LA-UR-20-22580

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Title: Supo Thermal Model Development IV

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Intended for: Report

Issued: 2020-03-27

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Introduction

This report describes the continuation of the Computational Fluid Dynamics (CFD) model of the Supo cooling system described in the reports, Supo Thermal Model Development¹, II², and III³. In the previous reports, the solution natural convection of Supo was simulated using a 2D, axisymmetric model that altered the actual geometry. A 3D geometry of Supo will more accurately estimate the natural convection heat transfer coefficient (HTC) of the system since Supo contains several non-symmetric internal components that can only be modeled in 3D. This, in turn, will improve the natural convection HTC results for comparison purposes with past operational data and previous 2D CFD results. Unfortunately, the complexities of performing multiphase 3D CFD simulations has proven too large of a task for our current capabilities. Instead, this report will focus on the 3D model development for the 2.39 kW/L (31.3 kW) case and limitations and challenges associated with the 3D simulations.

Background

Supo, or “Super-Power” was a 45 kW water boiler reactor that consisted of a uranyl-nitrate solution within a spherical vessel. Supo was operated from 1951 to 1974 at what is currently called Los Alamos National Laboratory. The vessel contained water-cooled spiral coils distributed throughout the solution to maintain desired operating temperatures, re-entrant thimbles containing boron control rods, and a “glory hole” allowing neutron data to be acquired. Supo was mainly used for neutron research, and proved to be a versatile and reliable research tool.

Geometry

The internal components of Supo have been updated from the previous reports to match the dimensions in the literature as accurately as possible. The dimensions of the cooling coils, control rod thimbles, outer sphere, and glory hole were gathered from reports by King⁴, Durham⁵, and Bunker⁶. A detailed description of the overall solution vessel geometry is also provided in Buechler’s report¹. Figure 1 shows the cross section of Supo with the internal cooling tubes and water level. Figure 2

Figure 1 – Cross sectional sketch of the internal components in the Supo reactor vessel⁵

¹ C. Buechler, LA-UR-16-29483, Supo Thermal Model Development, 2016.

² A. Wass, LA-UR-17-25822, Supo Thermal Model Development II, 2017.

³ A. Wass, LA-UR-18-25097, Supo Thermal Model Development III, 2018.

⁴ L. D. P. King, Design and Description of Water Boiler Reactor, Proceedings of the International Conference on the Peaceful Uses of Atomic Energy, 1955

⁵ F. Durham, Radiolytic-Gas Bubbling Improves Convective Heat Transfer in Supo, Nucleonics, 1955.

⁶ M.E. Bunker, LA-2854, Status Report on the Water Boiler Reactor, 1963.

shows the Solidworks 3D CAD model of Supo. Since the 3D locations of the cooling coils were not known, historical images and Fig. 1 were used to estimate the location of each tube along the cross section. The tube locations were then translated slightly along the plane 90 degrees from the original locations. This produced the spiral shape of the cooling coils. The cooling coils were modeled as solids since the tube thickness is defined in the CFD software. Since the glory hole was not included in Fig. 1, the cooling coils had to be shifted around the glory hole in an arbitrary manner to avoid interference. The cooling coils were modeled as three different coils (outer, middle, and inner) shown in Fig. 3. The length of each coil was 17.3, 25, and 17.2 ft for a total of 59.5 ft. The CAD model coil length was 0.5 ft less than the actual Supo geometry. The modeled solution volume was 13.115 L, a difference of 0.001 L from the actual steady state operating condition¹.

Figure 2 – Solidworks CAD model of Supo showing isometric (top left), front view cross section (top right), side view cross section (bottom left), and top view cross section (bottom right)

Figure 3 – Solidworks CAD model of Supo showing outer cooling tube (top left), middle cooling tube (top right), and inner cooling tube (bottom)

Mesh

In order to obtain a converged and accurate solution, the 3D mesh must be of high quality. The quality of the mesh is characterized by several parameters including aspect ratio, orthogonal quality, and skewness. For multiphase simulations, ANSYS recommends a very good maximum skewness of less than 0.5, an acceptable aspect ratio of less than ten, especially near the gas-liquid interface, and very good minimum orthogonal quality greater than 0.70⁷.

A simplified geometry was first meshed using ANSYS Mesher and contained only the basic outer sphere and the fluid region and can be seen in Fig. 4. No cooling coils or additional parts were added. The mesh contained tetrahedral and prism elements and the mesh size and quality information can be found in Table 1. Another 3D mesh of a simplified geometry of Supo was created that included the outer cooling coil only (with inflation layers around the cooling coil) and is also shown in Fig. 4 and mesh information and quality listed in Table 1. Inflation layers were

⁷ ANSYS, Inc., Modeling Bubble Columns – Best Practices, Presentation, May 27, 2015.

added to the outside surface of the cooling coils and had a first layer thickness of .04 mm, 12 layers, and a last aspect ratio of 3.

Mesh quality generally improves with the total size of the mesh, however, with the limitations on computational time, and additional complexity of the geometry, a limit had to be set on the mesh size. This limit was based on previous 2D simulation results, their mesh size, and solving time. Several attempts were made to develop a high quality mesh of the total 3D Supo geometry, including a polyhedral dominant mesh, yet, a tetrahedral and prism mesh was developed with the highest achievable quality with total node and element count in mind. The size and quality of the final mesh is listed in Table 1, and the mesh can be seen in Fig. 5. The inflation layers on the cooling coils, control rod thimbles, and glory hole had a first layer thickness of .04 mm, a total of 10 layers, and a growth rate of 1.15. Due to the complexities of the geometry, the final mesh quality was less than the ANSYS recommended quality.

Table 1: Mesh size and quality for three geometries with increasing complexity

Mesh	Nodal Count	Element Count	Min. Orthogonal Quality (Target >.7)	Max. Skewness (Target <.5)	Max. Aspect Ratio (Target <10)
Simplified	194,111	1,059,277	.474	.526	3.9
Simplified with Outer Cooling Coil Only	2,137,789	6,899,916	.212	.770	63
Full Geometry	7,555,411	22,493,334	.150	.850	50

Figure 4 - Simplified 3D mesh of Supo's fluid volume without internal geometry (left) and with the outer cooling coil only (right)

Figure 5 – Multiple views of the final 3D mesh of Supo

Properties, Profiles, and Wall Boundary Conditions

The material properties, heat and mass generation profiles, and wall boundary conditions were gathered from the previous report³, and modified slightly for the full 3D geometry (boundary conditions were applied to surfaces, not lines). However, the report by Buechler¹ explained the process for determining these model inputs in greater detail. The boron control rods and glory hole walls were modeled as adiabatic surfaces. Properties were determined for each power level using the appropriate fluid temperatures determined by Durham's and Bunker's experiment results^{5,6}. Buechler¹ also determined temperature-dependent polynomials of the radiolytic gas mixture properties⁸ for density, specific heat, thermal conductivity, viscosity, and molecular mass using mass fractions of H₂ and O₂.

The power and mass generation profiles were modeled as a 3D Gaussian profile within the solution portion of the vessel. Buechler determined these profiles from assumptions and examples in King's and Bunker's reports^{4,6,9}. Such assumptions included a power deposition in the liquid proportional to the neutron flux. A contour plot of the power deposition profile (W/m³) that was used for the 2.39 kW/L (31.3 kW) case is shown in Fig. 6. One should note that the peak power is higher in order to achieve the desired volume integrated power of Supo. The mass source was

⁸ Incropera and DeWitt, Fundamentals of Heat and Mass Transfer, 4th Ed., Wiley, 1996, p. 841-842.

⁹ King, et. al., Gas Recombination System for a Homogeneous Reactor, Nucleonics, Vol. 11, No. 9, 1953.

Figure 6 - Power deposition profile (W/m³) for the 2.39 kW/L (31.3 kW) case

introduced as a mixture of oxygen and hydrogen and proportional to the reactor power and power deposition profile.

Natural Convection Model

The commercial CFD software, ANSYS Fluent Version 2019 R1, was used to model the fluid flow of the fuel solution. Based on results from the previous work^{1,2,3}, the k-omega SST turbulent model with dispersed turbulence multiphase option was used in this work. Most of the bubble phase interaction models remained the same in this report as previously defined¹. The bubble drag model was set as the Schiller-Naumann drag model, the bubble lift force and vertical wall effects were modeled using the Tomiyama lift

force and Antal wall lubrication force models, respectively, and the multi-phase heat transfer was modeled using the Ranz-Marshall heat transfer model. Two turbulent based models were required for the multiphase, turbulent cases. The turbulent dispersion model was set as the Burns dispersion model, and the turbulence interactions were modeled using the Sato model.

Model Parameters and Solution Methods

Similar to the previous report³, the same model parameter and solution methods were used for each case from the Durham⁵ and Bunker⁶ reports. Also, the boundary conditions for each case remained unchanged. The results were considered fully converged when the power balance between the cooling tubes and the outer wall matched the total power generation to within 1%. Typically, mass balance is achieved faster than the energy balance, however, since the full geometry model never stabilized and diverged, it was difficult to gather useable mass and energy data. Ultimately, the mass flow of bubbles at the degassing boundary condition, maximum bubble velocity, maximum and average solution temperatures, cooling tube power and tube temperature, and volume fraction were recorded.

Bubble Size Determination

The method for determining radiolytic gas bubble size remained the same from the previous work^{1,2,3}. The bubble size was determined using experimental values from King's and Bunker's reports^{4,6}, as well as two bubble diameters measured at Argonne National Laboratory by Chemerisov et al.¹⁰ A linear relationship between bubble diameter and power density was developed that results in positive values for bubble diameter at all power densities, as shown in Fig. 7. The predicted bubble diameter is: Bubble diameter (mm) = 0.652*(Power density in kW/L) + 0.1099. For the 2.39 kW/L (31.3 kW) case, the bubble diameter was 1.67 mm.

¹⁰ Chemerisov et al., Experimental Results for Direct Electron Irradiation of a Uranyl Sulfate Solution: Bubble Formation and Thermal Hydraulics Studies, ANL/NE-15/19.

Figure 7 - Linear fit of bubble diameter using measured data and CFD results

Results & Troubleshooting

In order to make certain that the model was set up correctly, a 2.39 kW/L (31.3 kW) case simulation with no internal components (cooling coils, control rods, glory hole) was performed first. The model had very good mesh quality and was considered an optimal case. The heat transfer coefficient was set to 26,086 W/m²-K on the outer wall with an initial solution temperature of 308 K. The outlet boundary was set to outgassing. The simulation stabilized without issue, and was stopped after 4923 iterations. The next simulation was meshed with a single outer cooling coil, however, good mesh quality was much more difficult to achieve. The 2.39 kW/L case with the single outer cooling coil was successfully ran with the gas bubble generation turned off. However, when the gas bubble generation was turned back on in a separate simulation, the simulation ran unstable for 5781 iterations before diverging. Many attempts to improve the run time, such as modifying solution controls and settings, adjusting numerical schemes, and gradually increasing the gas generation rate were unsuccessful. It was determined that the poor mesh quality was to blame for the divergence of this simulation. Of course, adding the full 3D geometry of Supo, such as all the internal cooling coils, control rod thimbles, and glory hole, created additional challenges to develop a high quality mesh. Therefore, a successfully converged simulation of the 2.39 kW/L case was never achieved (as well as the 3.05 kW/L, 40 kW case).

Conclusion

The 3D geometry of the Supo solution reactor was developed using the dimensions and sketches from previous historical reports. The internal solution volume matched the historical data to within .001 L. Several 3D meshes were produced from the geometry. The first was a simplified version containing no internal components such as cooling coils, through holes, etc., and had a very good mesh quality. The 2.39 kW/L case simulation of the simplified model performed well and did not diverge or show significant signs of instability. The next simplified mesh included the outer cooling coil and inflation layers on the coil surface, and had a slightly poorer mesh quality. Due to the poor mesh quality, the multiphase simulation did not converge and was unsuccessful. Unfortunately, with each additional component included into the mesh, the mesh quality decreased. Therefore, the quality for the final 3D mesh with all components was quite poor, resulting in diverging simulations and instabilities in the calculations. Thus, no converged simulations of the full geometry of Supo were successfully completed.