CFD Modeling of a Simulated Protected Loss of Power in the Gallium Thermal-hydraulic Experiment (GaTE) using STAR-CCM+

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Abstract

This report presents the progress made by the University of New Mexico's Institute for Space and Nuclear Power Studies (UNM-ISNPS) in the first year of an Integrated Research Project (IRP) led by City College of New York (CCNY). The objective is to develop research capabilities in large scale Computational Fluid Dynamics (CFD) modeling and simulation and apply them to simulate thermal-hydraulics phenomena in advanced reactors. The performed CFD analyses model the Protected Loss of Power (PLOP) experiments conducted using the Gallium Thermal-hydraulic Experiment (GaTE) at Purdue University. The experiment investigates thermal stratification phenomena of liquid Ga akin to that in the upper plenum of sodium fast reactors. The performed CFD analyses of the upper plenum test vessel in the experiment use the STAR-CCM+ commercial Multiphysics code. The analyses modeled the conditions for both the pre-test isothermal flow in the PLOP experiment and the transients of injecting cooler liquid gallium at different velocities and lower temperature from 373.15 K to 323.15 K to induce thermal stratification within the upper plenum of the molten gallium test vessel.

The performed simulations using the Shear Stress Transport (SST) k-ω Reynolds Averaged Navier Stokes (RANS) and the Large Eddy Simulation (LES) turbulence models assume a rigid gallium free surface within the test vessel. In the CFD analyses of the pre-test isothermal flow conditions, the LES turbulence model shows intense swirling and the formation of eddies in the liquid gallium within the test vessel, compared to the simulations using the SST k-ω RANS model. Performed CFD simulations using the LES turbulence model of the transient PLOP experiment with a uniform inlet velocity of 10 mm/s of the cooler liquid gallium show intense mixing during the first ~100s of the transient. For longer times, however, the calculated spatial temperature distributions and the temperature gradient across the thermal stratification layer within the test vessel using the two turbulence models are nearly the same.

The greater mixing of the colder gallium injected into the hot gallium within the test vessel results in more uniform temperatures compared to the reported experimental measurements. The predicted mixing within the test vessel in the transient simulations may be due to using the sub grid model in the LES turbulence model or assuming a rigid liquid surface in the plenum. Future analyses will investigate the effects incorporating a liquid free surface using a Eulerian multiphase model in STAR-CCM+ on the comparisons of the CFD simulation results with the reported experimental measurements. These CFD simulations will also investigate the effects of increasing the injection velocity of the cold gallium into the test vessel of both the calculated temperature and flow fields in the experimental test vessel.

Nomenclature

CCNY	City College of New York
CFD	Computational Fluid Dynamics
D_{in}	inlet diameter (m)
DNS	Direct Numerical Simulation
DTS	Distributed Temperature System
ΔTp	difference between the radially innermost and outermost DTS probe temperatures, $\Delta T_p = T_{r = 11.75mm} - T_{r = 56.90mm}$
GaTE	Gallium Thermal-hydraulic Experiment
HEX	heat exchanger
HTGR	High Temperature Gas-cooled Reactor
IRP	Integrated Research Project
LES	Large Eddy Simulation
PLOF	Protected Loss of Flow
PLOP	Protected Loss of Power
r	radial coordinate (mm)
RANS	Reynolds Averaged Navier Stokes
Re_{in}	inlet Reynolds number ($U_{in}\, \rho_{Ga}\, D_{in} / \mu_{Ga}$)
SFR	Sodium Fast Reactor
SST	Sheer Stress Transport
T	temperature (K)
TC	thermocouple
U_{in}	uniform inlet flow velocity (mm/s)
UDV	Ultrasonic Doppler Velocimeter
UIS	Upper Instrumentation Structure
UNM-ISNPS	University of New Mexico's Institute for Space and Nuclear Power Studies
URANS	Unsteady Reynolds Averaged Navier Stokes
WALE	Wall-Adapting Local Eddy-viscosity
Z	axial coordinate (m)
μ_{Ga}	gallium viscosity (Pa-s)
ρ_{ga}	gallium density (kg/m^3)

1.0 Introduction

Thermal stratification is considered a key safety issue for pool-type Sodium Fast Reactors (SFRs) [Wu et al. 2020; Schneider et al. 2019]. The pool of hot liquid sodium above the reactor core provides a large thermal mass for limiting temperature changes during operation transients. The liquid sodium exiting the reactor core mixes into the hot upper sodium pool. The hot primary sodium flow in an intermediate Na/Na heat exchanger (HEX) within the liquid sodium pool transfers heat to the cooler intermediate loop liquid sodium flowing upward within the HEX. The cooled primary liquid Na enters the reactor core where it removes the thermal power generated by fission in the fuel elements.

A fast decrease in the reactor's thermal power decreases the temperature of the liquid sodium exiting the reactor core mixing into the hot sodium pool above the core. This can occur during a postulated Protected Loss of Flow (PLOF) accident, following a partial loss of the main coolant pump and a reactor scram to reduce the reactor power and avoid overheating the fuel elements in core. During a Protected Loss of Power (PLOP) accident the main coolant pump continues to circulate the primary liquid sodium through the reactor core. Following an unanticipated reactor scram, the flow rate of the colder sodium entering the pool decrease compared to a PLOF accident. In both events the cold, denser cooler sodium exiting the reactor core into the hot sodium pool forms a stratified sodium layer with the hot sodium at the top of the pool (Fig. 1.1).

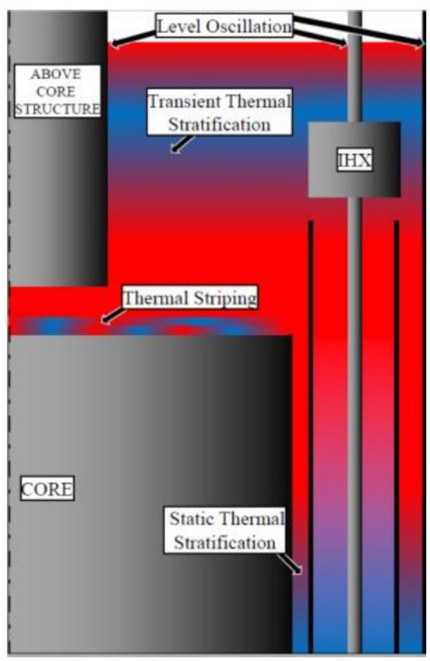


Fig. 1.1. Thermal-hydraulic mixing in a hot liquid metal pool resulting in a transient thermal stratification [Schneider et al. 2019].

Following a loss of forced circulation of the primary liquid sodium through the core during a PLOF accident, the reactor core would be cooled by natural circulation of the in-pool sodium and the formation of a thermally stratified layer could inhibit the development of steady natural circulation [Wu et al. 2020]. Thermal stratified layers in liquid metals have been observed to be unstable and could result in local temperature oscillations within the pool. These temperature oscillations can induce thermal stresses in the metallic components of the pool, such as the Upper Instrumentation Structure (UIS) above the core,

which contains the control element drives and in-core instrumentation tubes (Fig. 1.1), and the reactor vessel. The thermal fatigue cracking caused by these stresses may damage these components.
To quantify the extent of these risks, researchers have performed small scale experiments and numerical CFD simulations to predict thermal stratification. Transient simulation of thermal stratification phenomena in SFRs has proved challenging, with some approaches reporting significant differences in predictions compared to reported experimental results [Ohno et al. 2011, Mochizuki and Yao 2014, Sakamoto, et al. 2010, Zwijen, et al. 2019, Hu, et al. 2013]. The reported CFD simulation results of thermal stratification in SFR upper pools confirmed the importance of using fine numerical meshing with the appropriate turbulence models. This will help capture the flow details and simulate the formation and movement of stratified layer in the hot liquid sodium in the upper pool.

In addition, reported modeling approaches differed in how to model the inert cover gas layer above the liquid metal hot pool. Most assumed a rigid gas-liquid interface to simplify the analyses [Mochizuki & Yao 2014; Sakamoto et al. 2010; Zwijsen et al. 2019]. Others used multi-component flow models to simulate a dynamic interface that can move with temperature and interaction with the in-pool liquid metal flow [Hu et al. 2013]. However, there is a need to further understand and quantify the effects of these modeling approaches of the liquid metal gas interface in the upper plenum on the CFD simulations results and the flow within the upper pool of SFRs.

Simulating such complex thermal-hydraulic phenomena requires large scale CFD modeling and simulation capabilities to capture the fine details and of the liquid metal flows. The objective of this work is to develop and exercise advanced computing capabilities for simulating thermal-hydraulic phenomena in advanced High Temperature Gas-cooled Reactors (HTGRs) and SFRs. The commercial CFD code STAR-CCM+ [Siemens PLM, 2023] will be used to model the Gallium Thermal-hydraulic Experiment (GaTE) facility at Purdue University [Bindra, et al. 2020; Ward, Clark, and Bindra, 2019] and the obtained results will be compared to reported flow velocities and temperature measurements for selected transient experiments investigating thermal stratification in the molten gallium.

These simulation results will later be compared to those obtained by City College of New York (CCNY) using the NekRS code to investigate its capabilities for simulating transient thermal-hydraulic phenomena in the upper pools of pool-type SFRs and identify areas for potential improvements. The performed CFD simulation using STAR-CCM+ will investigate the effect of using the lower fidelity Sheer Stress Transport (SST) k-ω Reynolds Averaged Navier Stokes (RANS) turbulence model and the higher order Large Eddy Simulation (LES) turbulence model on the results. The results will be compared against the reported temperature and flow velocity measurements in the GaTE facility's liquid gallium pool at Purdue University.

The CFD simulation of thermal-hydraulic in nuclear reactors may select among different methods for modeling fluid flow with increasing sophistication and complexity. The direct Numerical Simulation (DNS) methods directly solve the Navier Stokes flow equations and require using a refined numerical mesh grid to resolve the formation of small eddies in the flow, at the expense of a high computational cost [Afgan, 2007]. The common two-equation RANS turbulence models, such as the k-ε and k-ω, do not directly solve the Reynolds stresses in the flow and instead use approximate models to compute the turbulent isotopic eddy viscosity [Launder and Spalding, 1974]. The RANS models have low computational costs but the isotropic turbulence approximations they employ can have difficulties modeling highly anisotropic flow behavior, such as swirling and jetting [Larocque, 2004; Rodriguez and El-Genk, 2011]. The LES turbulence method uses spatial filtering to solve the turbulence in the different regions of the flow. It directly solves for the formation of larger eddies in the flow as in DNS and uses a subgrid model to solve for the formation of small turbulent eddies below the scale determined by the filtering criteria [Smagorinsky, 1963]. The LES method can accurately than the simpler isotropic RANS models capture complex turbulent behavior, such as in swirling and jetting flows, but requires a refined mesh to directly solve for the eddies in the flow above the filter size [Taglia et al., 2004; Siemens PLM, 2023]. Therefore, large scale CFD simulations of advanced reactors need a balance between reasonable accuracy in modeling the essential physics and computational cost. It is important to investigate the effect and quantify the added value of employing a sophisticated turbulence model, such as LES, compared to a simpler, lower cost turbulence model for simulating the pertinent physics in the flow.

During the 1st year, the University of New Mexico's Institute for Space and Nuclear Power Studies (UNM-ISNPS) effort focused on **Task 1:** Recruitment of Graduate Students at UNM, **Task 2:** Selection and Preparation of Benchmark Data, and **Task 3:** Training on Use of STAR-CCM+. The subaward of the DOE IRP to UNM-ISNPS was delayed almost five months to start February 21st, 2024, instead of October 1st, 2023. This delayed the student recruitment and the data selection tasks.

The objective is to develop research capabilities in large scale Computational Fluid Dynamics (CFD) modeling and simulation and apply them to simulate thermal-hydraulics phenomena in advanced reactors. The performed CFD analyses model the Protected Loss of Power (PLOP) experiments conducted using the Gallium Thermal-hydraulic Experiment (GaTE) at Purdue University. The experiments investigate thermal stratification phenomena of liquid gallium akin to that in the upper plenum of sodium fast reactors. The performed CFD analyses of the upper plenum test vessel in the experiment use the STAR-CCM+ commercial Multiphysics code.

The analyses modeled the conditions for both the pre-test isothermal flow in the PLOP experiment and the transients of injecting cooler liquid gallium at different velocities and lower temperature from 373.15 K to 323.15 K to induce thermal stratification within the upper plenum of the molten gallium test vessel. The performed simulations using the SST k-ω RANS and the LES turbulence models assume a rigid gallium free surface within the test vessel.

2. Student Recruitment and Training

We conducted a comprehensive recruiting effort to identify potential graduate students for the planned research effort. This included posting information on the research assistantship opportunities on the UNM-ISNPS website and on the UNM nuclear engineering LinkedIn pages. UNM-ISNPS communicated the opportunity to 13 nuclear engineering programs around the country as well as CENA in Argentina so they can pass it on to students who may be interested in the opportunity. Recruiting is also done at the Sandia Graduate Student Fair held at the National Museum of Nuclear Science and History in Albuquerque, NM. The review of the received applications selected Mr. Keenan Kresl-Hotz, a recent graduate in Mechanical Engineering at the University of Wyoming, to join our team on the project. During a summer internship at Idaho National Laboratory, Keenen provided support to the Advanced Test Reactor program, and with another summer internship with BWXT he supported nuclear fuel modeling for high temperature gas cooled reactors. He joined our team on August 1, 2024. Keenen has received training on performing CFD simulations using the STAR-CCM+ and COMSOL CFD codes, both of which are available at UNM-ISNPS. His training with our team included using the high-performance computing recourses at UNM's Center for Advanced Research Computing on applying STAR-CCM+ commercial CFD Multiphysics code to modeling the liquid gallium experiments performed in the GaTE facility at Purdue University.

3. Identification of Benchmark Cases

The UNM-ISNPS team reviewed the reported results and measurements for the liquid gallium thermal stratification and mixing experiments performed using the Gallium Thermal-hydraulic Experiment (GaTE) facility at Purdue University. The GaTE facility is constructed to investigate thermal stratification within the upper plenum of SFRs. The geometry of the test vessel is a 1/20th scale version of the DOE Advanced Burner Test Reactor design [Bindra, et al. 2020]. Experiments simulated conditions analogous to Protected Loss of Power (PLOP) and Protected Loss of Flow (PLOF) accidents in a pool-type SFR and investigated the formation and behavior of thermal stratification layer in the liquid metal upper pool.

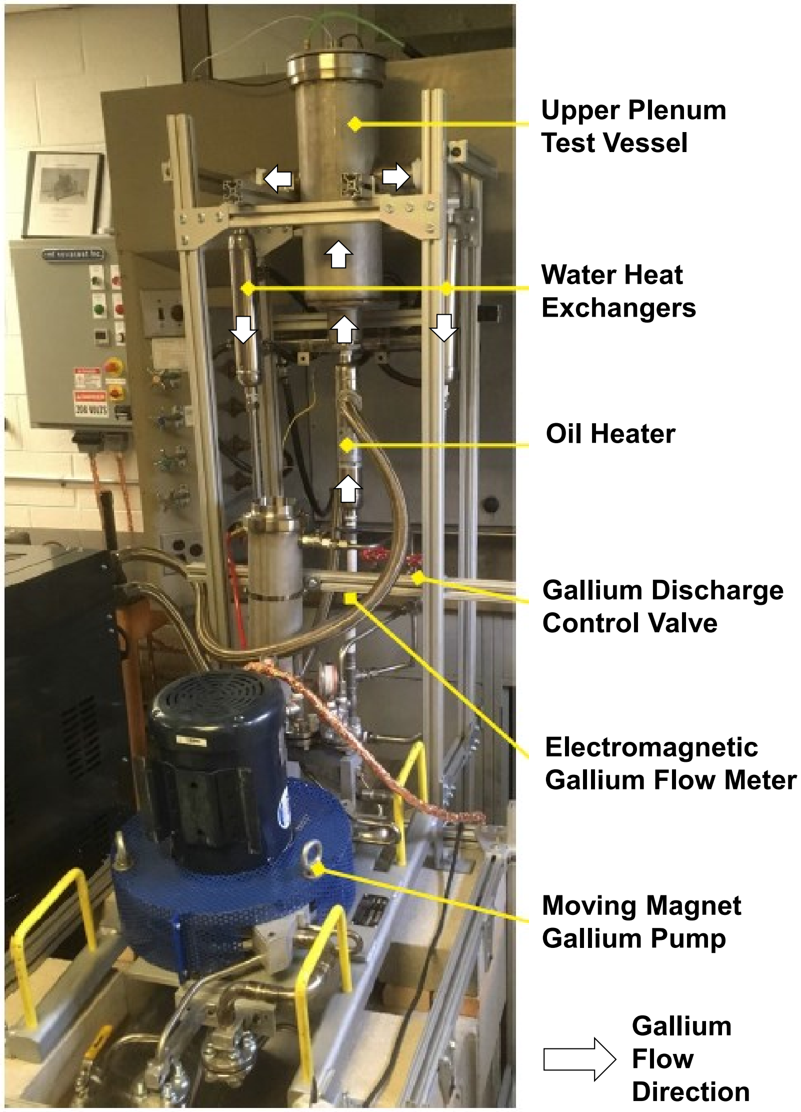


Fig. 3.1. Gallium Thermal-hydraulic Experiment Facility at Purdue University [Ward, Clark, and Bindra, 2019].

3.1 GaTE Facility at Purdue University

Figure 3.1 shows a photo of the integrated GaTE facility and Fig. 3.2 shows section views of the test vessel 316 stainless-steel plenum. The test vessel mounted on the top of the facility represents the upper pool of a SFR (Figs. 1.1, 3.1). The test facility circulates molten gallium in the loop using a moving magnet pump, which can control the flow rate to within < 2% of its programmed setpoint [Bindra, et al. 2020]. An electromagnetic flowmeter with reported accuracy to be within < 5% measures the flow rate of the liquid gallium exiting the pump [Bindra, et al. 2020]. A tube and shell oil circulation heat exchanger (HEX) heats the liquid gallium flowing on the tube side and therminol mineral oil heat transfer fluid flowing on the shell side (Fig. 3.1). The heater represents the reactor core in a pool-type SFR (Fig. 1.1).

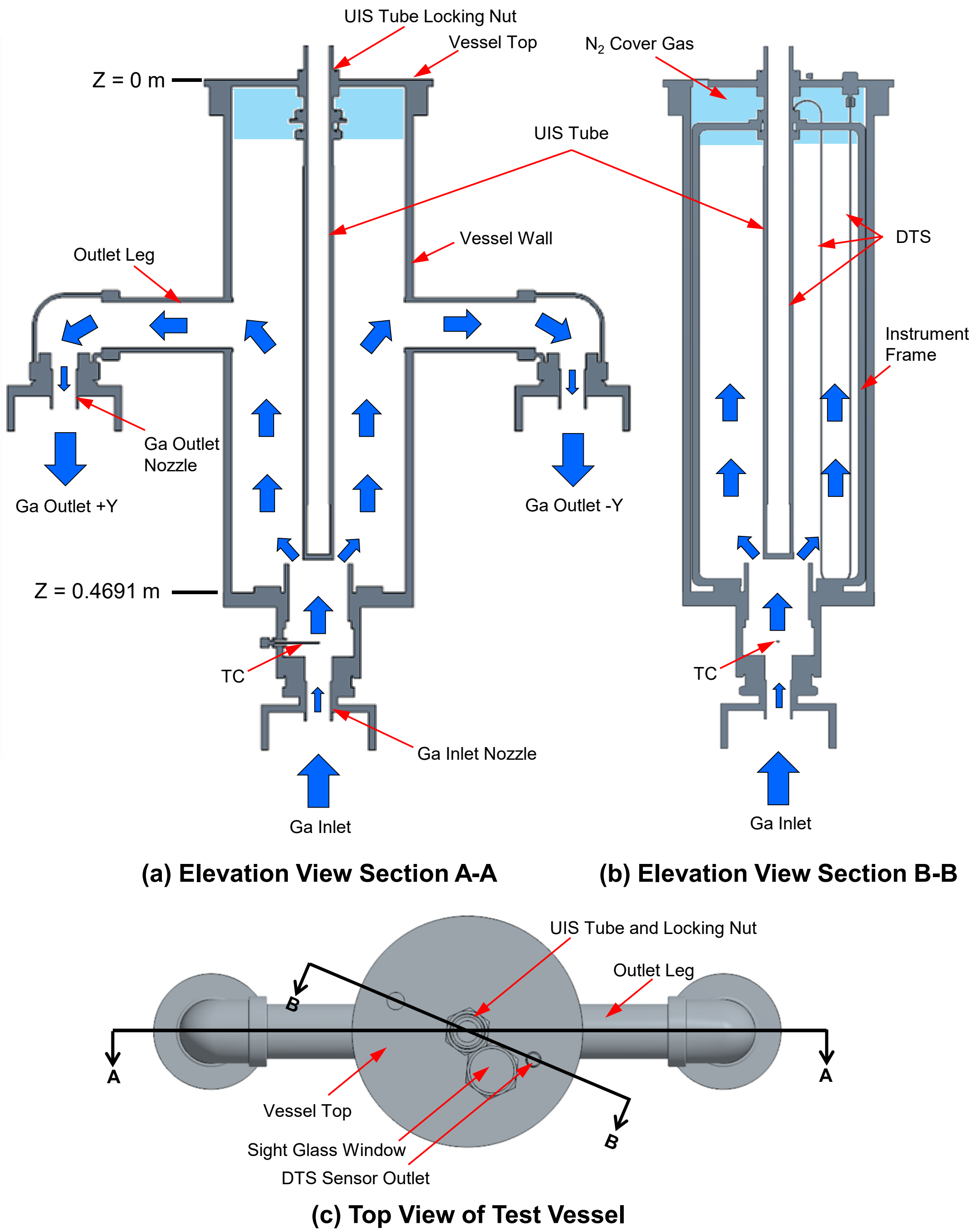


Fig. 3.2. Cutaway View of the upper plenum of the GaTE facility used in Present CFD Simulations.

The heated liquid gallium exiting the heat exchanger enters the test vessel through the inlet flow nozzle at the bottom of the upper plenum (Figs. 3.1 and 3.2). Liquid gallium flows up into the upper plenum of the test vessel and exits through two horizontal legs on either side of the test vessel (Figs. 3.1 and 3.2). To minimize oxidation of the liquid gallium at the free surface in the upper plenum of the test vessel has a layer of inert nitrogen cover gas at atmospheric pressure (Fig. 3.2) [Bindra, et al. 2020]. The central stainless-steel tube in the upper plenum of the test vessel (Fig. 3.2), which represents the Upper Instrumentation Structure (UIS) in an SFR, is sealed to prevent the liquid gallium from entering at the bottom. The liquid gallium exiting the horizontal legs flows through exit nozzles to the two tube and shell water HEXs (Figs. 3.1 and 3.2). The water circulating through the shell side of the HEXs cools the liquid gallium flowing downward through the tube-side. These are analogous to the intermediate HEX in the SFR hot pool (Fig. 1.1). The cooled liquid gallium returns to the pump to be recirculated within the test loop.

The GaTE test facility at Purdue University measures the temperature and velocity of the liquid gallium in the test vessel. A k-type 1/16" diameter thermocouple (TC) at the center of the inlet flow channel measures the inlet temperature of the flowing liquid gallium (Fig. 3.2), with reported uncertainty of ± 0.75% ºC [Bindra, et al. 2020]. Additional k-type thermocouples are located at the outlet of each of the water HEX and between the outlet of the electromagnetic flow meter and the inlet of the oil circulation heater (Fig. 3.1). A Distributed Temperature Sensor (DTS) system mounted to an internal rectangular instrumentation frame (Fig. 3.2) measures the liquid gallium temperature within the upper plenum of the test vessel. The instrumentation frame is rotated 23° from the plane that passes through the center of the two horizontal outlet legs in the upper plenum of the test vessel (Figs. 3.2c). This system measures the liquid Gallium temperature using optical frequency domain reflectometry through an optical fiber, which can measure temperatures with a spatial resolution of 0.625-1.4 mm with an uncertainty of ± 1.8°C [Bindra, et al. 2020]. The optical fiber is bent to form three straight vertical lengths: (a) an 'inner' located 11.8 mm from the centerline and inserted within a grove in the side of the UIS tube wall, (b) a 'middle' location 35.6 mm from the centerline, and (c) an 'outer' location 56.9 mm from the centerline of the test vessel (Figs. 3.2a and b). The DTS system measures the temperature at a frequency up to 250 Hz.

An Ultrasonic Doppler Velocimeter (UDV) mounted to the rectangular instrumentation frame on the side opposite to the DTS optical fiber measure gallium velocity within the upper plenum of the test vessel (Fig. 3.2). The sensor measures the axial component of the gallium flow velocity by measuring the ultrasonic waves reflecting off gallium-oxide particles within the molten gallium. The UDV sensor is mounted vertically in the test vessel at 281 mm from the bottom and can be moved radially 36, 47, and 58 mm from the centerline of the test vessel [Ward, Clark, and Bindra, 2019]. The UDV sensors were calibrated in a static tank of molten gallium. A motor moved the sensors at a fixed rate towards the bottom of the tank with an uncertainty < ±2.5 mm/s.

3.2 Protected Loss of Power (PLOP) Tests

The UNM-ISNPS team reviewed the experiments performed in the GaTE facility at Purdue University and identified the Protected Loss of Power (PLOP) experiment to be the focus of the present CFD simulation and modeling effort [Ward, Clark, and Bindra, 2019]. This experiment is of the liquid gallium initially circulating at a constant temperature of 373.15 K and a constant flow rate through the upper plenum of test vessel. The subsequent transient experiments begin by tripping the power to the oil circulation heater to decrease the temperature of the liquid gallium entering through the inlet nozzle by 50 degrees, from 373.15 K to 323.15 K. The pump maintains the selected mean inlet flow velocity throughout the transient. The cold gallium flowing into the hot gallium-filled vessel eventually develops a thermally stratified layer at the top of the upper plenum, above the side outlet ducts [Ward, Clark, and Bindra, 2019]. The transient experiments continue until the mean temperature of the liquid gallium flowing to the cold heat exchangers reaches 323.15 K. In these experiments, the power for the water cooling HEXs maintain a constant inlet temperature.

The performed PLOP experiments are for a wide range of liquid gallium average flow velocities at the bottom of the inlet duct (Table 3.1 and Fig. 3.2) [Ward, Clark, and Bindra, 2019]. The selection of the PLOP transient experiments with different inlet velocities cases will allow the present CFD simulation and modeling effort to examine the effects on the results for the inlet flow Reynolds number, Re_{in} both the laminar and turbulent flow regimes. Bindra, et al. [2020] reported that the time between tripping the heater and the inlet temperature dropping from 373.15 to 323.15 K is very short, and they modeled it as a step function in their CFD simulations of the experiments. The present simulations also use a step change in the inlet temperature of the entering liquid gallium at the beginning of the transient experiment (time t = 0.0 s).

Table 3.1. Reported experiment conditions of the inlet liquid Gallium flow in the PLOP experiments performed using the GaTE facility.

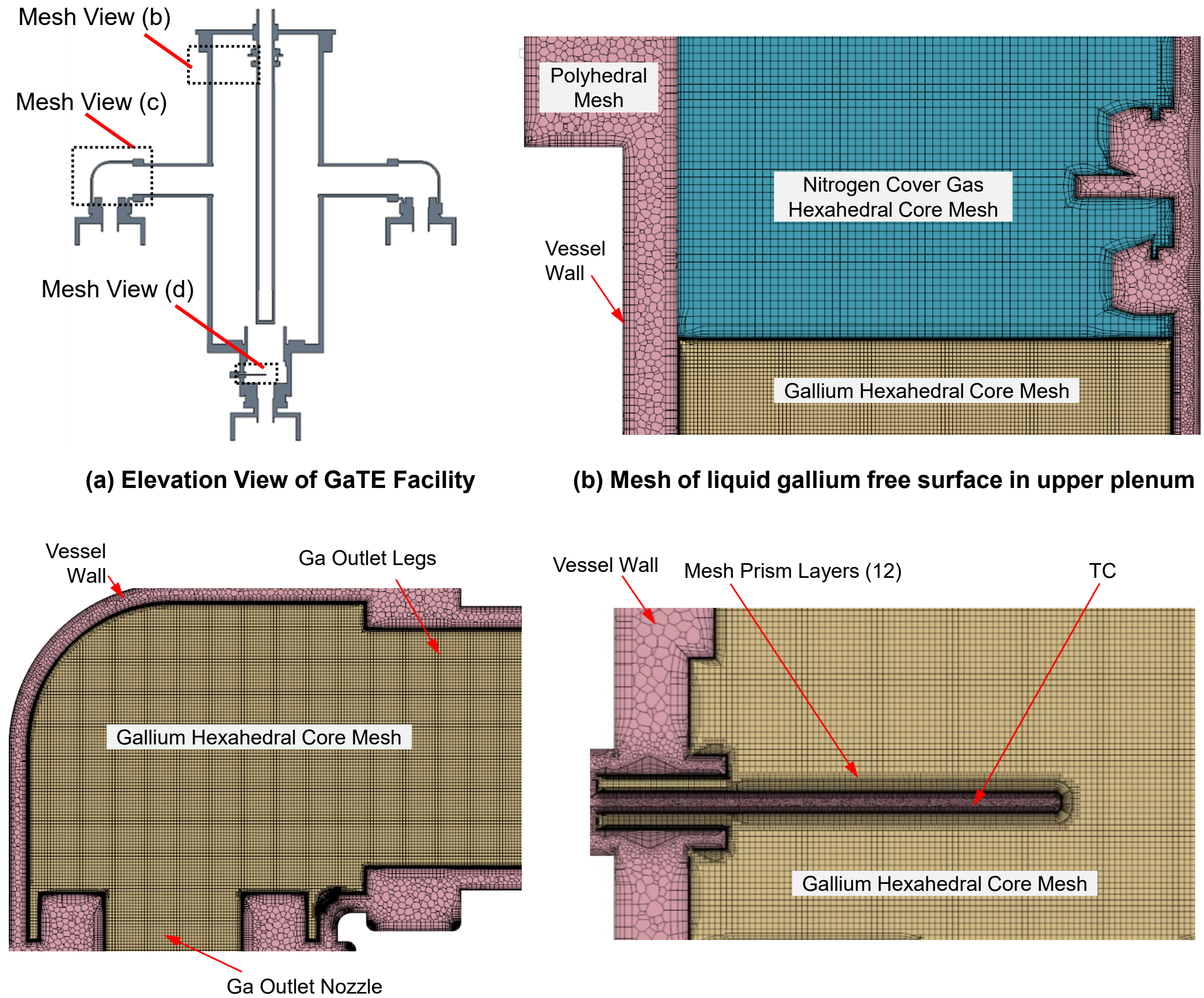
Inlet Velocity, U_{in} (mm/s)	Re_{in}	Initial T_{in} (°C)	Initial Mass Flow(kg/s)	Transients T_{in} (°C)	Transients Mass Flow (kg/s)
2.39	422	100	0.0895	50	0.0900
3.25	574	100	0.1217	50	0.1223
10	1770	100	0.3745	50	0.3764
20	3540	100	0.7491	50	0.7529
40	7070	100	1.4981	50	1.5057
60	10600	100	2.2472	50	2.2586
80	14100	100	2.9963	50	3.0114

4. CFD Methodology

The present CFD simulation and modeling effort of the performed experiments at the GaTE facility used the commercial CFD code STAR-CCM+. The simulated portion of the facility includes the stainless-steel plenum vessel shown in Fig. 3.2. Purdue University supplied the solid geometry files for the GaTE facility to UNM-ISNPS. The STAR-CCM+ meshing models had difficulty resolving the mesh along the threads from the solid geometry files without having to use a very small mesh size which significantly increased the computational cost. The geometry is simplified in parts to smooth the helical threading on some of the pipes, without affecting the CFD simulation. The outer surfaces of the 316 stainless-steel vessel and ducts are modeled with an insulated boundary condition, the inlet flow of the liquid gallium with a constant uniform velocity boundary, and a constant pressure boundary for the liquid gallium exiting the two side outlet ducts.

The performed CFD simulations begin with the level of the liquid gallium set at 0.0564 m below the top of the plenum vessel. This is the measured level reported by Ward, Clark, and Bindra [2019] in the experiments through a sight glass on the top of the vessel (Fig. 3.2c). The present simulations assume a rigid liquid free surface in the upper plenum between the liquid gallium and the nitrogen cover gas. This simplifying assumption will be examined in future modeling to evaluate the effects of on the calculated temperature and liquid flow fields, and on the stability of the thermally stratification layer of the liquid gallium in the upper plenum of the test vessel.

The present CFD simulations used both the Sheer Stress Transport (SST) k-ω Reynold's Averaged Navier-Stokes (RANS) turbulence model and the more sophisticated Large Eddy Simulation (LES) turbulence model. RANS turbulence models are widely used to provide adequate turbulence modeling for many thermal-hydraulic applications. They are computationally inexpensive but the approximations in solving the Reynolds stresses for the flow result in a poor performance when modeling flows with high swirl and mixing [Rodriguez and El-Genk, 2011]. The present simulations using the SST k-ω turbulence model used either the steady state solver or the implicit unsteady solver. The unsteady cases use a timestep size of 0.025s with 10 inner iterations per timestep. The RANS CFD cases utilize the All y+ Wall Treatment as the wall model. The implemented initial condition for the simulations is an isothermal temperature of 373.15 K with an initial velocity of 0 m/s.



(a) Elevation View of GaTE Facility **(b) Mesh of liquid gallium free surface in upper plenum**

(c) Mesh in elbow of horizontal outlet leg **(d) Mesh in gallium Inlet with TC**

Fig. 4.1. Numerical mesh grids used in the present CFD simulations in different regions of the Upper Plenum of theTest Vessel (Fig. 3.2a).

The LES turbulence model has a higher computational cost compared to the RANS models but is capable of superior performance in modeling swirling and mixing flows [Siemens PLM, 2023]. The LES model uses a Direct Numerical Simulation (DNS)-like solver to directly solve for the largest turbulent eddies in the flow, and a sub grid scale model for the smaller eddies. The present simulations use the Wall-Adapting Local Eddy-viscosity (WALE) subgrid scale model in STAR-CCM+ with the default input parameters. The wall is modeled using the All y+ Wall treatment model. The performed CFD simulation cases with the LES turbulence model use the implicit unsteady solver with the same 0.25s timestep as the Unsteady RANS (URANS) cases. The LES turbulence model requires a more developed field data for the initial condition for the stability of the solution [Siemens PLM, 2023]. Therefore, the present simulations are first modeled using an isothermal flow with the SST k-ω model to generate the numerical cell field data for the steady state condition. This CFD solution is input as the initial condition for the transient simulations using the LES turbulence model.

4.1 Numerical Mesh Grid

The implemented numerical mesh grid uses the Trimmer meshing model in STAR-CCM+ to generate a regular hexahedral cell elements in the fluid region with a base size of 0.5 mm (Fig. 4.1), selected to better capture the turbulent eddies in the CFD simulations using the LES turbulence model. The prism layer meshing model used generates 12 prismatic layers in the liquid hydrodynamic and thermal boundary layers adjust to the solid boundaries. The 1.0 mm thick prism layers have an exponential stretching factor of 1.2 between layers. The Polyhedral masher model in STAR-CCM+ uses a base cell element size of 2.0 mm in the solid stainless-steel wall of the upper plenum in the test vessel (Fig. 4.1). The solid mesh includes 6 prism layers to accurately calculate the interface temperature of the stainless-steel wall and the heat transfer by conduction from the vessel wall to the liquid gallium. The present CFD simulations use a fine mesh grid to ensure sufficient refined for the LES turbulence model to resolve the larger eddies in the flow. The fine mesh grid has 97.75 million volume cells in the liquid gallium region, 16.83 million mesh cells in the stainless-steel vessel and ducting, and 1.85 million mesh cells in the static nitrogen cover gas.

5. Numerical Simulation of the PLOP Experiments

This section presents the results of the performed STAR-CCM+ simulations in three of the PLOP experiments. In the PLOP10 experiment, the uniform gallium inlet velocity, U_{in} , is 10 mm/s, compared to 40 mm/s in the PLOP40 experiment, and 60 mm/s in the PLOP60 experiment (Table 3.1). Each experiment is first simulated with a uniform initial temperature of 373.15 K to establish the simulated flow patterns of liquid gallium within the upper plenum of the test vessel prior to the start of the transient. The results are then used for the initial condition for the transient simulation of the PLOP experiments. Section 5.1a compares the obtained simulation results for the isothermal flow of 373.15 K molten gallium through the upper plenum of the test vessel at different inlet flow velocities of the liquid gallium. Also compared are the obtained results of simulating the liquid gallium flow using the SST k-ω and LES turbulence models. Section 5.1b compares the obtained results of the performed CFD transient simulations of the PLOP10 experiment using both the SST k-ω URANS and LES turbulence models at a liquid gallium inlet flow velocity, U_{in} = 10 mm/s. The calculated temperature values of the liquid gallium in the plenum of test vessel are compared to the reported experimental measurements. These simulations assume a rigid and stationary free surface of the liquid gallium.

5.1a Simulation Results of Isothermal Experiments

The performed CFD simulations of isothermal liquid gallium in the upper plenum of the test vessel are during the pre-test startup phase when the oil heater and water HEXs maintain the molten gallium within the test vessel at a uniform temperature of 373.15 K. The results presented in Figs. 5.1 and 5.2 are of the calculated patterns using the SST k-ω URANS turbulence model of the liquid gallium flow within the upper plenum at three different inlet velocities, U_{in} = 10 mm/s, 40 mm/s, and 60 mm/s. The transient results are for 120s simulation time, which was considered sufficient for the CFD simulation residuals to converge. The plots in Fig. 5.1 show velocity contour plots for a plane section through the center of the two horizontal outlet legs (Section A-A in Figs. 3.2a and 3.2c). Fig. 5.2 shows line-integral-convolution plots of the flow vector field, detailing the formation and extent of the turbulent eddies within the liquid gallium flow in the upper plenum of the test vessel.

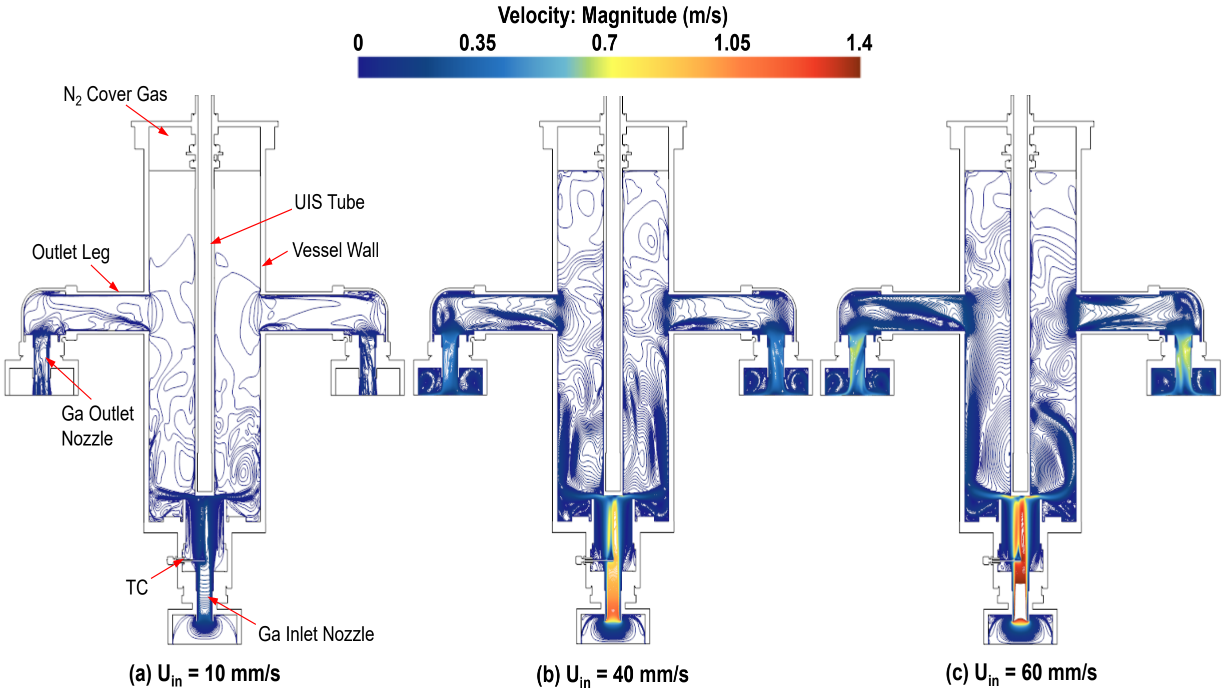


Fig. 5.1. Calculated flow velocity contours in CFD simulations using URANS SST k-ω turbulence model of pre-test isothermal conditions for the three selected PLOP experiments with different liquid gallium inlet velocities of 10, 40, and 60 mm/s.

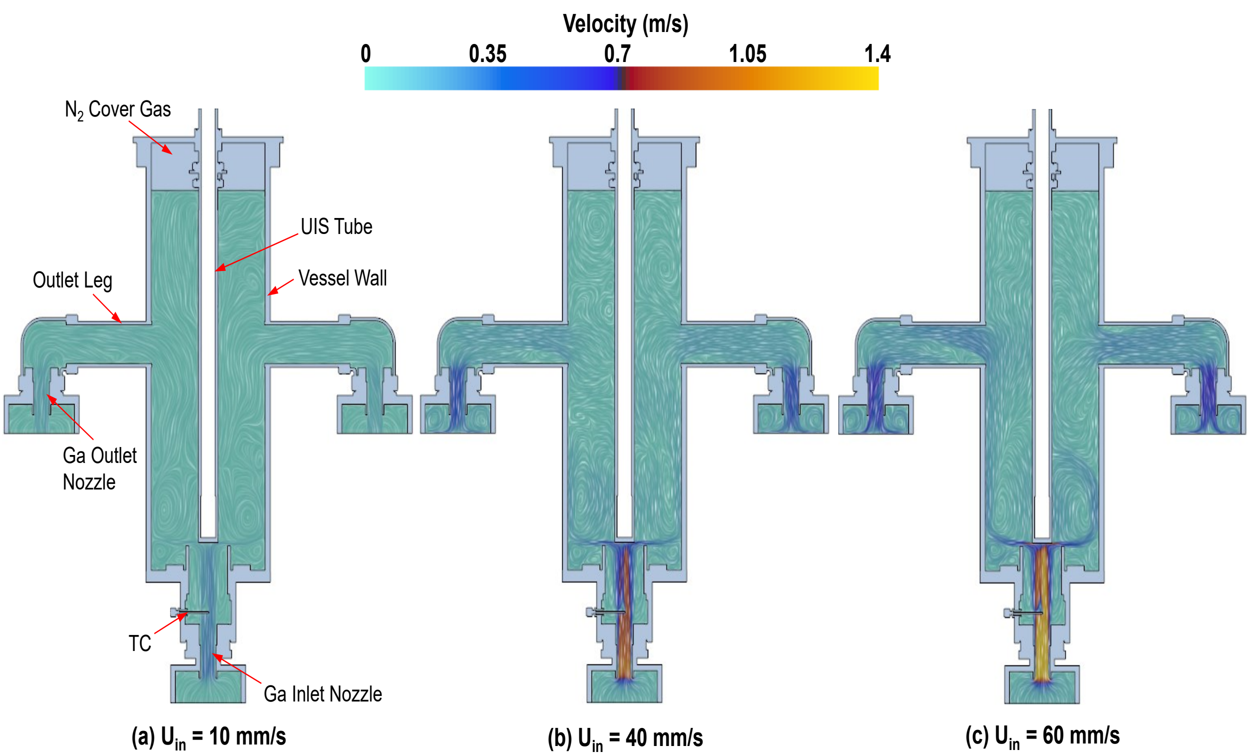


Fig. 5.2. Line integral convolution vector plots of the CFD simulations results using URANS SST k-ω turbulence model of pre-test isothermal conditions for the three selected PLOP experiments with different liquid gallium inlet velocities of 10, 40, and 60 mm/s.

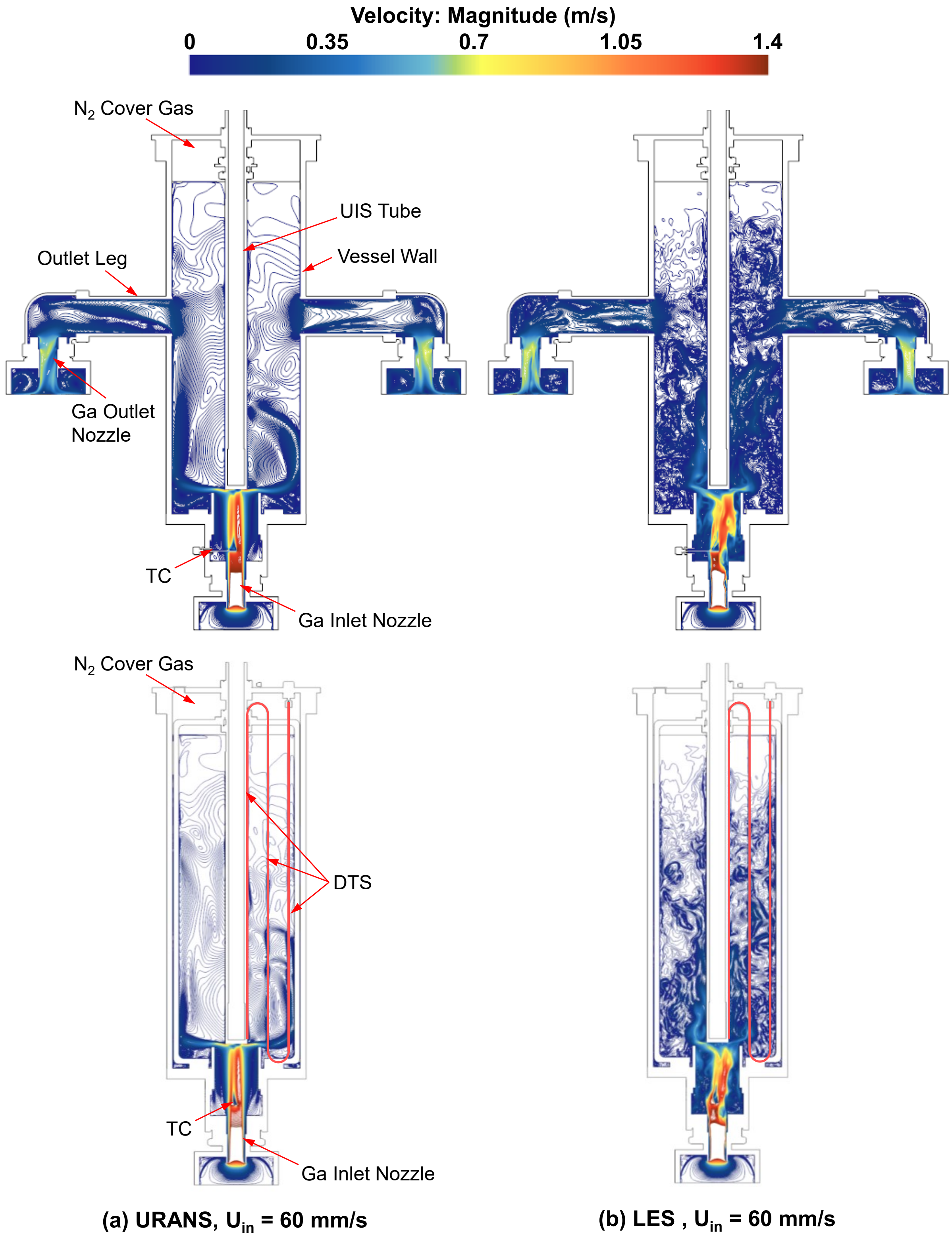


Fig. 5.3. Calculated velocity contour plots of the CFD simulations using: (a) URANS k-ω and (b) LES turbulence models of pre-test isothermal condition with liquid gallium inlet flow velocity of 60 mm/s.

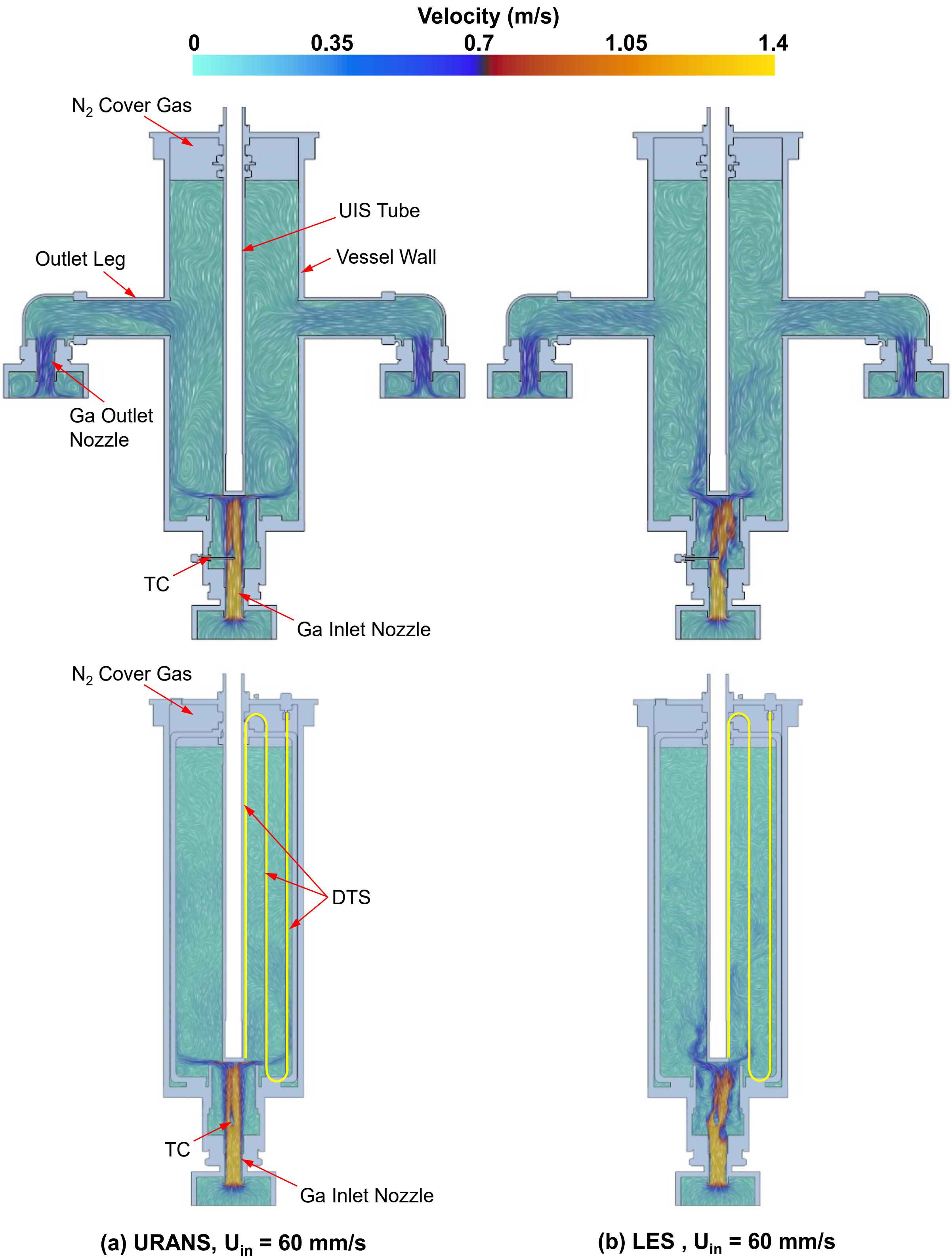


Fig. 5.4. Calculated line integral convolution vector plots of the CFD simulations using: (a) URANS k-ω and (b) LES turbulence models of pre-test isothermal condition with liquid gallium inlet flow velocity of 60 mm/s.

Liquid gallium entering through the inlet nozzle at the bottom of the test vessel flows upward in the entrance section. The gallium flow velocity is highest in this region, reaching 0.292 m/s for an inlet velocity U_{in} = 10 mm/s, 1.18 m/s for U_{in} = 40 mm/s case, and 1.77 m/s for U_{in} = 60 mm/s (Figs. 5.1a-c). The blue color in the image of inlet flow jet in Figs. 5.1b and c is of the wake as the flow moves past the inlet thermocouple. The inlet flow jet stagnates as it reaches at the bottom of the UIS tube and flows radially outwards towards the test vessel wall. The flow plots in Figs. 5.1 and 5.2 show the flow eddies within the test vessel before exiting through the two horizontal outlet legs and the constricting outlet nozzles. The velocity contour plots of the liquid gallium in the region extending from above the discharge to the outlet legs to the rigid free surface show comparatively little turbulence and similar overall flow patterns for the three different inlet velocities. However, the level of turbulence of liquid gallium in the upper plenum generally increases with increasing the inlet velocity. The flow images for U_{in} = 40 mm/s (Fig. 5.2b) and U_{in} = 60 mm/s (Fig. 5.2c) show larger numbers of flow eddies within the upper plenum compared to that for the lowest inlet velocity, U_{in} = 10 mm/s (Fig. 5.2a).

Figures 5.3 and 5.4 present the calculated velocity contours and the line integral convolution plots for the transient CFD simulations at U_{in} = 60 mm/s using the SST k-ω URANS turbulence model (Figs. 5.3a and 5.4a) and the LES turbulence model (Figs. 5.3b and 5.4b). The performed CFD simulations using the LES turbulence model predict more chaotic turbulent flow patterns within the upper plenum of the test vessel compared to the URANS turbulence model. The LES model shows that the high velocity flow exiting the inlet nozzle breaks up within the lower section of the upper plenum vessel, and intensely swirls as it enters the test vessel past the UIS tube (Fig. 5.3b). These results contrast with the those of the calculated flow patterns for the performed simulations using the URANS model, showing that the inlet liquid jet maintains its shape and does not break up (Fig. 5.3a). For the increased turbulence within the main volume of the test vessel, the line integral convolution plots show the formation of a greater number of smaller flow eddies (Figs. 5.4a and b). The predicted flow patterns by the two turbulence models become similar as the liquid gallium flow through the horizontal legs and exits through the two downward pointing outlet nozzles. The LES turbulence models have been reported to better simulate jetting and swirling flows [Rodriguez and El-Genk, 2011]. Therefore, the complex turbulent flow pattern obtained in the present simulation using the LES model could be because it captures more flow details than the simpler URANS model.

5.1b Transient Simulation of PLOP Experiment

This subsection presents the results of the present simulations of the PLOP10 experiment with a uniform inlet velocity of 10 mm/s using both the URANS and LES turbulence models. The simulated transient begins (t = 0 s) with liquid gallium, stainless steel vessel, and nitrogen cover gas at a uniform temperature of 373.15 K. The liquid gallium inlet temperature then decreases from 373.15 K to 323.15 K while the inlet velocity is maintained constant at 10 mm/s throughout the transient. The colder liquid gallium at 323.15 K continues to flow into the upper plenum test vessel throughout the duration of the transient.

The colder molten gallium entering the test vessel through the inlet nozzle located at the bottom mixes with the hotter gallium in the lower section of the test vessel (Fig. 5.5). At time t = 20 s the simulation using the URANS turbulence model shows the gallium flow entering the main volume of the upper plenum as a radial jet, compared to the case using the LES model which shows more chaotic flow mixing (Fig. 5.5a). As the simulated transient progresses in time, a stratified layer begins to form within the upper plenum of the test vessel, with the colder gallium progressing upwards through the vessel until it reaches the horizontal discharge legs on either side of the vessel (Figs. 5.5b and c). At t = 100 s, the colder gallium is still mixing in the lower portion of the vessel and the stratification layer extends beyond the side discharge outlets (Fig. 5.5b). At t = 200 s, the stratification layer moves above the axial location of the discharge outlets, with molten gallium being close to the inlet temperature (Fig. 5.5c). The thermal stratification layer slowly progresses upward with time (Fig. 5.5d) as the heat conducts downward from the hot gallium in the stratified layer at the top of the upper plenum of the test vessel to the colder gallium flow below. The simulation results using the LES and URANS models show differences in the first 100 s of the transient (Figs. 5.5a-b), but as the transient continues the calculated temperature fields for the two turbulence models become nearly identical (Figs. 5.5c-d).

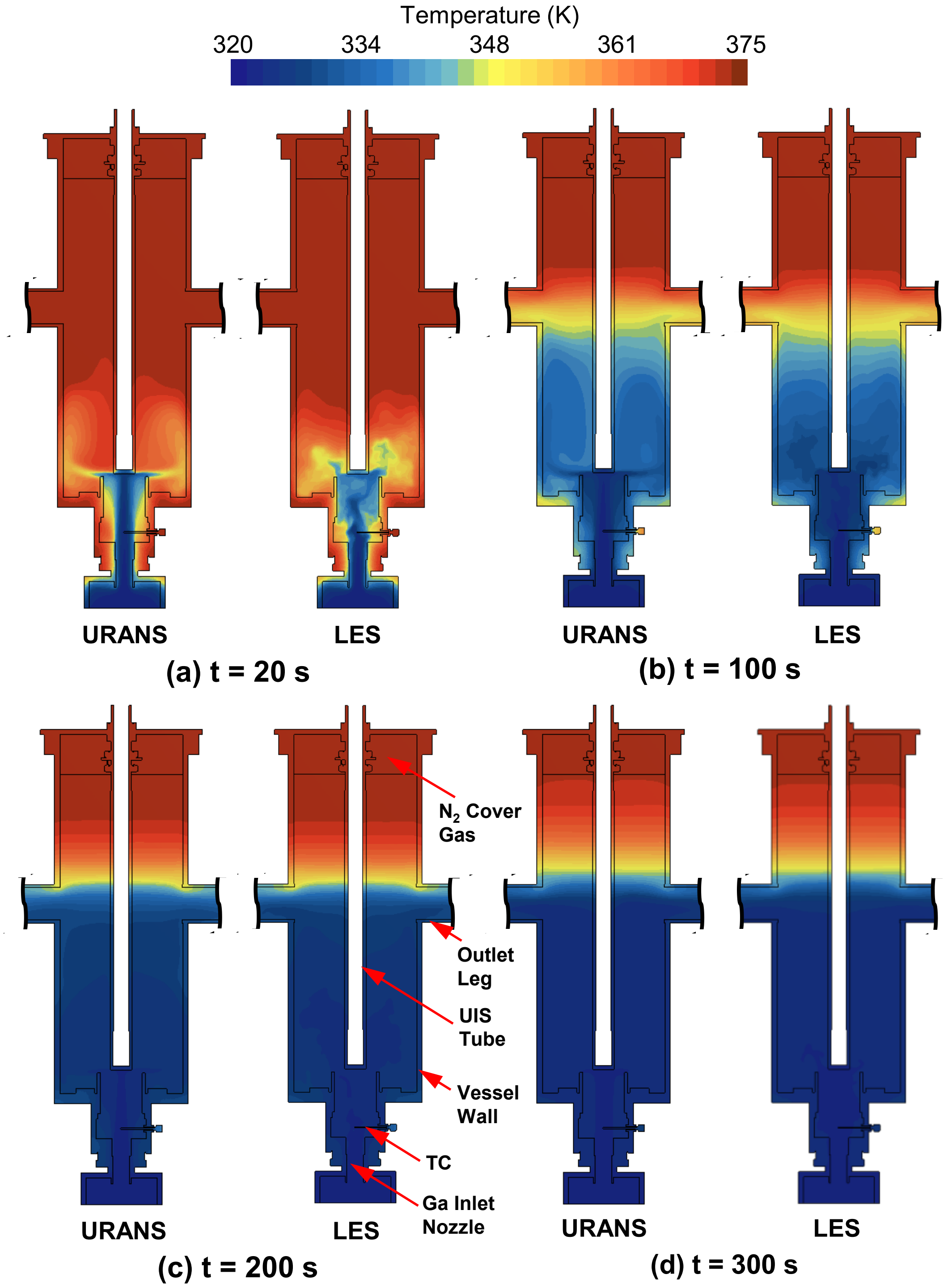


Fig. 5.5. Calculated Gallium temperature field in the CFD simulations of the PLOP10 experiment using the URANS k-ω and LES turbulence models.

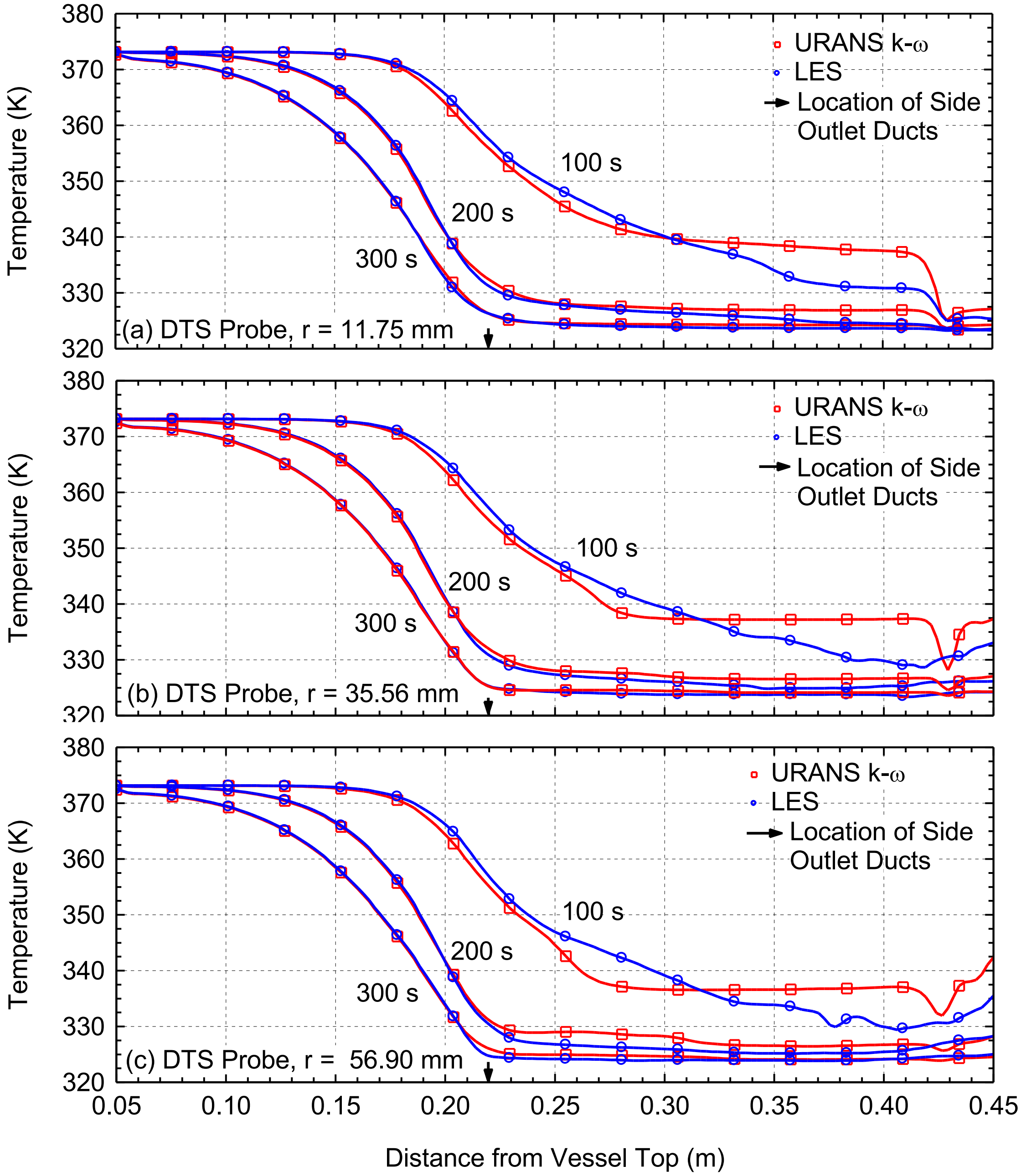


Fig. 5.6. Comparison of the calculated gallium temperatures in the simulated transient of the PLOP10 experiment using the URANS k-ω and LES turbulence models for the PLOP10 experiment at the three different radial locations of the DTS fiber tube.

Figure 5.6 plots the calculated molten gallium temperature along the three vertical sections of the DTS fiber tube at t = 100, 200, and 300 s during the simulated transient of the PLOP10 experiment. At time t = 100 s, the DTS probe at a radial distance, r = 11.75 mm and inserted into a groove in the wall of the UIS tube (Fig. 5.6a) records lower temperatures near the bottom of the test vessel than the probes that immersed fully in the flow at radial distances r = 35.56 mm (Fig. 5.6b) and r = 56.90 mm (Fig. 5.6c). The calculated temperatures in the present CFD simulation using the URANS turbulence model are largely flat in the portion of the vessel 0.3 m the vessel top. This is except for a narrow region where the inlet gallium jets flow radially outward in the gap between the top of the inlet pipe and the bottom of the UIS tube (Figs. 5.1a, 5.6a-c).

The performed CFD simulations using the LES turbulence model calculate low temperatures in the lower section of the test vessel and predict intense mixing of the hot and colder liquid gallium. At t = 100 s the formed thermal stratification layer is located between 0.13 m and 0.27 m below the vessel top. The temperature gradient between the hot and colder liquid gallium moves upwards and becomes steeper at t = 200s and 300 s (Fig. 5.6). At t = 200 s, the mixing of the colder and hot gallium in the upper plenum of the test vessel results in an almost uniform temperature in the region below the stratified liquid layer. The calculated temperatures in the CFD transient simulations using the LES and URANS turbulence models at time t = 300 s along the DTS probes are nearly the same (Fig. 5.6).

The measured temperature differences between the innermost (r = 11.75 mm) and outermost (r = 56.90 mm) vertical sections of the DTS tube, $\Delta T_p = (T_{r = 11.75mm} - T_{r = 56.90mm})$ are reported for the PLOP10 experiment at an axial location 0.2564 m from the top of the vessel [Ward, Clark, and Bindra, 2019]. The reported values are compared to the values of ΔT_p calculated in the present CFD simulations at the same axial location, z = 0.2564 m (Fig. 5.7). The reported experimental values of ΔT_p that are initially ~ 2 K steadily increases to a peak of ~4K during the first 300 s of the simulated transient, then decreases steadily to ~ 2 K at t = 500 s (Fig. 5.7). The calculated values of ΔT_p in the present CFD simulations start = 0 K, near the initial isothermal temperature, increases during first 100-140 s to ~ 2K, then decreases to 0 K at t > 300 s, due to the mixing of the colder and hot gallium in the test vessel. The present CFD transient simulation using LES turbulence model predicts that the temperature difference, ΔT_p, decreases faster with time than that predicted in the CFD simulation using the URANS turbulence model, due to a stronger flow mixing for the former. The predicted temperature difference in the CFD simulation using the URANS model becomes slightly negative for t > 180 s, due to insufficient flow mixing (Fig. 5.7).

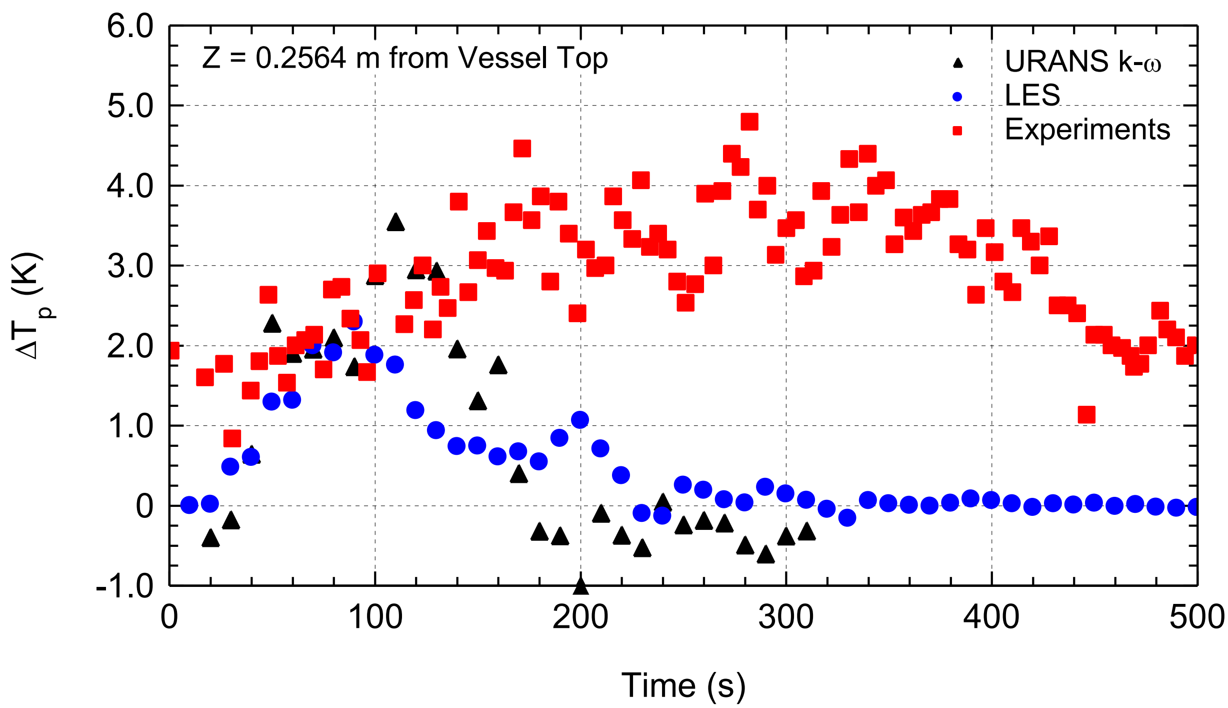


Fig. 5.7. Comparison of the calculated and measured gallium temperature difference ΔT_p the PLOP10 experiment at an axial location of 0.2564 m from the top of the test vessel.

Figure 5.8 compares the calculated values in the present CFD transient simulation of ΔT_p along the length of the DTS fiber tube at times t = 100, 200, and 300 s. The value of ΔT_p is near zero in the hot gallium at the top of the test vessel before it becomes slightly positive, then becomes negative across the thermal stratified layer (Figs. 5.8a and b). The performed CFD simulation using the LES turbulence model predicts larger fluctuation in ΔT_p in the region below the stratified layer, for all three time, reflecting the predicted intense flow turbulence and mixing. The performed CFD simulations using both the LES and URANS turbulence models predicts smaller values of ΔT_p than those reported in the experiment, due to predicting higher flow mixing in the simulations. This mixing results in a more uniform temperature for the liquid gallium in the test vessel with smaller values of ΔT_p (Figs. 5.7 and 5.8).

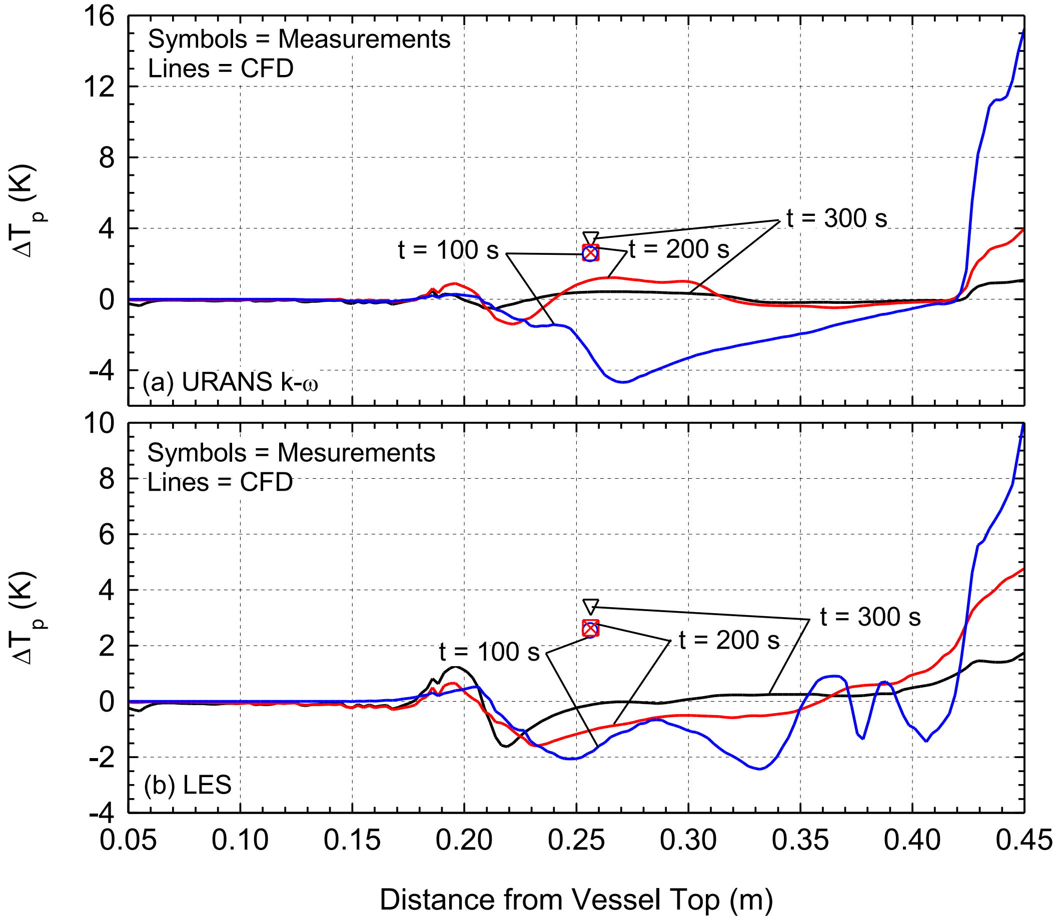


Fig. 5.8. Gallium temperature difference ΔT_p for CFD simulations using the URANS k-ω and LES turbulence models and reported measurements of the PLOP10 experiment.

Figure 5.9 plots of the calculated axial velocity of the molten gallium in the upper plenum test vessel in the performed CFD transient simulations at the three radial locations of the UDV probe. The presented CFD results are for both the LES and URANS turbulence models for time t = 300 s. The measured values of this velocity are not reported for the PLOP10 experiment, so the presented comparison in Fig. 5.8 is between the CFD results using the two turbulence models.

The calcuted velocity profiles in the transient CFD simulation using the URANS model are smoother than those calculated using the LES model (Fig. 5.9), which reflects the less chaotic gallium flow predicted by the URANS model. The calculated values of the axial velocity component at the radial location, r = 36 mm (Fig. 5.9a), are higher than those calculated at larger redial distances of r = 47 mm (Fig. 5.9b) and 58 mm (Fig. 5.9c) from the center of the vessel. The calculated velocity in the performed transient CFD simulation using the URANS model near the bottom of the test vessel (at > 0.42 m from the vessel top) are higher than those predicted using the LES model. This could be attributed to the jetting flow that turns upwards within the test vessel (Figs. 5.1a and 5.2a). Both turbulence models predict variation in the axial component of the flow velocity with axial location, from 0.42 m from the top to the location below the side outlet ducts. The negative axial velocity values calculated in the CFD simulations using with the LES turbulence model at r = 57 mm are because the larger number of the predicted flow swirling eddies in the test vessel causes the flow to move downward at several locations (Fig. 5.9c).

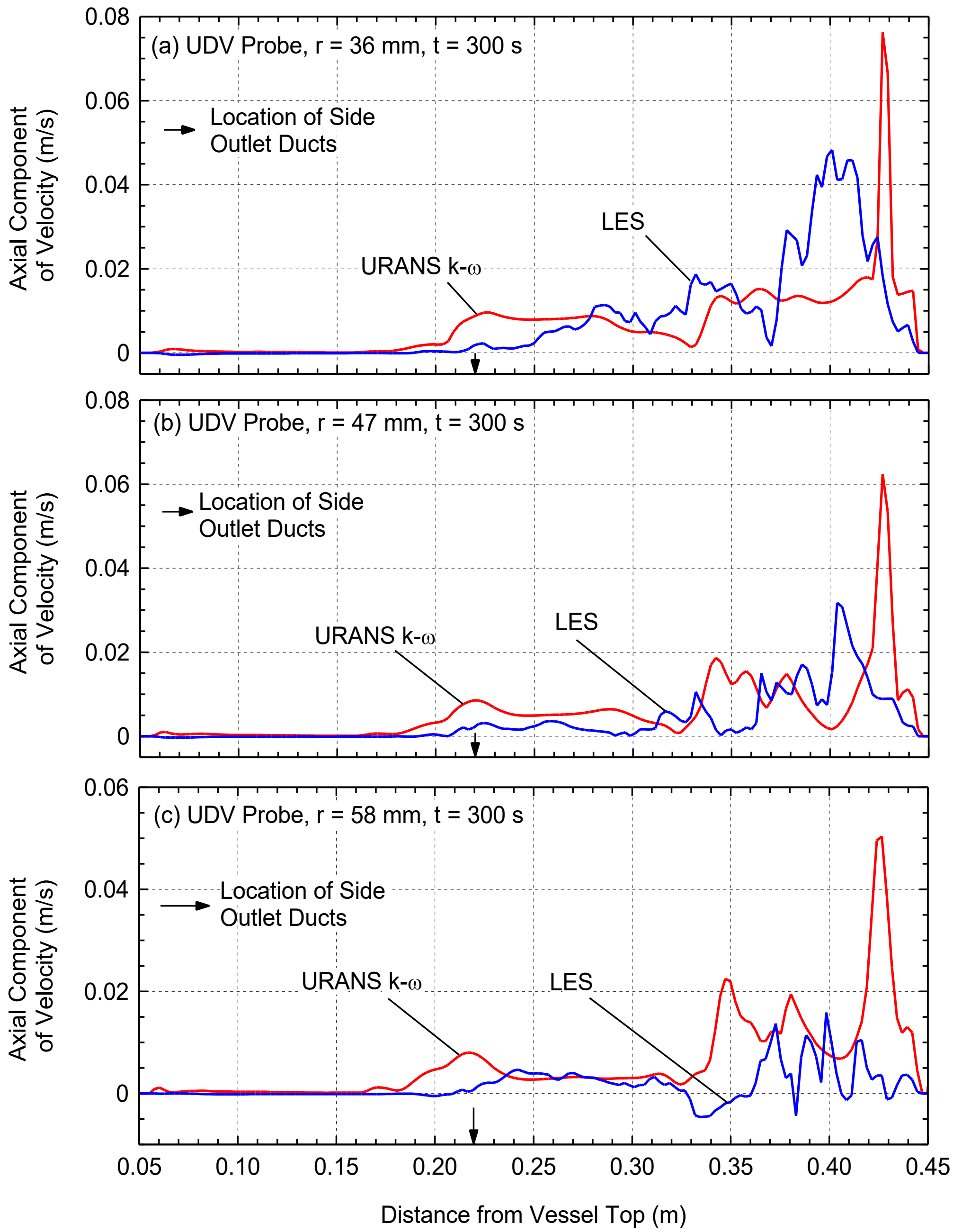


Fig. 5.9. Comparison of the calculated axial velocity component of liquid gallium in the performed CFD transient simulations using the URANS k-ω and LES turbulence models, at the three radial locations of the UDV probe in the PLOP10 experiment at time t = 300 s.

6. Summary and Future Work

This work presents the results of the first-year CFD simulation effort by the UNM-ISNPS for the 2023 DOE NUEP IRP *Exascale Simulation of Thermal-Hydraulics Phenomena in Advanced Reactors and Validation Using High Resolution Experimental Data*. This project aims to build expertise and capabilities for large scale CFD modeling and simulation of thermal-hydraulic phenomena in advanced SFRs and HTGRs at UNM and CCNY. During the 1st year of the project, the UNM-ISNPS team focused on recruiting and selected a graduate student for the project, identifying liquid gallium thermal stratification experiments conducted at the GaTE facility by Purdue University for the performing the CFD simulations, and training the graduate student on CFD modeling using the STAR-CCM+ commercial code.

The performed STAR-CCM+ CFD simulation simulations are first for the pre-test conditions for the PLOP experiments conducted in the GaTE facility. These are of isothermal conditions and gallium flow inlet velocities of 10, 40, and 60 mm/s. The performed CFD simulations with the STAR-CCM+ code used both the URANS SST k-ω and LES turbulence models to investigate the effects of the choice of turbulence model on the calculated flow patterns. The predicted flow in the CFD simulations using the URANS SST k-ω are similar for the three inlet flow velocities, but with increasing number of the turbulent eddies forming in the upper plenum test vessel with increasing inlet velocity. The LES turbulence model predicts more complex flow patterns with intense flow mixing of liquid gallium in the upper plenum test vessel than those predicted in the simulations using the URANS model.

Performed CFD simulations of the PLOP10 experiment investigated the effects of using the URANS SST k-ω and LES turbulence models on the development and the extent of forming a thermal stratification layer within the test vessel during the transient. The URANS and LES turbulence models predict different temperature profiles during the early periods of the PLOP10 transient, due to the higher liquid mixing predicted by the LES model. Once the thermal stratification layer develops early in the transient at times > ~100 s, the predicted temperature profiles by the two turbulence models become nearly the same.

The comparison of the performed CFD simulation results to the reported temperature measurements in the PLOP10 experiment shows the effect the simulations predicted flow mixing of the liquid gallium in the upper plenum of the test vessel. The predicted values of radial temperature difference across the test vessel are compared to those measured using the DTS fiber tube. The predicted values in the CFD simulations are consistently smaller than the reported measurements in the experiment.

Future work will simulate the PLOP40 and PLOP60 transient experiments with higher inlet flow velocities of 40 and 60 mm/s and compare predictions to the reported experimental measurements of the liquid gallium temperatures and velocities. We also plan to investigate the effects of modeling the free surface interactions of the liquid gallium in GaTE test vessel and the nitrogen cover gas on the transient temperature and flow velocity predictions of the PLOP experiments. The predictions will be compared to the reported experimental measurements, The Volume of Fluid (VOF) Eulerian Multiphase model in STAR-CCM+ will be used to simulate the movement of the gallium free surface in the upper plenum of the test vessel surface. The results will help quantify the effects of assuming a rigid surface in the CFD simulations and of incorporating a free surface on the behavior of the thermally stratification and flow field of the liquid gallium in the upper plenum of the test vessel.

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