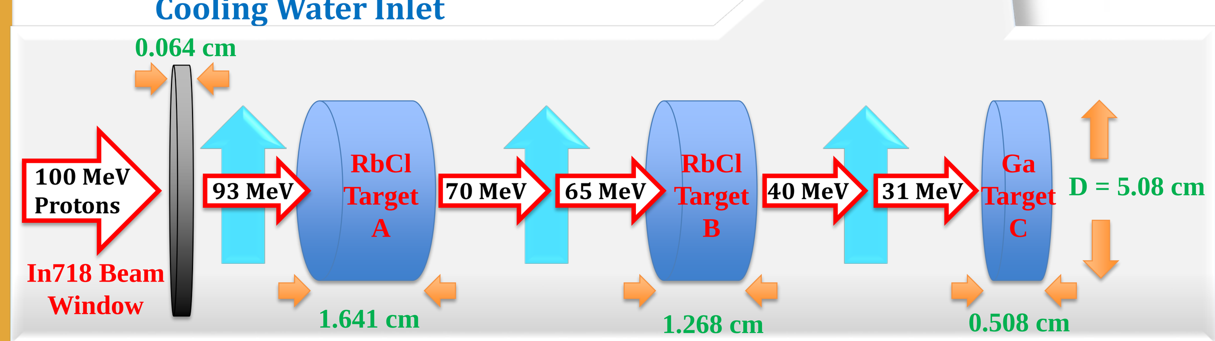


Figure 3. Cut-out of target capsules with dimensions and average incident and exiting energies crossing target faces.

- 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

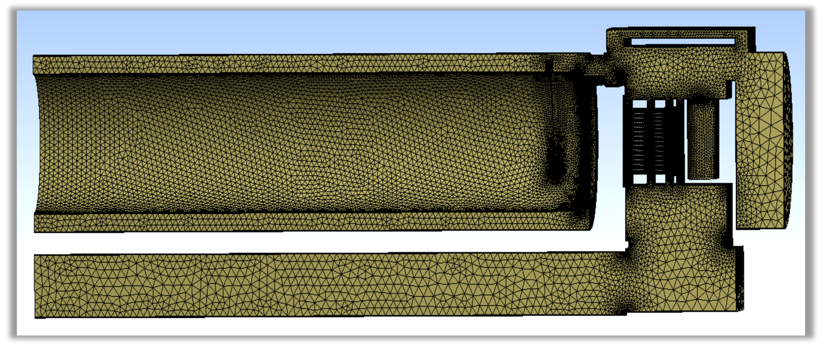


Figure 4. Cross-sectional image of full model mesh including cooling water domain.

- **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.
- **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.

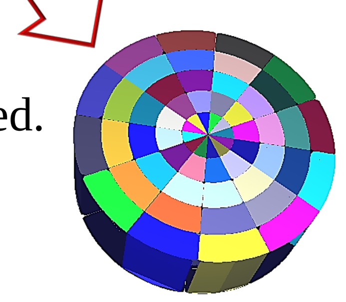


Figure 5. Simplified version of MCNP mesh for RbCl Target A with defined radial, angular, and axial planes.

References
[1] ANSYS CFX version 17.0.
[2] MCNPX User's Manual v. 2.7.0. Distributed by Los Alamos National Laboratory.
[3] MATLAB version R2016a.
[4] J.L. Peeples, M. Magerl, E.M. O'Brien, J.M. Doster, I.A. Bolotnov, B.W. Wieland, M.H. Stokely, 2016, "High Current C-11 Gas Target Design and Optimization Using Multi-Physics Coupling", in *16th Proceedings of Workshop on Targetry and Target Chemistry*, (Santa Fe, N.M., US, 2016).
[5] IAEA database: https://www-nds.iaea.org/medical/rbp82sr0.html.
[6] N. Otuka, S. Takács: Definitions of radioisotope thick target yields. *Radiochim. Acta* **103**, 1-6, (2015).

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]

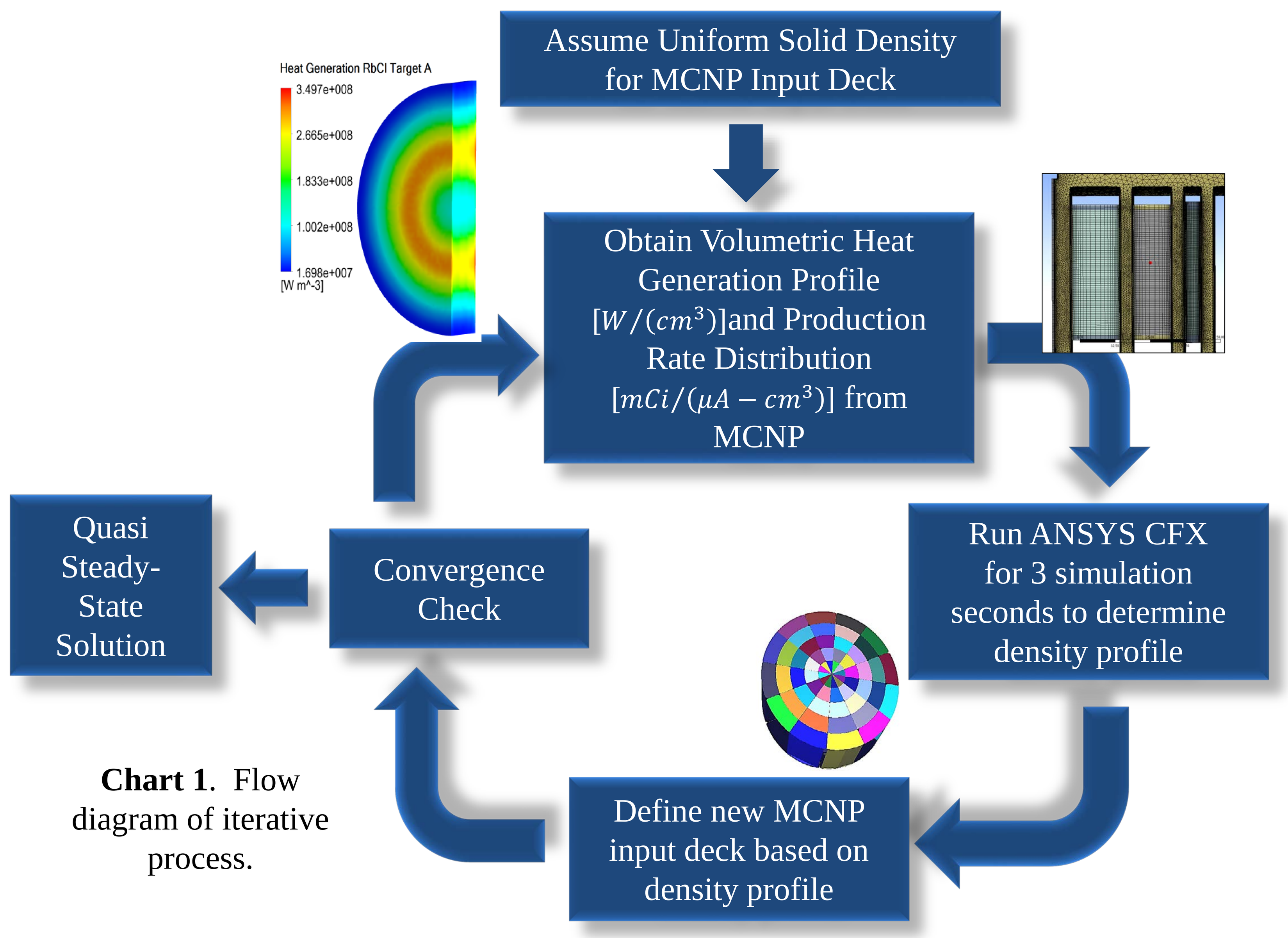


Chart 1. Flow diagram of iterative process.

Yield and Production Rate Calculations

- Net yield and production rates – Quantifiable means of comparing computational results to experimental data.
- Reaction of interest: ^{nat}Rb(p,xn)^{82}Sr.
- 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]:
  - $A(t_{irr})[Ci]$ =
    - $A_{sat}\left[\frac{mCi}{\mu A}\right] \cdot I_{beam}[\mu A] \cdot (1 - e^{-\lambda t_{irr}})$
    - $A_{physical}\left[\frac{\mu Ci}{\mu A \cdot hr}\right] \cdot I_{beam}\,[\mu A] \cdot \frac{(1-e^{-\lambda t_{irr}})}{\lambda}$
- Source Intensity: $I_{beam} = \left[\frac{particles}{sec}\right]$
- Irradiation time: t_{irr}

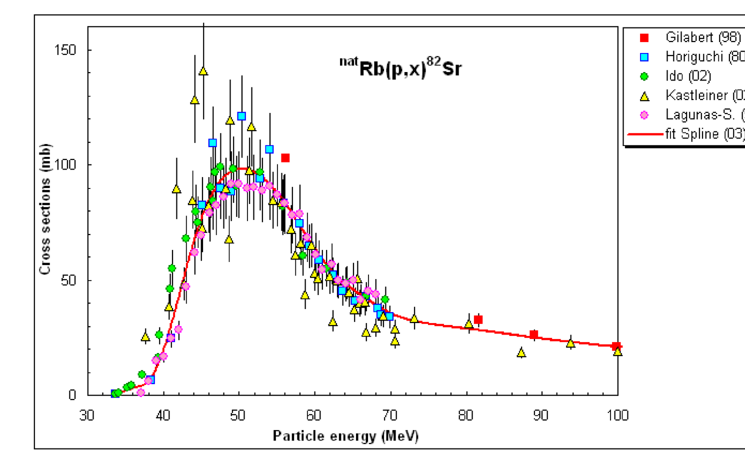


Figure 6. IAEA database cross-section data used for all yield and production rate calculations in MCNP.[5]

- Reaction Rate: $R = \int_{\vec{r}} \int_E \phi(E,\vec{r})\Sigma(E) dE\, d\vec{r}$
- Flux: $\phi = \left[\frac{particles}{cm^2 \cdot sec}\right]$
- Macroscopic Cross-Section:
  - $\Sigma = N\sigma$
- Microscopic Cross-Section:
  - $\sigma = [cm^2]$
- Number density: $N = \left[\frac{atoms}{cm^3}\right]$
- Half-life of ^{82}Sr: $t_{1/2} = 25.4\ day$
- Decay Constant: $\lambda = \ln(2)/t_{1/2}$

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- BTI Targetry LLC is acknowledged for assistance in the development of FORTRAN codes.

Results and Conclusions

Table I. Heat deposition in target bodies.

Target Domain	Heat Deposition [kW]
In718 Window	0.353
RbCl Target A	4.7256
In625 Capsule A	0.7019
RbCl Target B	4.9137
In625 Capsule B	0.9582
Ga Target C	5.0648
Niobium Capsule C	0.7240

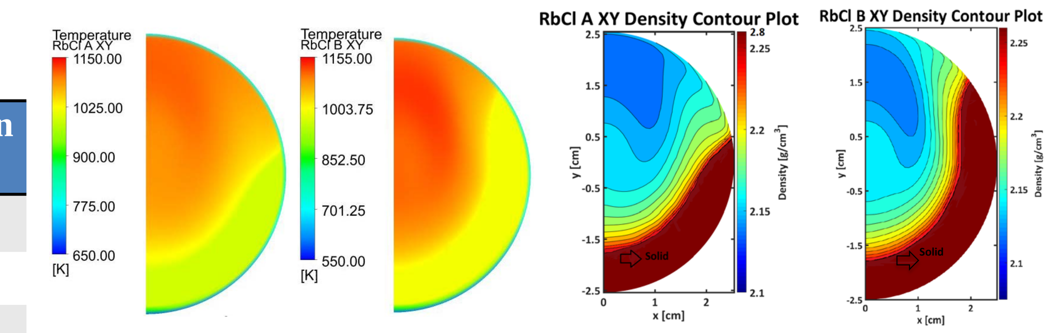

Figure 7. RbCl Targets A and B mid-plane temperature and density distribution profiles for a quasi steady-state solution.

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

Parameters	RbCl Target A	RbCl Target B
E_{in} [MeV]	90.832	70.389
E_{out} [MeV]	61.949	39.812
$\frac{Yield_{MCNP}}{Yield_{LANL}}$	0.962	0.948

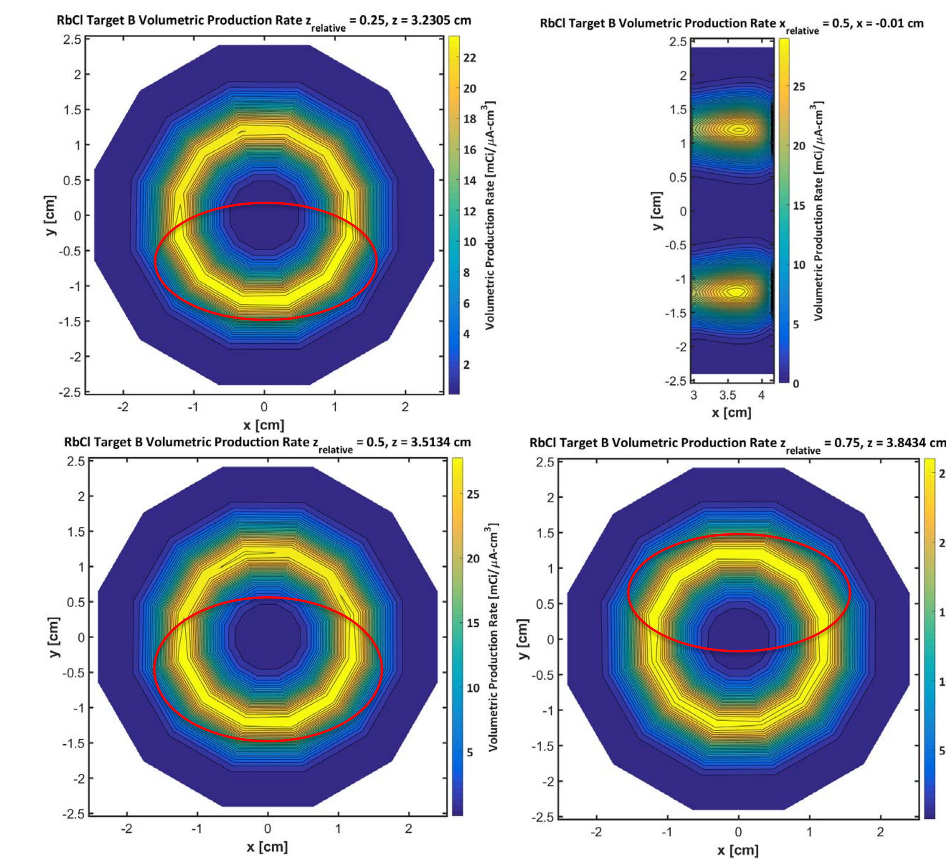

Figure 8. Volumetric production rate distributions at a YZ mid-plane in RbCl Target B and at various axial locations in XY planes with regions of highest production circled in red.

- The given E_{in} and E_{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.

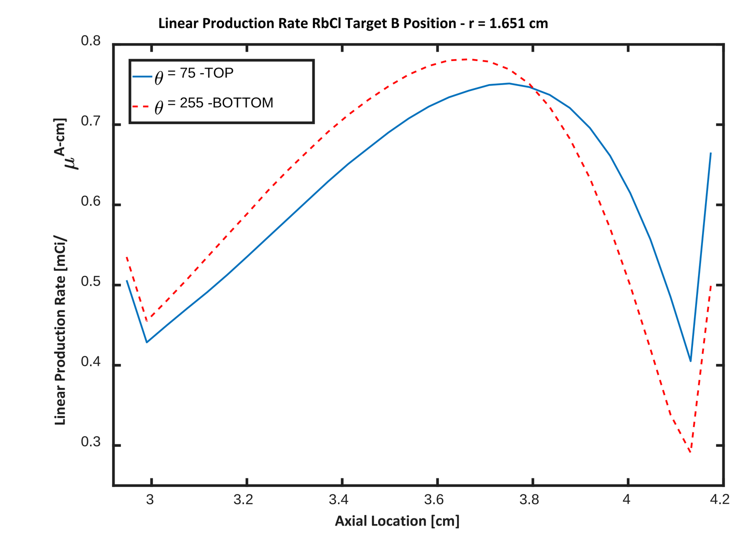

Figure 9. Linear production rate distribution at the top and bottom of RbCl Target B.

- 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

- Alter 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.