ORNL/TM-2022/2627

Validation of Thermohydraulic Simulations using RELAP for Critical Dual Purpose Canisters

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Nuclear Energy and Fuel Cycle Division

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Prepared by
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managed by
UT-Battelle LLC
for the
US DEPARTMENT OF ENERGY
under contract DE-AC05-00OR22725

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ABBREVIATIONS

ORNL	Oak Ridge National Laboratory
CFD	computational fluid dynamics
RELAP	Reactor Excursion and Leak Analysis Program
US	United States
DOE	US Department of Energy
MPC	multipurpose canister
CAD	computer-aided design
PWR	pressurized water reactor
TH	thermal hydraulics

NOMENCLATURE

μ	Dynamic Viscosity [Pa-s]
ρ	Density [kg/m^3]
k	Thermal Conductivity [W/m-K]
α	Thermal Expansion Coefficient [1/K]
C_p	Heat Capacity [J/kg-K]

ABSTRACT

Simulations using the RELAP5-3D systems analysis code and STAR-CCM+, a high-fidelity computational fluid dynamics code, were performed on a model of a real-scale MPC-32 dual-purpose canister undergoing a criticality event. These simulations were performed to provide code-to-code verification of the natural convection capabilities in RELAP5. The STAR-CCM+ simulations revealed various natural convection flow patterns that aided in the cooling of fission heat produced in the fuel rods in the canister. Negligible spatial temperature variations were observed across the canister in the STAR-CCM+ results, supporting the use of RELAP5 in predicting the sub-cooled regime. The surface-averaged rod temperature predicted by RELAP5 compared well with STAR-CCM+, verifying the predictive capability of RELAP5 for sub-cooled conditions.

1. BACKGROUND

The United States consumes about 37 quads of thermal energy annually for electricity production, out of which 8.42 quads (22%) comes from nuclear fission [4]. It is anticipated that the demand for nuclear energy will significantly increase in the next decades because nuclear energy, along with wind and solar, is categorized as one of the clean forms of energy (no CO_2 emission) that will advance the nation's mission of achieving net zero carbon emissions by 2050. This expected surge in demand for nuclear energy will likely increase the volume of nuclear waste substantially. Regulatory agencies are currently formulating strategies to manage this waste. Storing nuclear waste in geological repositories is one of the options under consideration. One risk with a geological repository is flooding of the nuclear canisters by ground water. The water entering can create conditions such that the canisters will go critical. To simulate a critical event in a flooded spent nuclear fuel canister, a combination of a neutron transport solver and thermal hydraulic solver can be adopted to predict the sustainable power level and nuclide inventory. The thermohydraulic solver under consideration in this study is RELAP5-3D [8]. To our knowledge, the use of RELAP5 for a critical spent nuclear fuel canister under sub-cooled conditions has not been verified. Therefore, the main goal of this work is to compare the thermal hydraulic predictive capability of RELAP5 with the prediction of a high-fidelity computational fluid dynamics (CFD) solver, STAR-CCM+ [7], for sub-cooled conditions while analyzing the detailed flow and heat transfer patterns in a canister using CFD.

The remainder of this report is organized as follows: in Section 2., the capabilities of STAR-CCM+, the models used for the CFD simulations, and the flow and heat transfer patterns predicted by STAR-CCM+ are discussed. In Section 3., the RELAP5 modeling details are given and the the RELAP5 simulation results are discussed. In Section 4., the results between RELAP5 and STAR-CCM+ are compared, and finally in Section 5. conclusions are drawn and future work is discussed.

2. CFD MODELING AND SIMULATION

Simcenter STAR-CCM+ [7] is a multiphysics CFD software package for the simulation of thermohydraulic systems operating under real-world conditions. The single integrated environment includes everything from CAD, automated meshing, multiphysics CFD, and sophisticated postprocessing. This enables efficient high-fidelity exploration of the flow, heat transfer, and structural characteristics of devices used in many applications. An extensive validation of flow and heat transfer predicted by the code for a nuclear canister can be found in [1].

2.1 GEOMETRY AND MESH

The geometry used for the simulations is a quarter of a full-scale MPC-32 dual-purpose canister, as shown in Figure 1. There are eight pressurized water reactor (PWR) fuel assemblies in the quarter portion of the canister. Each assembly has 17×17 rods, with a total of 264 fuel rods, 24 guide tubes, and one instrument tube per assembly. Each assembly is surrounded by a stainless steel basket with neutron absorbers. The basket and the assemblies are surrounded by an outer cover made of stainless steel (see properties in Table 1). Due to the complexity involved in constructing a computational mesh, the upper plug and the lower nozzle geometry (a subset of the original geometry) shown in Figure 2 are neglected under the assumption that the inclusion of these elements would have minimal impact on the simulation results. Additionally, the interior of the rods are not meshed so as to reduce the number of computational cells and thus the computational expense of the simulations. The power generated within the fuel rods are simulated by a heat flux boundary.

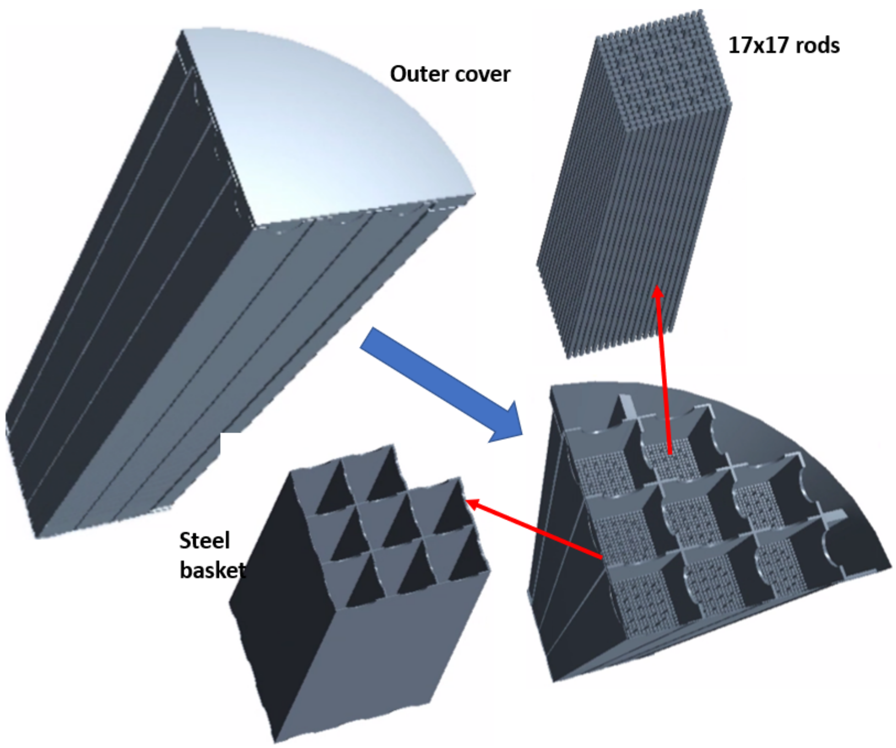


Figure 1. Quarter geometry of an MPC-32 canister.

Polyhedral mesh elements are known for their ability to provide accurate solutions with a minimal mesh count compared to other types of mesh elements. Thus, the “polyhedral mesher” within StarCCM+ was used to generate the mesh for this study. For a sufficiently accurate solution, a mesh count of 140 million cells was required. These calculations were run on Oak Ridge National Laboratory’s (ORNL’s) Panacea

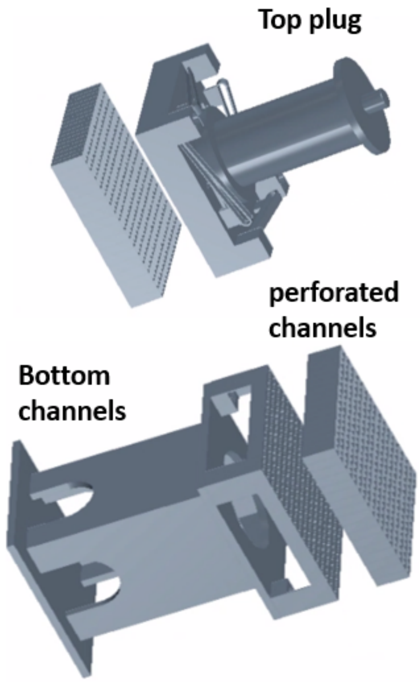


Figure 2. Parts excluded from PWR assemblies for the MPC-32 modeling.

cluster with 270 cores for 3 days. A “thin mesher” module capable of meshing very thin geometries while keeping the number of mesh elements low was used to generate mesh for the steel basket.

Bulk mesh elements (see Figure 3) away from the rods had a size of 2 cm, whereas the mesh elements around the rods were 3 mm thick. The maximum cell size in the inter-rod channels (refer to Figure 4) was limited by the rod spacing; a minimum of two cells were required for reasonable resolution (based on the coarsest mesh used in [6]), which led to a high mesh count. Unfortunately, the majority of the canister space is occupied by these rods; hence, the final mesh count for this quarter geometry of the canister reached 140 million cells. Two prism layers were generated around the tubes as shown in Figure 5 to accurately capture the boundary layer heat transfer from the rods to the fluid.

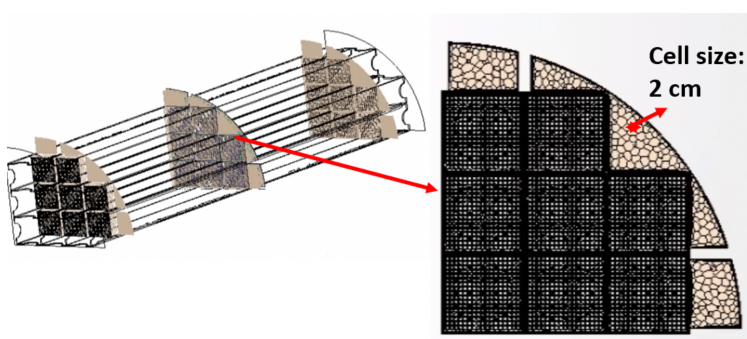


Figure 3. Illustration of mesh resolution in the radial plane.

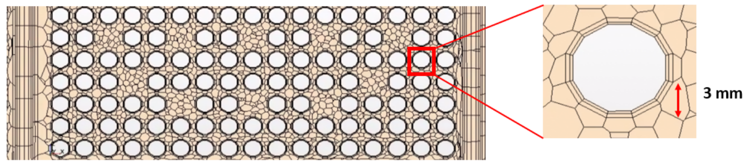


Figure 4. Meshing around fuel rods in the radial plane.

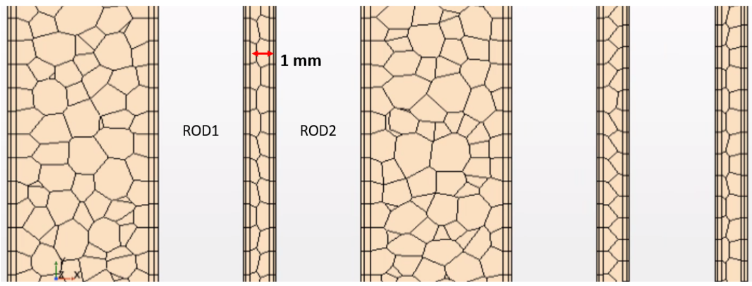


Figure 5. Mesh between fuel rods in the axial plane.

2.2 MODELING AND SETUP

The CFD computational cost involved in simulating a full canister is very high. Therefore, only a quarter portion of the canister is considered, and similarity of the flow in other quarters of the canister is assumed. To mimic the way DPCs are typically loaded in a geological repository, the canister geometry was arranged horizontally (as seen in Fig. 3) such that the gravitational force acts perpendicular to the rod length. For this investigation, the canister was assumed to be fully submerged in water (see water properties in Table 1) with no water entering or leaving the system, and with a water temperature below the boiling temperature at the operating pressure of 50 bars. The temperature inside the fuel rods was not computed to reduce computational cost. Therefore, in these simulations, the power generated by the fuel rods was specified as heat fluxes (in kW/m^2) on the rod surfaces in contact with the water. Three different total power levels were simulated: 4 kW, 6 kW and 8 kW. Since only a quarter of the geometry is considered, the power levels were divided by four when used to compute rod surface heat flux.

Table 1. Thermophysical properties

Materials	ρ	μ	**k**	C_p	α
Water	812	0.000888	0.62	4181	0.00039142
Stainless Steel	8055	-	15.1	480	-

The boundary conditions used for the simulations are provided in Table 2. The thermal boundary condition for the canister outer boundary is unknown, since this boundary is coupled to the repository rock. Therefore, in this investigation an approximate canister boundary temperature, calculated using the PFLOTRAN code [5], with thermal inputs matching plausible repository conditions, was used on the outer cover. Adiabatic boundary conditions were used on the surfaces that are assumed to be symmetric. For flow calculations, a no-slip boundary condition is applied on all the solid walls of the canister (i.e, the outer

Table 2. Boundary conditions

Governing Equations	Outer cover	Rods	Symmetry surfaces
Heat	238 C	heat flux calculated from power	adiabatic
Flow	no-slip	no-slip	no-slip

cover, rods, and symmetry surfaces).

Natural circulation is generated inside the canister due to the heating of the water by the rods. The water density variation across the canister due to the heating will induce a buoyancy effect. The accurate capture of this buoyancy effect is crucial to predict the steady-state rod temperatures. Typically, in CFD simulations, the effect of the liquid density variation with temperature or pressure is captured using a compressible solver. However, since compressible solvers are prone to divergence and computationally very expensive, an incompressible solver was used, and the buoyancy effect was approximated by the Boussinesq model [3] given by

$$\mathbf{Fb} = \alpha \rho_{\text{ref}} \left(T - T_{\text{ref}} \right) \ , \tag{1}$$

where α is the thermal expansion coefficient of water, T_{ref} is the reference temperature, and ρ_{ref} is the reference density. The Boussinesq model is valid for flows with very low $T - T_{ref}$. In this study, for all power levels, the reference temperature is the canister boundary temperature 238 °C, and the reference density is the density of water corresponding to the reference temperature. The temperatures inside the canister are only 2–3 °C above the boundary temperature. Thus, this model is applicable for capturing the buoyancy effect in the range of power levels considered. All the results reported in the next section are for steady-state conditions with an initial temperature of 238 °C. The simulation was stopped when the surface averaged rod temperature reached a steady value.

2.3 RESULTS AND DISCUSSION

The temperature distribution inside the horizontally oriented canister for three different planes along the axial direction, for powers 4 kW and 8 kW, is shown in Fig. 6. Hot spots are observed for the assemblies in the middle compartment. The temperatures on the bottom sides of all the bottom assemblies or compartments are small compared to liquid around other assemblies, due to the behavior of the natural convection of the water around the assemblies as discussed below.

The natural circulation in the radial plane for 4 kW and 8 kW power levels are given in Figure 7. Based on the liquid velocity magnitudes, the circulation is stronger for 8 kW, as expected. For both power levels, the clockwise circulations near the outer wall in the assembly-free spaces seem to drive some of the heat away from the assemblies in its vicinity toward the outer wall. The heated fluid rejects its heat to the outer wall, becomes heavier, and comes down to carry more heat. These radial circulations are found only in the empty assembly-free spaces of the canister. As discussed in the next paragraph, the regions with assemblies have circulations only in the axial direction and do not have radial vortices in these empty spaces.

The natural circulation currents produced inside the canister is illustrated on an axial plane in Figure 8 (top). The circulation is oriented in the y-direction and symmetric across the z-axis. It is evident from the contour of the velocity component along the y-axis (Figure 8 (bottom)) that a pair of symmetric counter-current vortices are generated in each assembly compartment, oriented in the y-direction with axes in x-direction. An investigation was also performed to detect other dominant vortices inside the assemblies

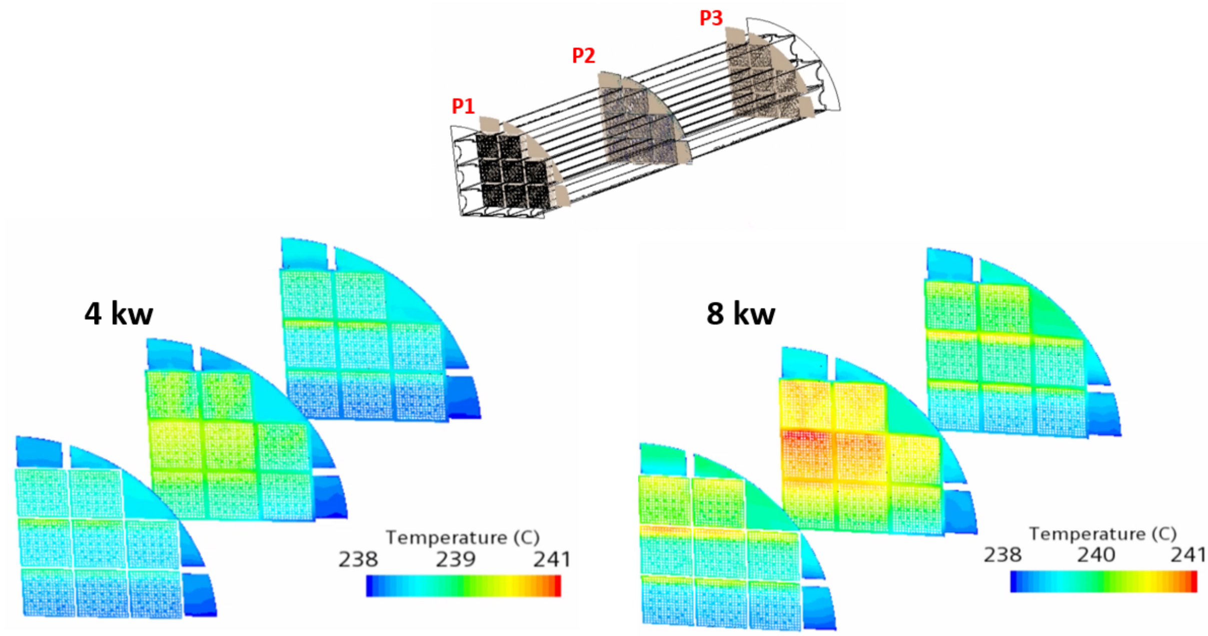


Figure 6. Temperature on three planes along the axial direction for 4 kW (left) and 8 kW (right).

by analyzing cut planes oriented in other directions. However, it seems that the one in the y-direction shown in Figure 8 was the only dominant vortex that existed in the assemblies and contributed significantly to heat transport. The heat generated by the rods in each assembly or compartment is carried by this circulation from the bottom side to the top side of each compartment in the positive z-direction, as seen in Figure 10. The circulation rejects its heat to the top side while traveling in the y-direction; thus, the temperature of the liquid progressively decreases in both y-directions (see Figure 8 (bottom)). The decreased temperature results in heavier fluid, which comes down to the bottom side of the compartment due to gravity acting in the negative z-direction and repeats the cycle of heat transport every time. The same cycle of heat transport is repeated in all the assemblies of the canister. Then, the heat accumulated in the top most compartment of the canister is rejected to the outer wall (at 238°C) by the vortices in the empty assembly-free spaces.

The RELAP5 thermal calculations are typically valid for applications with small spatial temperature variations. To investigate the validity of this assumption for the canister, multiple sample planes were generated in both the axial and radial directions, and plane surface–averaged temperature variation in both directions are plotted and reported in Figure 10 (top and bottom). It can be inferred from the plots that the spatial variation of temperature is small inside the canister.

The level of detail obtained from CFD simulations, along with its utility in verification, can also be used in diagnosing the problems related to canister cooling and discovering new designs for resolving it.

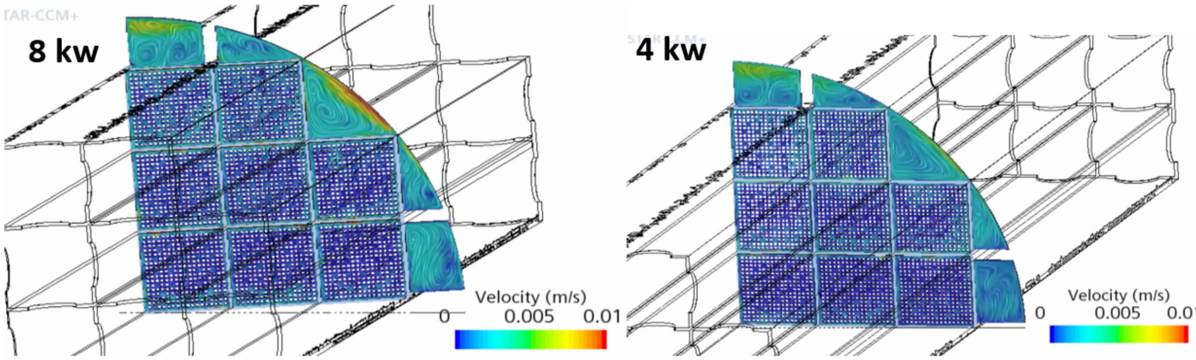


Figure 7. Natural circulation velocity on a radial plane 8 kW (left) and 4 kW (right).

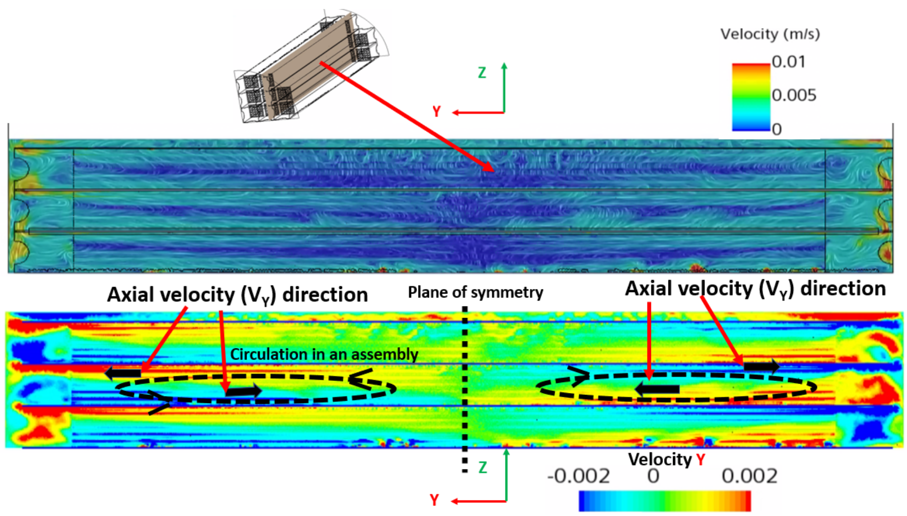


Figure 8. Natural circulation on an axial plane for 8 kW: velocity magnitude (top) and velocity component Y (bottom).

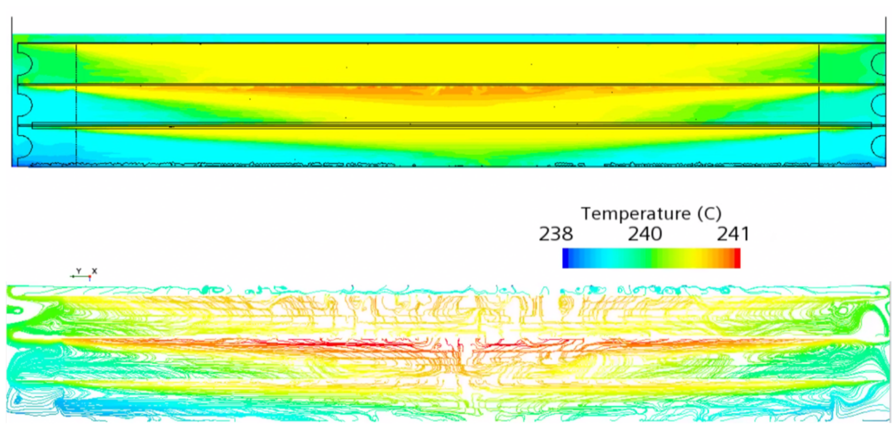
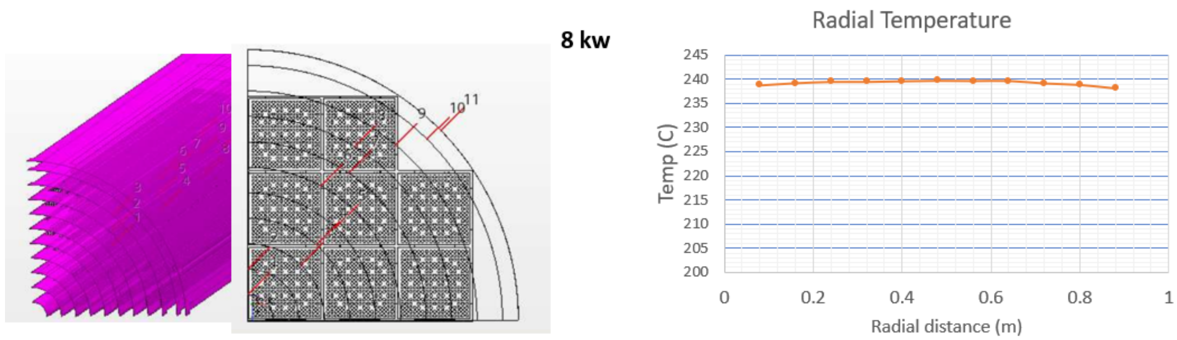


Figure 9. Temperature profile on an axial plane: contour (top) and stream lines (bottom).



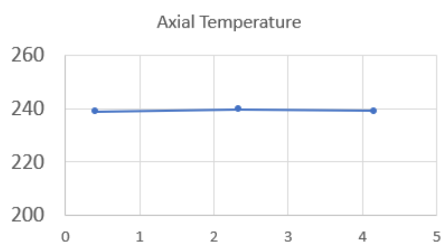


Figure 10. Radial and axial temperature profiles.

3. RELAP5 MODELING AND SIMULATION

3.1 CODE DESCRIPTION

RELAP5-3D [8] is a standard system analysis simulation code developed by Idaho National Laboratory. This code has been developed to analyze steady-state and transient TH behavior in light-water reactors (LWRs). It is a best-estimate code developed for transient simulations of LWR coolant systems during operational transients and postulated accident scenarios, and it can be used for modeling other nuclear systems. RELAP5-3D has a fully integrated, multidimensional TH and kinetic modeling capability, making it applicable to a wide range of systems and applications. The code is extensively validated in [2] and is widely accepted in the nuclear industry for system analysis applications. The code can be used to simulate a wide variety of thermal transients in nuclear and non-nuclear systems that involve mixtures of vapor, liquid, non-condensable gas, and nonvolatile solute.

3.2 MODEL OVERVIEW

The RELAP5-3D model developed for this study is composed of a series of hydrodynamic components, control volumes, heat structures, junctions, and other components. The model is used to calculate fluid temperatures at different power levels for an assumed fixed repository temperature.

It is computationally inefficient to model the entire waste package system at a subchannel level of detail in RELAP5-3D. The fuel basket in the RELAP5-3D model is modeled as a series of concentric regions, each representing a number of basket cells. Each basket region consists of a pipe representing the fluid volume, a heat structure representing the basket walls, and a heat structure representing the heated rods of the assemblies within that region. The innermost 4 basket cells are modeled as a single pipe, and the rods in these four assemblies are represented by a single heat structure inside the pipe; the intermediate 12 basket cells and the outermost 16 basket cells are modeled in this same manner. The rod and basket wall heat structures are thermally connected to the appropriate pipes representing the fluid volumes of each basket region. The basket regions as they are grouped in RELAP5-3D are identified in Figure 11.

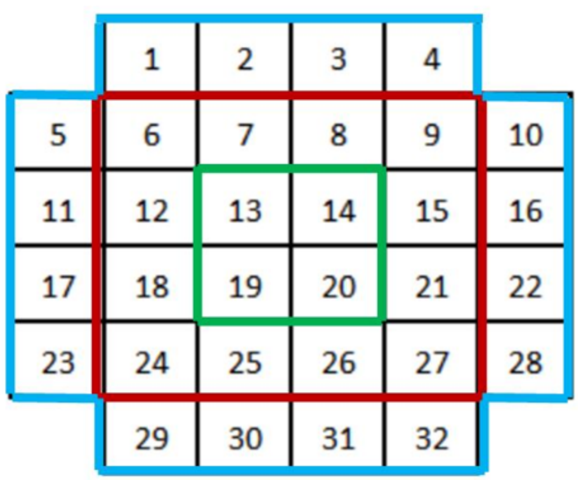


Figure 11. Basket and assembly model in RELAP5-3D.

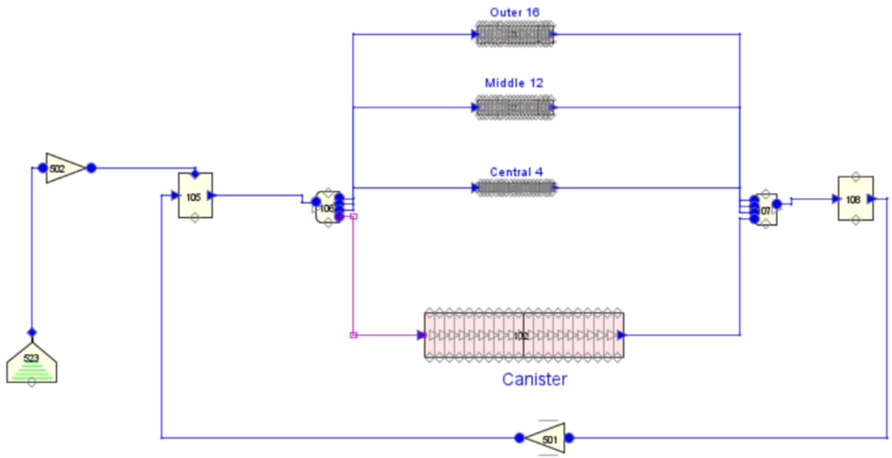


Figure 12. Model of an MPC-32 as Represented in RELAP5-3D

The portion of the canister surrounding the basket is modeled using a pipe representing the fluid volume and a heat structure representing the canister wall. Upper and lower regions in the canister are modeled using branches and pipes to facilitate flow distribution among the different basket regions. For this verification effort, the waste package is not included in the model. The canister is modeled in the horizontal orientation. The configuration of the RELAP5-3D model is provided in Figure 12.

3.3 GEOMETRY AND BOUNDARY CONDITIONS

Various assembly dimensions and geometry parameters calculated for use in RELAP5-3D are provided in Table 3. RELAP5-3D allows the user to define natural circulation lengths for the left and right boundary of each heat structure in the model. If the natural circulation lengths are not defined, then the heat transfer hydraulic diameter is used. The natural circulation length represents the vertical distance over which natural circulation occurs in a given fluid region. Consistent with this definition, the natural circulation length of all basket cell regions in this analysis is assumed to be the inner flat-to-flat width of a single basket cell.

Because each fuel rod heat structure represents multiple rods, RELAP5-3D's *cylinderheight* parameter for these heat structures is scaled based on the number of rods it represents. Each heat structure is separated into 20 axial segments in RELAP5-3D. The cylinder height of each fuel rod heat structure is provided in Table 4. Solid materials used in the RELAP5-3D model are provided in Table 5. These are standard materials with properties built in to RELAP5-3D. The system is modeled at a system pressure of 50 bar and is assumed to be completely filled with water. Initial fluid temperature and boundary conditions are provided in Table 6. For all power levels analyzed, the outer canister wall is set to a constant temperature equal to the assumed repository temperature.

Table 3. Fuel Rod Heat Structure Cylinder Heights in RELAP5-3D

Assembly parameters	
Rod Diameter (mm)	9.502
Rod Length (m)	3.8354
Heated Length (m)	3.8354
Rods Per Assembly	289
Heated Rods Per Assembly	264
Number of Assemblies	32
Inner Basket Cell Width (flat-to-flat) (cm)	22.479
Basket Wall Thickness (mm)	9.347
Area (m^2)	0.030035
Wetted Perimeter (m)	9.526579
Hydraulic Diameter (m)	0.012611
Heat Transfer Hydraulic Diameter (m)	0.013683
Innermost 4 Assemblies	
Fluid Area (m^2)	0.120141
Effective Radius of Fluid Area (m)	0.195556
Area of Basket Walls (m^2)	0.017159
Effective Outer Radius of Basket Walls (m)	0.209055
Intermediate 12 Assemblies	
Fluid Area (m^2)	0.360423
Effective Radius of Fluid Area (m)	0.338713
Area of Basket Walls (m^2)	0.034667
Effective Outer Radius of Basket Walls (m)	0.354628
Outermost 16 Assemblies	
Fluid Area (m^2)	0.480564
Effective Radius of Fluid Area (m)	0.391112
Area of Basket Walls (m^2)	0.051476
Effective Outer Radius of Basket Walls (m)	0.411526

Table 4. Fuel Rod Heat Structure Cylinder Heights in RELAP5-3D

Heat Structure	Number of Rods	RELAP5-3D Cylinder Height (m)
Innermost 4 Assemblies	1056	202.5091
Intermediate 12 Assemblies	3168	607.5274
Outermost 16 Assemblies	4224	810.0365

Table 5. Solid Materials used in RELAP5-3D

Component	Material
Fuel Rods	UO_2
Basket/Canister Walls	Stainless Steel

Table 6. Inital and boundary temperatures

Initial water temperature (C)	27
Canister Wall Outer Surface Temperature (C)	238

4. COMPARISON OF RESULTS BETWEEN RELAP5-3D AND STAR-CCM+

The surface-averaged rod temperatures predicted by RELAP5-3D and STAR-CCM+ for different power levels are given in Figure 13. It is interesting to note that the temperature increases linearly with power. The temperatures computed by RELAP5-3D deviate slightly from those computed by STAR-CCM+. This deviation could be attributed to the natural convection correlation used in RELAP5-3D. However, the deviations between RELAP5-3D and STAR-CCM+ are within 1.5% relative difference for all powers. Therefore, it was concluded that the RELAP5-3D predictions match well with the STAR-CCM+ predictions. The water density comparison between the two codes would yield the same conclusion because density is a function of temperature. Furthermore, based on this comparison, it can be inferred that the natural convective cooling predicted by RELAP5-3D should also be reasonably close to the high-fidelity CFD simulations performed by STAR-CCM+.

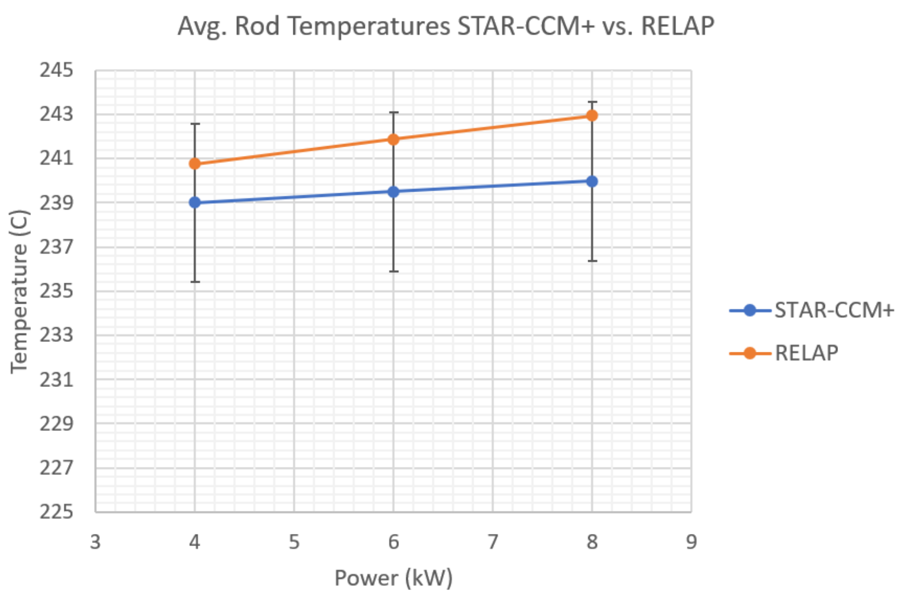


Figure 13. CFD vs. RELAP: Surface-averaged rod temperature for various power levels for subcooled flow with error bars that represent 1.5% **deviation from CFD.**

5. CONCLUSION AND FUTURE WORK

High fidelity CFD simulations using STAR-CCM+ and systems-level simulations using RELAP5-3D were performed for an MPC-32 canister filled with spent nuclear fuel in a critical configuration to understand the natural circulation-based cooling of the fuel rods and to verify the accuracy of RELAP5-3D in these scenarios against CFD. Three different canister power levels with flow at subcooled conditions were investigated. The flow pattern computed by STAR-CCM+ reveals a pair of counter-rotating axial circulation patterns in each assembly compartment and multiple radial patterns in the empty (assembly-free) spaces of the canister. The axial circulation pattern transports heat generated in the assemblies placed in the lower compartments to the higher compartments and subsequently rejects it to the outer wall, which is held at the boundary temperature. The negligible liquid temperature variation along the radial and axial directions of the canister justifies the use of RELAP5-3D for subcooled conditions. Additionally, the comparable rod temperatures predicted by RELAP5-3D and STAR-CCM+ verify the predictive capability of RELAP5-3D at subcooled conditions.

Future work will involve the verification of RELAP5-3D against CFD for boiling conditions. Also, the prediction of vapor fraction evolution after boiling and its impact on the fission and decay power, along with the stress exerted by the vapor on the canister walls, will be investigated.

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