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Two-way multi-physics coupling for modeling high power RbCl isotope production targets

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ABSTRACT

This work shows successful first application of two-way multi-physics coupling to model RbCl targets in a three-stacked target configuration used at Los Alamos National Laboratory's (LANL) Isotope Production Facility (IPF). Targets are known to melt at production level beam currents and as in-beam monitoring of the targets in this configuration is not possible, high-fidelity simulation has been utilized to gain insight into target thermal behavior. Thermal hydraulic modeling was performed with ANSYS CFX and particle transport with the Monte Carlo N-Particle (MCNP) code. Multi-physics coupling of these two codes was employed to fully capture the highly coupled nature of the problem physics. Both transient and equilibrium thermal hydraulic results were obtained using this process. The equilibrium thermal hydraulic results were then employed to predict measured ^{82}Sr yields in molten RbCl targets. This technique demonstrates promise as a tool to investigating, understanding, and enhancing high power targetry behavior and limitations.

1. Introduction

RbCl salt targets are often used to produce ^{82}Sr via the ^{nat}Rb (p,xn)^{82}Sr reaction by proton bombardment. The development and design of these targets has been predominantly empirical. Heightened interest in modeling the thermal processes and radiation transport mechanisms at work [1,2] has led to a push in model development to accurately represent radioisotope targetry behavior for different applications.

Phase and density changes seen in targets are known to impact beam penetration and distribution [1,3]. In addition, the incident and exit energy distributions seen in experimental measurements are more complex than those seen in previous predictions assuming uniform average densities. Accurately modeling the thermal behavior of these targets and the corresponding impact on beam behavior will improve understanding of how density variation in upstream targets impacts both incident and exit energy distributions in downstream targets.

Strong coupling between density and heat deposition impacts proton energy loss along the beam track, affecting radionuclide yields and target design. Thus, multi-physics coupling of the energy deposition and density distribution within a target medium is necessary to accurately capture the effects of a proton beam impinging upon a target.

2. Target geometry and materials

At the Los Alamos Isotope Production Facility (IPF) ^{82}Sr and ^{68}Ge are routinely produced in a configuration which consists of two inconel-encapsulated RbCl salt targets and one niobium-encapsulated gallium target separated by water cooling channels. This target stack configuration is shown in Fig. 1.

The three targets (RbCl, RbCl, Ga) depicted in Fig. 1 are housed in aluminum holders and are labelled as the A, B, and C slot targets corresponding to their order in the target stack. Target encapsulation is necessary as these targets are at least partially molten during irradiation.

All targets have a radius of 2.49 cm. The targets are progressively thinner as per their order in the target stack, ranging from 1.6 cm to 0.5 cm in thickness. The front and back target capsule faces are thinner than the radial face as these are the surfaces through which the beam passes. A scale is included in Fig. 1 to provide an idea of target size.

Cooling water flows between the targets through four 50 cm long rectangular channels each 0.5 cm in width. The net mass flow rate for the entire cooling water system is 2.52 kg/s, resulting in an average channel velocity of 2.45 m/s.

Protons with 100 MeV energy strike an upstream inconel beam window (not depicted) prior to entering the target stack as indicated in

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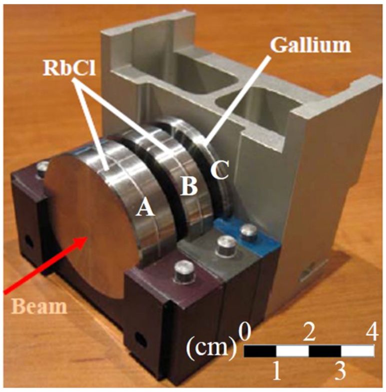

Fig. 1. Target stack geometry configuration in use at IPF.

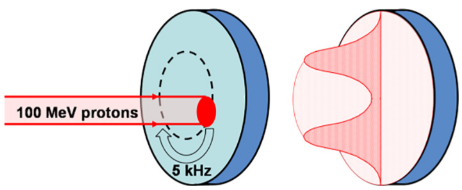

Fig. 2. Beam distribution [4].

Fig. 1. This beam window separates the beamline vacuum from the targets and the cooling water. The beam pulses at a rate of 120 Hz, delivering 100 pulses per second to the target stack with every sixth pulse sent to a downstream facility. This beam sweeps around the target at a rate of 5 kHz, creating a ring shaped profile with a radius of 1.27 cm as depicted below in Fig. 2.

The average operating temperature of RbCl targets ranges from ~1100 to 1250 K. Given this range and given an expected average temperature rise of ~5 to 8 K per beam pulse, temperature oscillations due to the beam time structure are less than ~0.5%.

In addition, given that the gate length of each pulse is 625 μs and the thermodynamic time response of the system is on the order of tenths of a second, it is clear that thermal time scale is significantly slower than the beam pulse frequency.

Therefore assuming an effective continuous beam current equal to the average nominal beam current of 230 μA introduced minimal error.

3. Multi-physics coupling methodology and tools

Thermal hydraulic modeling, including computational fluid dynamics (CFD) and heat transfer, was performed with the commercial ANSYS CFX version 18.1 package [5] while particle transport was examined with the Monte Carlo N-Particle (MCNP) version 6.1.1 package [6].

This work employs a very similar iterative methodology to that applied at CERN using FLUKA for particle transport and BIG2 for thermodynamic simulation of GeV and TeV proton beams incident on cylindrical copper targets [7,8]. However, ANSYS CFX is a 3D CFD code employing Eulerian methods while BIG2 is a 2D numerical simulation software employing Lagrangian methods and moving grids more applicable to high-velocity impact problems [9]. The use of ANSYS CFX is ideal for scenarios in which 3D thermodynamic behavior becomes important, as is the case for the target stack configuration at LANL's IPF. ANSYS Fluent, another 3D CFD code with capabilities similar to CFX, has been coupled with MCNPX to model the SINQ neutron source at PSI, though without performing any iteration [10].

3.1. Thermal hydraulic modeling

The system geometry as defined in ANSYS CFX is presented below in

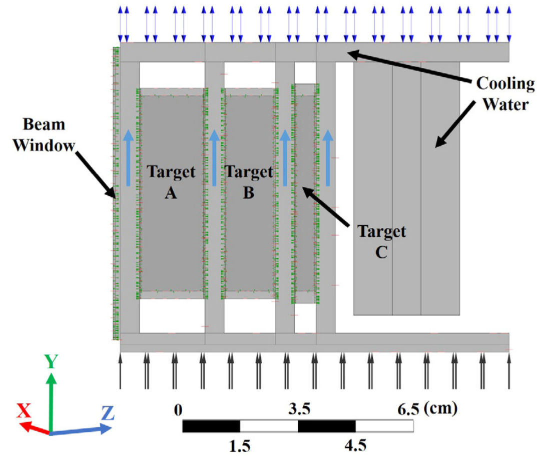

Fig. 3. Geometry in ANSYS CFX with assigned boundary conditions.

Fig. 3. As indicated by the axes, the beam travels in the positive z-direction. The size of the cooling water domain was significantly reduced by including only the four cooling water channels and an arbitrary 0.5 cm distance on either side of the inlet and outlet to the channels. The reduction in the cooling water domain was performed to strike a balance between optimized resolution in the cooling water channels and total problem size and run time. In addition, the problem geometry was reduced by a factor of two by slicing the geometry in half along the YZ midplane and applying a symmetry boundary condition.

The static pressure was supplied as a function of position for the inlet boundary condition. An opening type outlet boundary condition was defined with the (u,v,w) velocity components as a function of position. The converged hydraulic solution of a finely meshed full cooling water domain model with no heat transfer present was used to supply these boundary conditions. The full cooling water domain geometry as defined in ANSYS CFX is provided in Fig. 4.

Discretization of the problem was performed using the meshing tools provided in ANSYS. To ensure that the boundary layers were fully resolved, mesh optimization was performed in the cooling water channels in the vicinity of the target capsule walls. The y^+ value is a dimensionless quantity that is the perpendicular distance from the wall measured in terms of viscous lengths [5,11]. Using a first layer mesh height that provides a y^+ value of one ensures that the boundary layers are fully resolved. Application of boundary layer theory allowed for determination of the wall frictional velocity and desired first layer height of $\Delta y = 7 \times 10^{-3}$ mm. Meshing to this criteria ensured that the first layer height used was fine enough that wall heat transfer and any small scale turbulent effects were captured by the model. The optimized mesh is shown in Fig. 5 with the corresponding mesh statistics given in Table 1.

Orthogonality describes how close the angles between adjacent element faces or edges are to the optimal angle for a specific mesh element and its value should be as close to one as possible. Skewness is a measure of how close a face or cell is to ideal (quadrilateral or equiangular) [5]. This value should be as close to zero as possible.

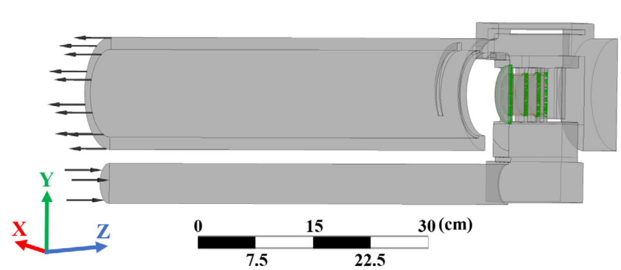

Fig. 4. Full cooling water domain model in ANSYS CFX.