Fermi National Accelerator Laboratory

High Pressure Rinsing of Accelerator Cavities: Computational Fluid Dynamic Simulation

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Abstract

PIP-II is a new system upgrade to the accelerator complex used at Fermilab, with the goal of increasing the energy of particles transported to several experiments. The last two sections of the PIP-II linear accelerator (linac) contain elliptical niobium cavities for particles to pass through and gain energy. During the fabrication process of the cavities, particle contaminants can be introduced and produce electron field emissions, limiting performance. High-Pressure Rinsing (HPR) is the process used to reduce such contaminants by spraying high-pressure, ultra-pure water in the walls of the cavities for hours at a time. In order to better understand and improve the rinsing process, computational fluid dynamics (CFD) can be used. Finding proper settings is a crucial step in creating a meaningful simulation with accuracy and computational ease.

Background

PIP-II

Each segment of PIP-II is cooled to 2 K to provide efficient, high-powered, acceleration. The final two segment types, LB650 and HB650, contain elliptical niobium cavities with a low β and high β respectively. Niobium was selected because it is a superconducting material with desirable mechanical and thermal properties. The iris position of the cavity experiences the highest electric field; therefore, it is potentially the highest field emitting site. While comparatively lower, the wall beginning at the iris and traveling towards the equator may also contribute to electron field emissions, as shown in Figure 1. Constructing the niobium cavities begins at the initial formation of the cavity shapes and includes chemical processing, heat treatments, tuning, and HPR steps. During these steps, chemical residuals and foreign particle contaminants are introduced. Particle contaminants are sources of undesired electron field emitters which limit the performance of the linac. HPR is used to remove the contaminants before the final assembly of the cavity in a cryomodule.

Figure 1. Cross-section for HB650 (left). High-beta niobium cavities (center). Contours of electron field emissions (right).

HPR is performed to remove particle contaminants from the cavity surface. When a cavity is rinsed, ultrapure water with resistivity of 18 MΩ.cm at a rate of 4.17 L/min is sprayed on the interior walls of the cavity. The nozzle head rotates to rinse the cavity moving in a vertical direction. HPR tool is shown in Figure 2. Rinsing takes hours and the cavities are left to air dry. The iris and the wall of the cavity are the locations prone to electron field emissions, so they are the most important areas of the cleaning process. Computational Fluid Dynamics (CFD) can be used to understand how water interacts with impacted surfaces.

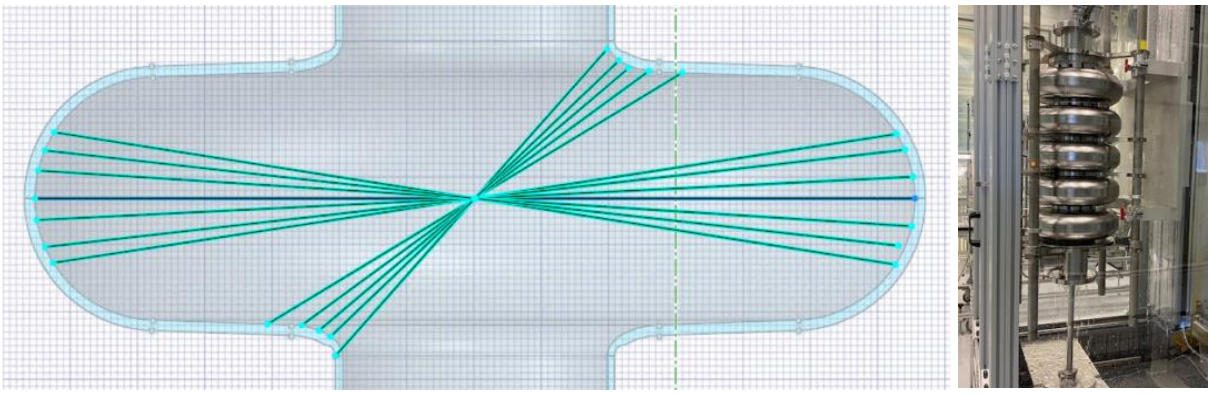

Figure 2. Potential spray pattern (left) and Niobium cavities on rinsing stand (right).

Fluid Calculation

Water jet spray can be separated into a potential core region, a main region, and a diffused-droplet region, as shown in Figure 3 [1]. The potential core region is primarily used in water jet cutting, the main region is used for cleaning or surface finishes, and the diffused droplet region is used for aspirating [2]. Cylindrical-converging nozzles have a constant cross-section beginning at the inlet and have a steep slope near the orifice. Tapered-converging nozzles have a gradual slope from the inlet to the orifice. Stepped nozzles have two constant sections, with a larger inlet section leading to a step down to the orifice section. Each shown in Figure 3. The cylindrical-converging and tapered-converging nozzles have comparatively higher peaks of fluid velocity, while the stepped nozzle is expected to maintain a high fluid velocity with less dependence on distance [2]. The cavity rinsing stand has the spray head fixed along the center line, so a stepped nozzle would allow for a more evenly distributed cleaning without adding a degree of freedom to the station.

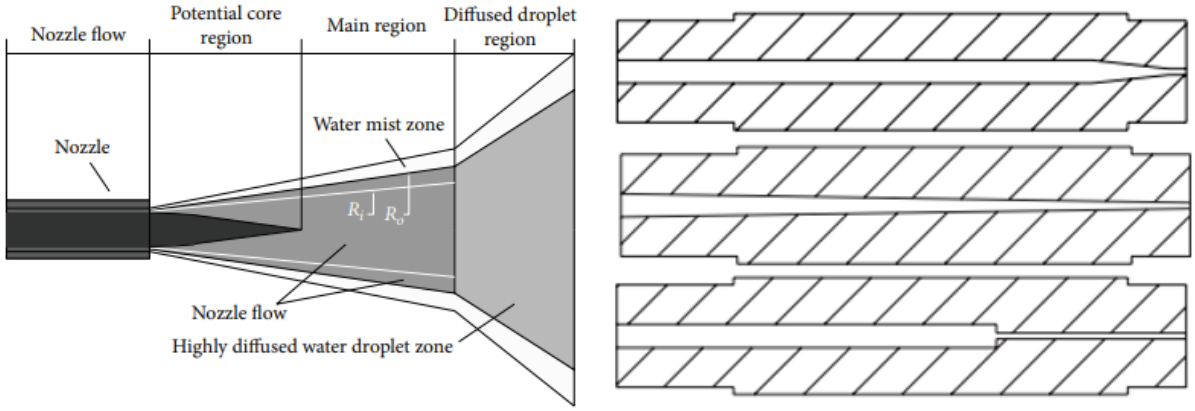

Figure 3. Water jet regions defined by [1] and visual by [2] (left). Cylindrical-converging (top right), tapered-converging (center right), and stepped nozzle (bottom right) [2].

At wall boundaries in CFD code, the software guesses for a shear stress the fluid applies to the wall and calculates for a Y+ value. Then the software iterates until the solution converges. The Y+ value is important for capturing the velocity gradient of the fluid near the wall. For each cell in the mesh, the simulation registers the fluid velocity at the centroid. More cells close to the wall creates more cell centroids for the software to calculate conditions and output datapoints. Increasing the number of datapoints near walls aids in resolving the velocity gradient for the boundary layer [3], depicted in Figure 4. Resolving the viscous sublayer of fluid motion is especially important when calculating shear stress, and a smaller Y+ represents a better resolution of the viscous sublayer [4]. The shear stress calculations are then used to understand how well the nozzle is cleaning the impacted wall.

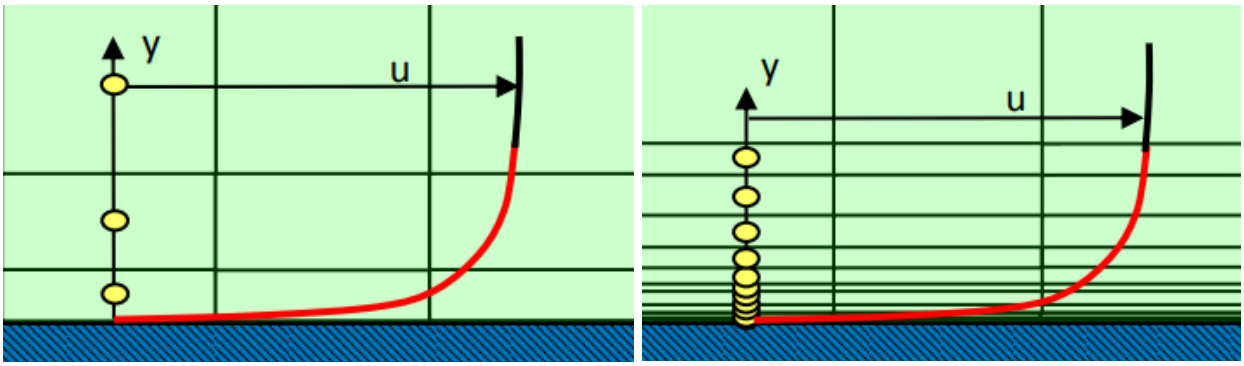

Figure 4. Coarse mesh (left) vs fine mesh (right) to visualizie how inflation layers can better capture fluid boundry layers near a wall, improving Y+. [5]

Setup

Inlet Boundary Condition

From physically collected data, the water upstream from the inlet is set to an operating pressure of 8.62 MPa (1250 psi). Bernoulli's equation and conservation of mass are used to calculate the expected inlet velocity, as shown in the appendix. Ansys Fluent depends on either a defined total pressure or a defined inlet velocity as a boundary condition for converging on a solution. The software will solve for a pressure given a velocity and vice versa. The velocity inlet type was chosen since a user-defined velocity should result in an expected pressure. Another physical data point considered is the volumetric flowrate of the water. The expected volumetric flow rate is 1.1 gal/min (4.17 L/min). Using the known mass flow rate and the geometry of the nozzle, the velocity of the fluid at the inlet can be calculated, as shown in the appendix. While these two methods are expected to confirm each other, the required velocity at the inlet is different. An inlet velocity of 2.8 m/s was chosen because the water pressure will decrease from the location of measurement

and the nozzle inlet, but the mass flow rate will stay constant regardless of losses due to the pipes.

Geometry

To begin simulating with CFD, a straight jet nozzle geometry was chosen. The internal volume of the nozzle was attached to a cylindrical control volume of 75 mm in radius and 100 mm in height. The control volume allowed a volume for water to expand to atmospheric pressure before making impact with the face furthest from the inlet. A straight jet geometry was chosen for its simplicity and to compare with test data, as shown in Figure 5.

Taking advantage of symmetry is valued because it decreases computation requirements. Since the chosen geometry is axisymmetric, the geometry was simplified to a 2D shape. During rinsing, the water flows through pipes before reaching the nozzle, allowing the velocity profile to develop. To simulate the already developed velocity profile, the nozzle was extended by 20mm.

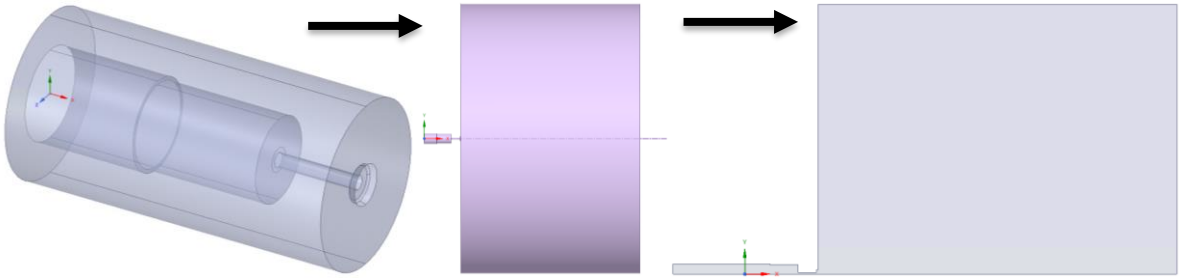

Figure 5.Geometry of a straight jet nozzle (left), 3D internal fluid volume (center), 2D simplification with extended inlet region (right).

Mesh Computational advantages are also found with intelligent meshing. The water is expected to occupy a narrow region of the shape, the mesh can contain larger cells in areas where only air is expected and smaller cells in areas of interest. The critical areas are the central axis, the back wall, and the nozzle. All cells target a quadrilateral shape with a 5% growth rate. The non-critical area targeted an element size of 0.25 mm. The inlet, axis, and impacted wall all targeted an element size of 0.025 mm. Additionally, 10 inflation layers were added to the inlet walls and the impacted wall to improve resolution of the fluid exiting the nozzle orifice and the pressure applied to the wall respectively, as shown in Figure 6. A fine mesh on the wall results in a desired Y^+ value.

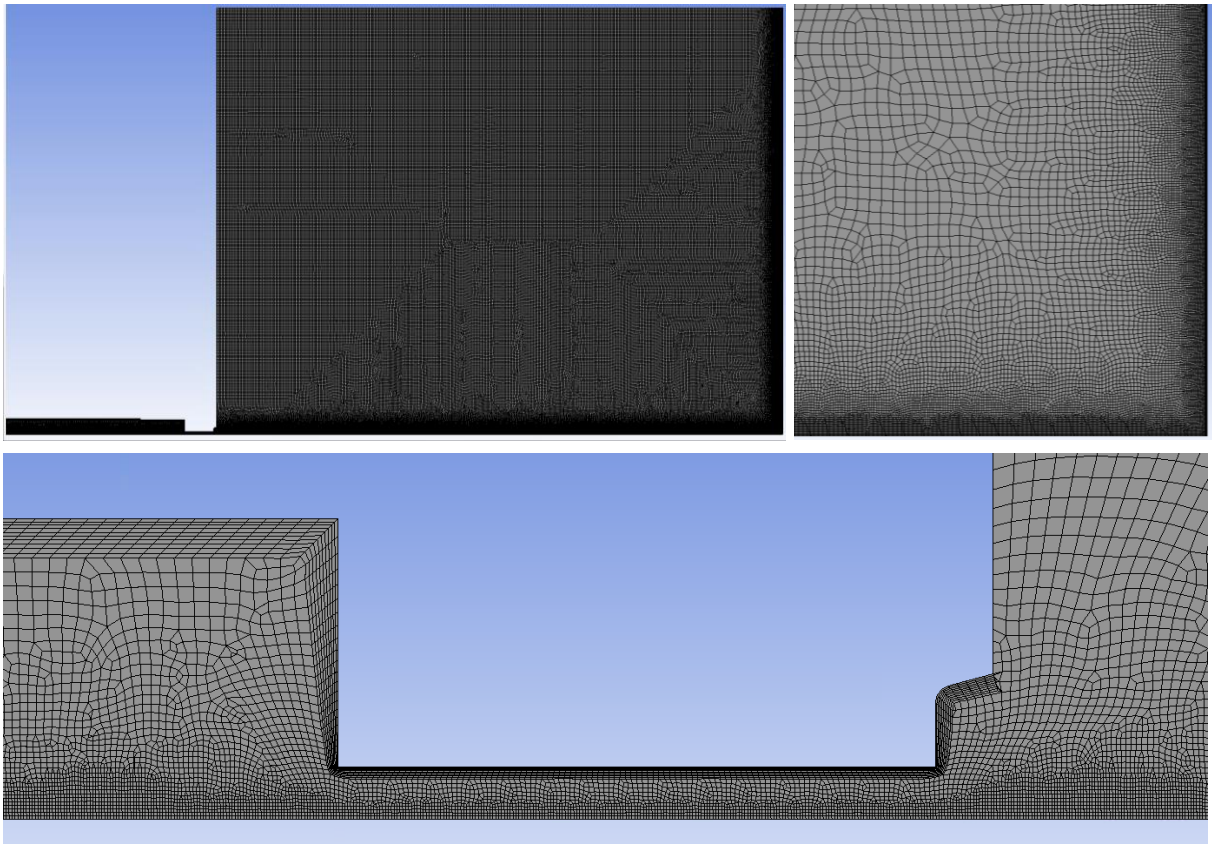

Figure 6. Meshed area (top left). Mesh of the corner between the axis and the impacted wall (top right). Mesh of the nozzle orifice (bottom).

Fluent Settings

In Ansys Fluent, a multiphase simulation can be represented as a volume of fluid (VOF), mixture, wet stream, or the Eulerian models. The Eulerian model is the most complex and computationally most expensive, the momentum equations for each phase, which is for inhomogeneous flows. The wet stream model is optimized for natural fluid flow (rivers, lakes, oceans, etc.). The VOF model is a surface-tracking technique applied to a fixed Eulerian mesh, ideal for tracking of any liquid gas interface (filling, sloshing, flow with large bubbles, and prediction of jet breakup). Lastly, the mixture model is a simplification of the Eulerian model, only one set of momentum equations is solved, and the other phases momentum equations are coupled. [3] The mixture model was chosen, as seen in Figure 7, because the behavior of the water phase is driving the solution and the air behavior is reactive. Ansys also recommended using the mixture model in [4].

The k-epsilon model was chosen for with the enhanced wall treatment option to better resolve the fluid boundary layer near walls, as shown in Figure 7. The Y^+ value in turbulent flows is calculated in one of two methods. The standard method is used when a mesh is too coarse to resolve the boundary layer and standard wall functions attempt to predict the boundary layer based on the free stream dynamics and the

no-slip condition at the wall. The enhanced wall functions method is used when the mesh is fine enough near the wall to resolve the boundary layer and provides a more accurate prediction. The enhanced comparison between these methods is shown in Figure 8. [3]

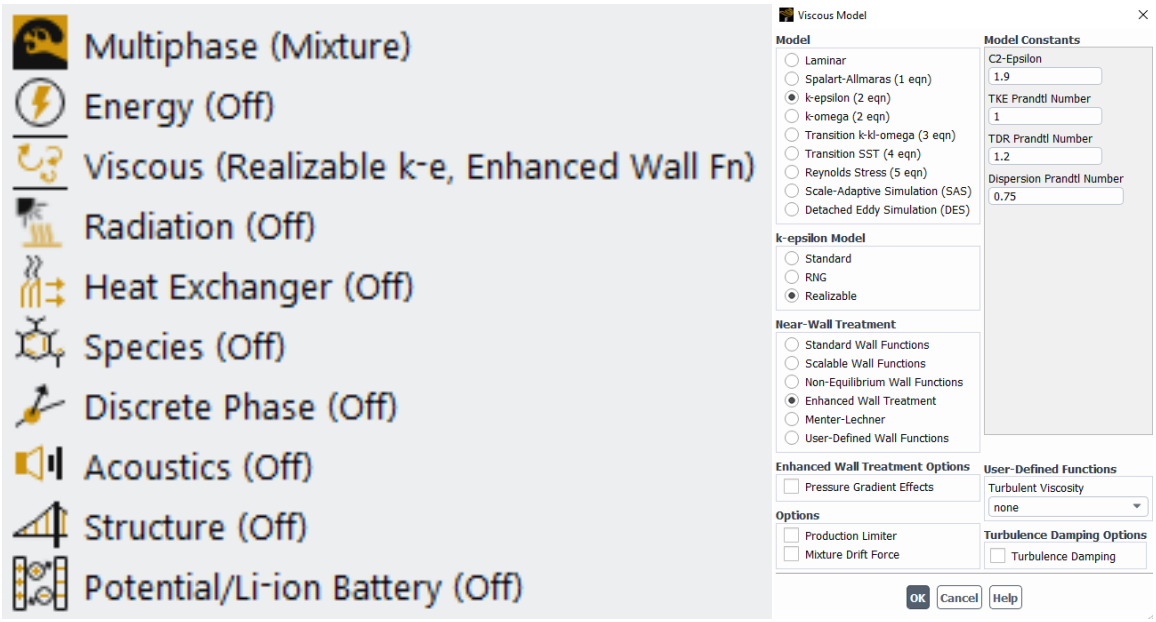

Figure 7. General model settings (left) and viscous model settings (right).

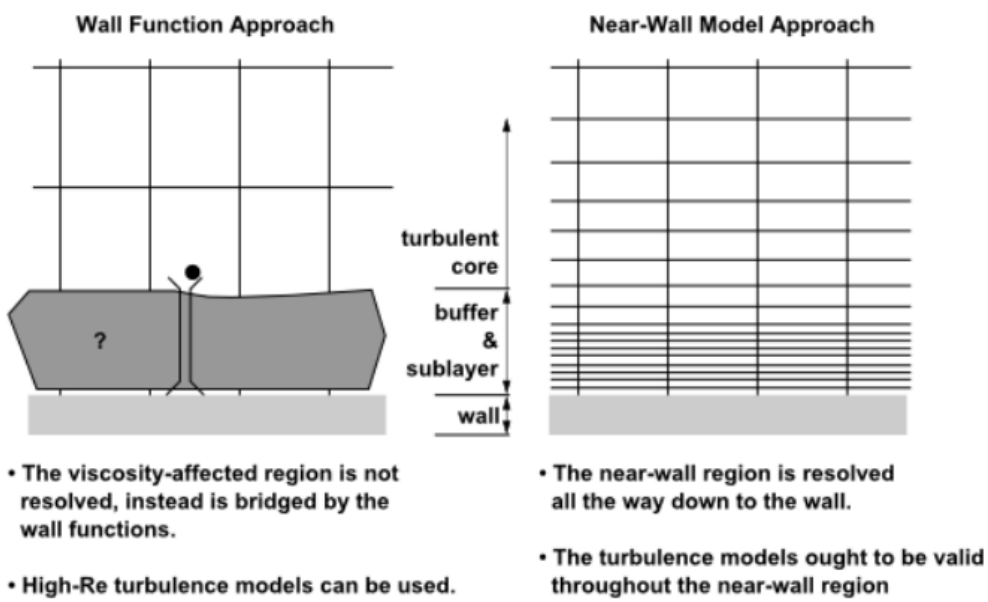

Figure 8. Standard wall function approach (left) vs enhanced wall function approach (right). [3]

The simulation was set for a pressure based, axisymmetric, with absolute velocity formulation. The velocity inlet was set to 2.8 m/s with a water volume fraction of 1. The remainder of the volume was sent to a volume

fraction of 0, entirely air. The pressure outlet was defined to have 0 gauge pressure, representing an open atmosphere. Figure 9 depicts the boundary conditions.

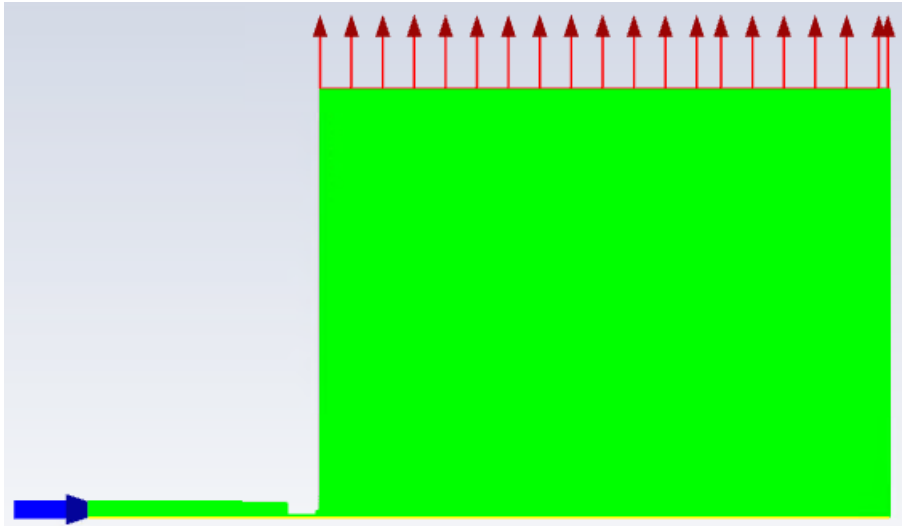

Figure 9. Boundary conditions for the geometry. The blue arrows indicate the inlet, the red arrows indicate represent the outlet, the green area indicates is the fluid volume, and the yellow line indicates the center axis.

Results

The images shown in Figure 10 depict the coupled air and water velocity contours for the simulated geometry. The top image shows the entire control volume with a higher velocity near the orifice and lower near the wall. The jet broadens as expected and the velocity slows away from the central axis, as expected the water is slowed by the air and disperses radially outward. The bottom right image shows a close up near the impacted wall. The wall has a no-slip condition applied so the velocity is zero at the wall. The velocity contours also show the end of the main rejoin and the beginning of the diffused droplet region shortly before the wall, both regions are shrouded by the water mist zone. The bottom right image shows an area near the inlet where the potential core region is better defined and disperses into the main jet region, as seen in Figure 3. In the appendix, a phase contour diagram shows the volume fraction of water to visualize what area contains the most concentrated water.

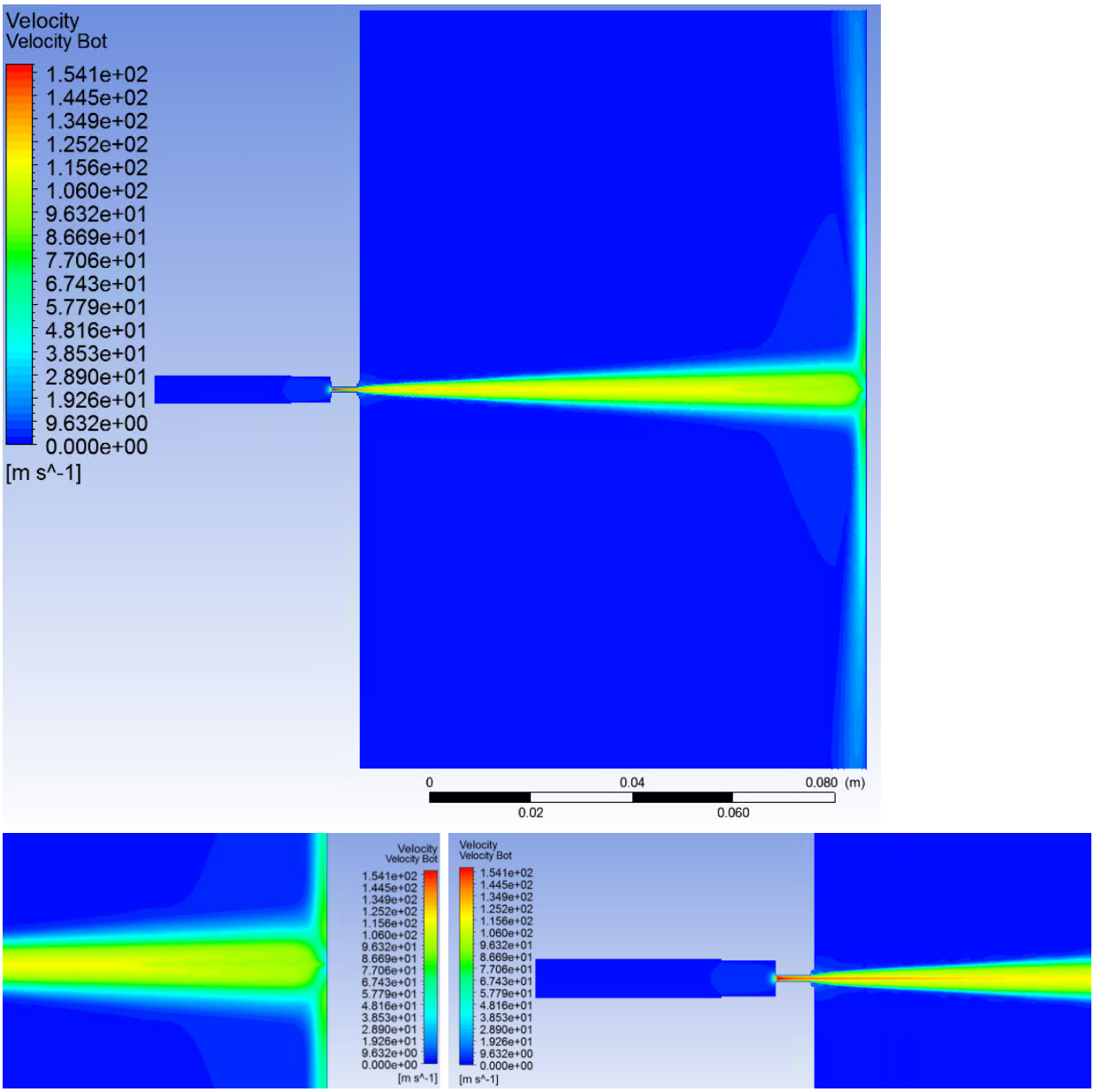

Figure 10. Velocity contours of entire fluid volume (top), near the impacted wall (bottom left), and near the inlet (bottom right).

The Y^+ value is reasonable for ranges 3-11 as stated in [4]. The Y^+ value in the center of the jet is highest, slightly above 11 and the remainder of the primarily impacted area is within the desired range, as shown in Figure 11. A logarithmic contour of the pressure on the impacted wall allows for a visualzation of the jet spot size. Using a full width at half maximum approach, the spot size is predicted to be 1.2 mm in radius, shown in Figure 12.

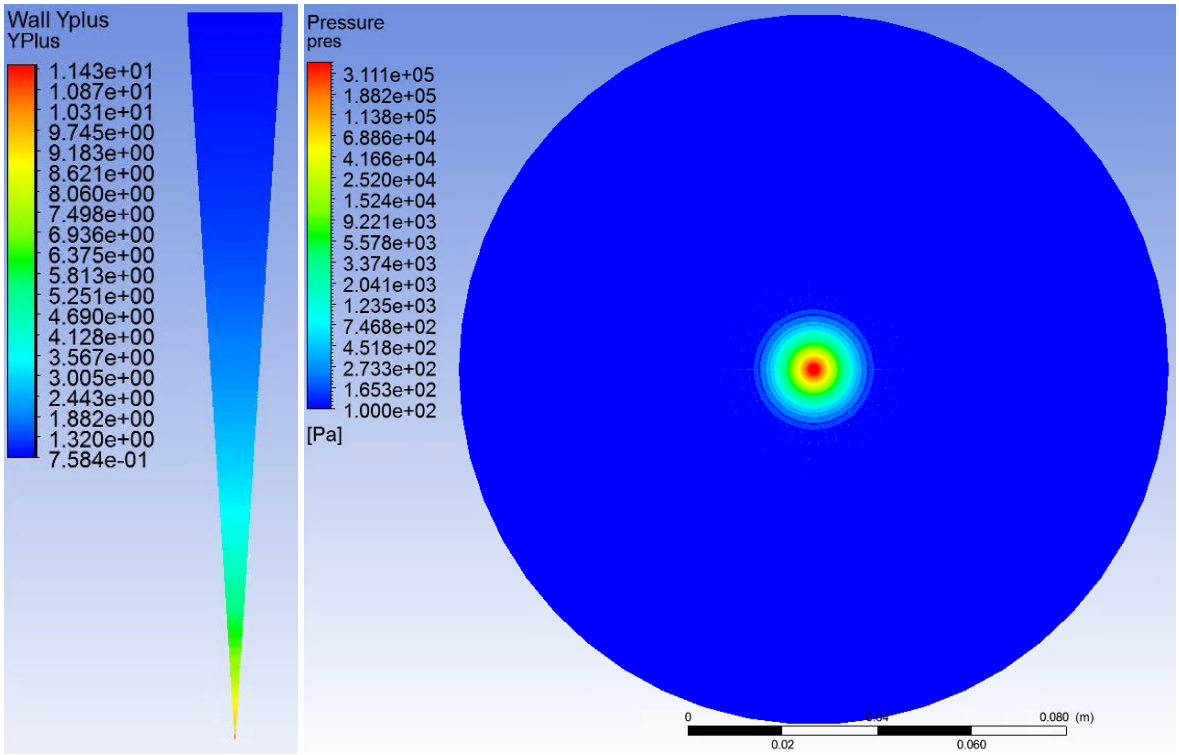

Figure 11. Section of wall Y^+ (left) and logarithmic pressure contours (right).

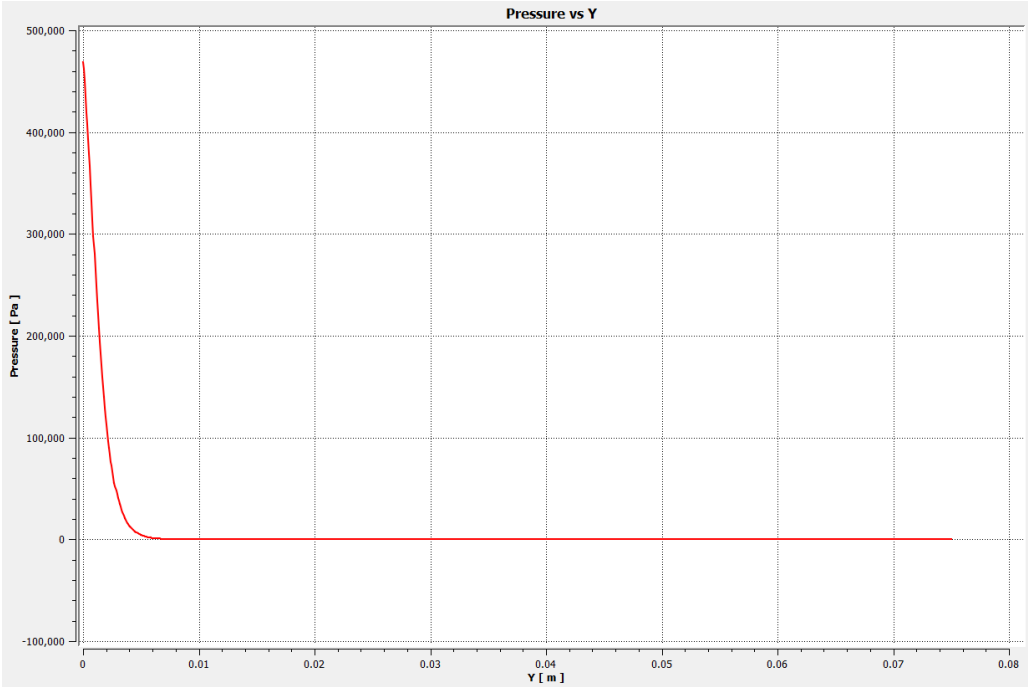

Figure 12. Plot of the pressure on the impacted wall beginning at the center axis and progressing radially outward.

Conclusion

When producing CFD simulations, determining the proper settings is crucial. A mesh that is too coarse will fail to capture the fluid mechanics, while a mesh that is too fine will waste computation time and unnecessarily delay results. Identifying boundaries or regions of interest can save computation requirements while still providing the desired model fidelity. For wall boundaries with fluid flow, inflation layers should be added to improve the Y+ and better resolve the viscous sublayer. The resolution of cells in an inlet influences the shape of the jet, and the cells near an impacted wall influence the spot size prediction.

The major limitation for using a 2D axisymmetric geometry is the conical symmetry requirement. In application, the nozzle will not always impact the Niobium cavities in an axisymmetric space. To better understand how water will behave when impacting the Niobium cavities of PIP-II, an angled wall simulation is required. Shear stress applied to an angled wall would provide a better representation for what the cavities would experience. In future simulations, using a 3D geometry would allow for more freedom with the nozzle shape and spray patterns. Creating transient simulations could also lead to a better understand of the water behavior.

References

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[3] SAS IP, Inc. (2013). Ansys Fluent Theory Guide (15.0).

[4] SAS IP, Inc. (2013). Ansys Fluent User's Guide (15.0).

[5] Lecture 7: Turbulence Modeling. (2022, August). Introduction to ANSYS Fluent.

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Appendix

Pressure calculation of inlet velocity

Continuity Equation:

$$A_i v_i = constant$$

A_i Cross-sectional area

v_i Fluid velocity

Bernoulli's Equation:

$$P_i + \frac{1}{2}\rho {v_i}^2 + \rho g y_i = constant$$

P_i Static pressure of the fluid

g Acceleration due to gravity

ρ Fluid density

y_i Fluid velocity

v_i Fluid velocity

Known:

P_{inlet} = 1250 psi ≈ 8.62 MPa

ρ = 998 kg/m

$P_{orifice}$ = 0

$\frac{A_{inlet}}{A_{orifice}}$ = 39

Solution:

$$\frac{A_{inlet} v_{inlet}}{A_{orifice}} = v_{orifice}$$

$$P_{inlet} + \frac{1}{2}\rho {v_{inlet}}^2 + \rho g y_{inlet} = P_{orifice} + \frac{1}{2}\rho {v_{orifice}}^2 + \rho g y_{orifice}$$

$$P_{inlet} + \frac{1}{2}\rho {v_{inlet}}^2 + \cancel{\rho g y_{inlet}} = P_{orifice} + \frac{1}{2}\rho {v_{orifice}}^2 + \cancel{\rho g y_{orifice}}$$

$$P_{inlet} - P_{orifice} + \frac{1}{2}\rho\left({v_{inlet}}^2 - {v_{orifice}}^2\right) = 0$$

$$P_{inlet} - P_{orifice} + \frac{1}{2}\rho\left({v_{inlet}}^2 - \left(\frac{A_{inlet} v_{inlet}}{A_{orifice}}\right)^2\right) = 0$$

$$v_{inlet} = \sqrt{\frac{2\left(P_{inlet} - P_{orifice}\right)}{\rho\left(\frac{A_{inlet}}{A_{orifice}}\right)^2}} = \sqrt{\frac{2(8.6 * 10^6 - 0)}{998(39)^2}}$$

$$\boldsymbol{v_{inlet} = 3.37\ m/s}$$

Volumetric flowrate derived calculation of inlet velocity

Volumetric Flow Rate:

$$Q = vA$$

Q Fluid volumetric flowrate

v Fluid velocity

A Cross-sectional area

Known:

A = 2.488 m^2

Q = 1.1 gal/min = 4.17 L/min

Solution:

$$Q = vA$$

$$v = \frac{Q}{A} = \frac{4.17}{2.488 * 10^{-5}}\left(\frac{1000\ L}{1\ m^3}\right)\left(\frac{1\ min}{60\ s}\right)$$

$$\boldsymbol{v = 2.8\ m/s}$$

Y+ formula

$$y^+ = \frac{u_\tau \rho y_P}{\mu}$$

ρ *fluid density*

y_P *distance from point P to the wall*

μ *fluid viscosity at point P*

u_τ *friction velocity* $\sqrt{\frac{\tau_w}{\rho_w}}$

τ_w *shear stress at the wall*

ρ_w *shear stress at the wall*

Phase Contour

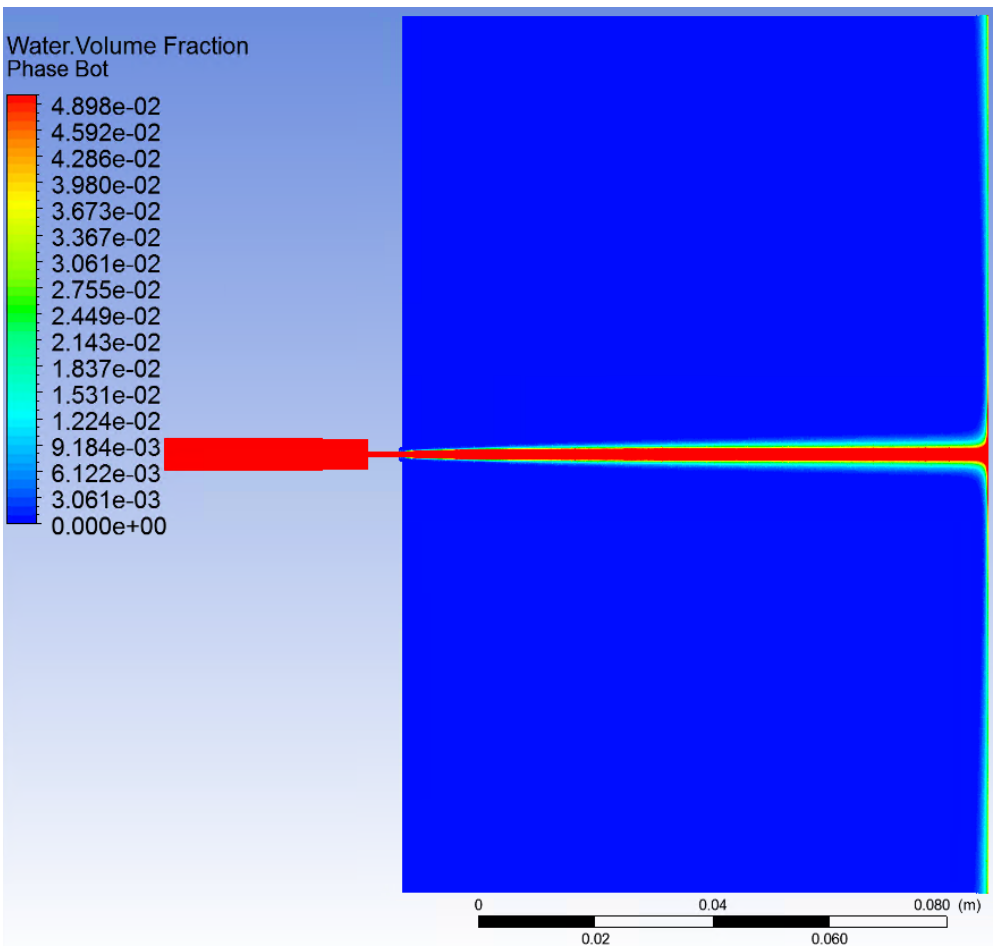

Figure 13. A volume fraction phase contour shows the area with a high concentration of water.