URANS SIMULATIONS OF THERMAL STRATIFICATION IN A LARGE ENCLOSURE FOR SEVERE ACCIDENT SCENARIOS

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ABSTRACT

The introduction of a jet of fluid into a more or less stationary body fluid at a different temperature can lead to thermal stratification, and these processes are expected to be important in some severe nuclear accidents. Thermal stratification within the secondary containment could affect the ability of the containment to reject decay heat, for example. An ability to predict the behavior of the fluid under these circumstances is thus important. Such flows are complex, and computational fluid dynamics approaches are needed to resolve them, but they do present modeling challenges that go beyond those of more common 'forced' flows.

In an effort to develop a computational methodology for CFD analyses of thermal stratification within large enclosures, the Twin Jet Water Facility (TJWF), discussed in previous works, was constructed to provide experimental data against which to assess the performance of various CFD modeling approaches. The TJWF allows for one or two heated jet(s) to enter vertically from below into a cooler pool of water, with either water recirculated, or with the water level allowed to rise. This work focuses on a single slender planar heated jet entering cooler water, and in which stratification is then seen to occur with a raising water level.

In this study, CFD analyses using unsteady Reynolds averaged (URANS) turbulence models such as low-Re κ-ε and SST-κ-ω are conducted, and the experimental data from the TJWF for the same test cases are compared to the computational results. The modeling deficiencies and potential causes of errors arising from the use of each approach is discussed. The results and conclusions for this work provide guidance for URANS simulations of such circumstances. This work was performed using the CD-adapco's STAR-CCM+ v9.04 CFD code.

KEYWORDS

Thermal Stratification, Thermal Mixing, Computational Fluid Dynamics, URANS, Turbulence Modeling

1. INTRODUCTION

The propensity for thermal stratification during some severe accidents can be a significant determinant of the severity of their consequences. Such stratification can reduce passive heat transfer, contribute to structural damage, and lead to high concentrations of hazardous chemical and radioactive species [1]. In large enclosures such as the containment building or spent fuel pool, a single jet of hotter fluid can lead to a large layer of hot fluid building up in the top of control volume. This phenomenon is very difficult to model accurately using computational fluid dynamics (CFD) approaches, because of the complexity of the flow caused by the entry of a highly turbulent thermal jet into a previously quiescent cooler temperature volume.

Recent efforts under the Department of Energy (DOE) Nuclear Energy Advanced Modeling and Simulations (NEAMS) initiative to develop and strengthen computational tools for reactor modeling motivated the present work. The thermal stratification experimental and computational research is being performed with the support of DOE NEAMS to provide high fidelity experimental data to benchmark and validate new tools against, and investigate modeling approaches. The current data sets were created in the Twin Jet Water Facility (TJWF) at the University of Tennessee, Knoxville and provide the basis for validation in this paper. The simulations are being conducted jointly by researchers at Texas A&M University and Imperial College London.

In Section 2, we present a brief summary of the main literature in this area. The experimental facility is described in Section 3, and the approach adopted in the modeling is outlined in Section 4. The comparison of the measured behavior, and predictions using the various approaches, is presented in Section 5, and the conclusions are drawn in Section 6.

2. LITERATURE REVIEW

The modeling of buoyant and momentum-driven jets is at the heart of the study of thermal stratification. Improper modeling of the physics governing these complex jets gives misleading predictions of how thermal stratification develops, and how it dissipates or grows [1]. For this work, a jet that is initially buoyancy and momentum driven which then develops into predominately buoyancy-driven jet is studied. An extensive review of pre-1980 experimental data on turbulent buoyant jets is provided by Chen and Rodi [2]. This review includes a discussion of the transition from momentum-driven jets to buoyancy-driven plumes and correlations for predicting centerline velocity and temperature behavior for jets and plumes that involve buoyancy effects. Kumar and Dewan [3] discuss the early and more recent advances in computational modeling applied towards turbulent thermal plumes. This review includes modeling efforts using direct numerical simulations (DNS), large eddy simulations (LES), and Reynolds averaged Navier-Stokes (RANS) approaches. The RANS investigation covered the standard κ-ε [4] and realizable κ-ε [5] turbulence models and includes different approaches to the modification required to account for the buoyancy terms. The different modifications mostly involved accounting for a changing density through the introduction of a source term in the turbulence kinetic energy equation. These source terms are modeled by the simple gradient diffusion hypothesis (SGDH) or the generalized gradient diffusion hypothesis (GGDH). This is required due to the κ-ε family being mostly based on a constant density formulation. The mean flow characteristics of mixed jets and turbulent plumes were able to be more accurately simulated using these modifications. Additionally, Kumar and Dewan summarize experimental developments concerning thermal jets and plumes after 1980 which were used to further drive LES and RANS modifications. Outside the κ-ε turbulence model family, the κ-ω turbulence model has been used to simulate both turbulent jets and plumes by Malin and Spalding [6] and found this model was in decent agreement with experiment data. The previous efforts to model these jets are used as guidance for the selection of the turbulence models used to properly simulate jet behavior seen in the experiments discussed later in this paper. This allows the focus of the work presented below to be primarily on simulating the enclosure behavior (i.e. buildup of the stratified thermal layer). It is plainly desirable to investigate the ability of other turbulence models, beyond these, to simulate thermal turbulent jets and thermal plumes. This is discussed in a qualitative manner while the thermal stratification is discussed in a quantitative manner using comparisons to experimental data.

With particular relevance to the thermal stratification in large enclosures using a mixed driven jet, previous efforts to model this behavior using a Finite Element Method (FEM) and deformable meshing were reported by L. B. Carasik, S. Walker, and A. E. Ruggles [7]. The behavior due to buoyancy was modeled using the Boussinesq variable density approximation. To model the increasing water level height throughout the simulation, the mesh was deformed vertically with a speed corresponding to the experiments. The authors concluded that the Shear Stress Transport (SST) [8] turbulence model was better suited to simulate this behavior as opposed to the Spalart-Allmaras [9], [10] turbulence model.

3. TWIN JET WATER FACILITY AND THERMAL STARTIFICATION EXPERIMENTAL STUDY

The TJWF was originally developed at the University of Tennessee, Knoxville to develop high-resolution temperature and velocity data sets in various conditions involving vertical jets impinging into a pool of fluid. The fluid can be quiescent or turbulent before the jet is admitted. Data is acquired using a variety of measurement techniques. For the thermal stratification studies, type T thermocouples were used to acquire point temperature measurements at different heights during the experiments. The TJWF and the thermocouple instrumentation is shown in Fig. 1. Further information is given in previous publications [11], [12].

3.1. Thermal Stratification Experimental Study

The thermal stratification experimental study was conducted with one (of the two possible) hot jets being injected into a quiescent, ambient temperature body of water. A hot jet of water was injected into the volume for a specified time during which stratification was made visible by dye injections, and temperature measurements were acquired. The experimental tests were conducted for a duration of 2-3 minutes and involved temperature differences of 25-45 C between the jet and tank volume. Temperature data sets for different inlet flow rates and temperature differences were developed and are being used for the computational studies being conducted. Further discussion of the thermal stratification experiments can be found in previous works [7], [11].

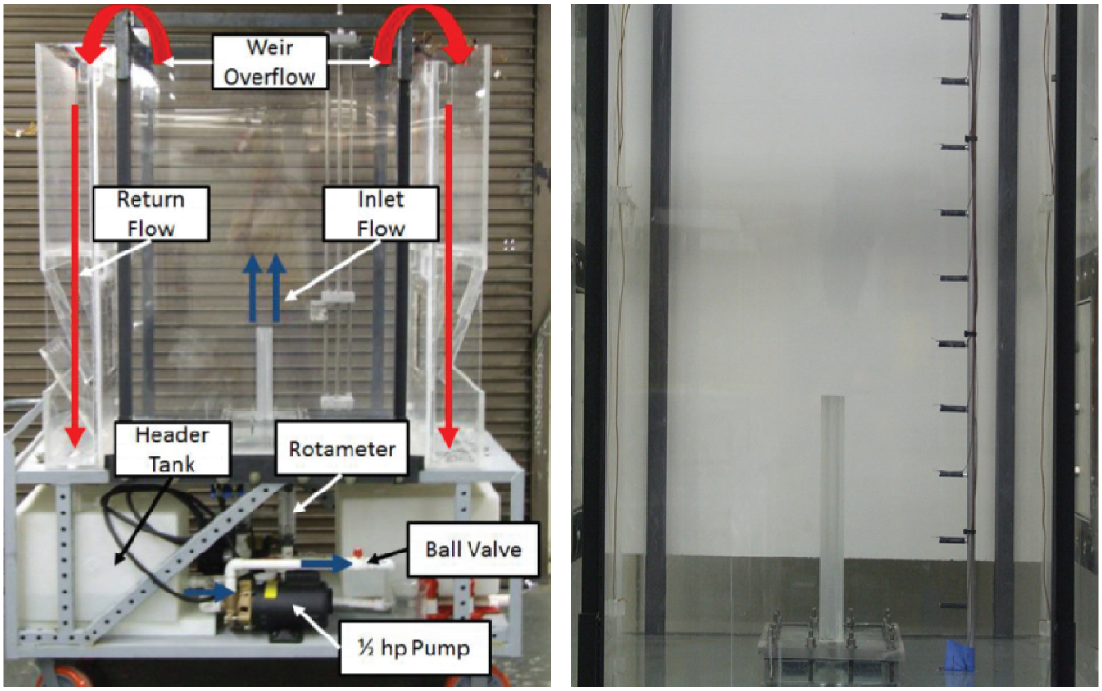

Figure 1. Twin Jet Water Facility and Measurement Instrumentation for Thermal Stratification Studies

An initial experimental trial to prove that thermal stratification can occur within the TJWF is shown with the aid of red dye in Fig. 2.

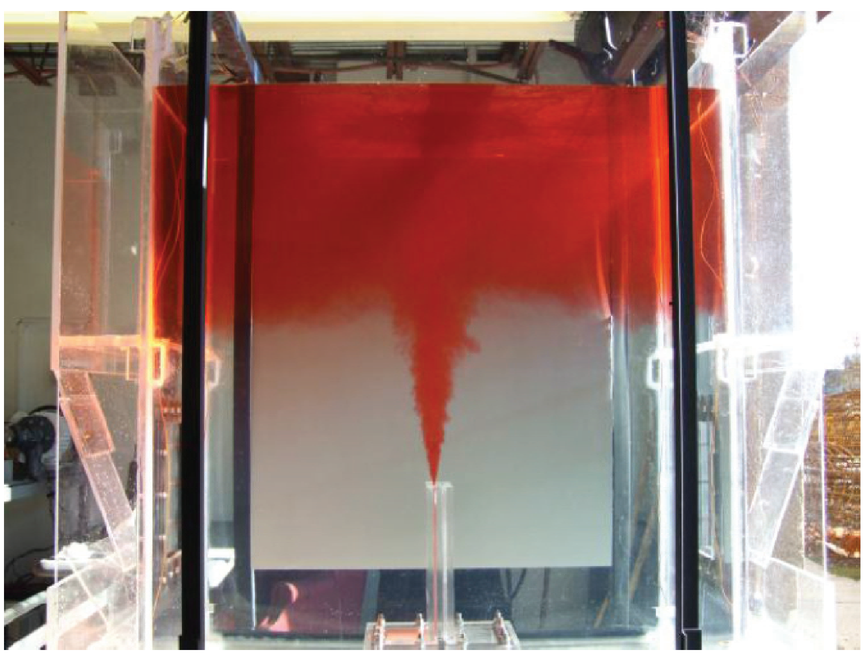

Figure 2. Initial Trial showing Thermal Stratification within the TJWF

The specific trial used for comparison with the simulations is summarized in Table I which is the same one used by L. B. Carasik, S. Walker, and A. E. Ruggles [7].

Table I. Thermal Stratification Trial Conditions

Condition	Value
Inlet Mass Flow Rate	0.248 kg/s
Inlet Jet Temperature	58.5 C
Tank Volume	20.8 C
Height of Starting Water Level	0.66 m
Height of Ending Water Level	0.71 m

4. COMPUTATIONAL METHODOLOGY AND SET UP

4.1. Computational Domain and Meshing

The computational domain for the TJWF was split into two subdomains, the inlet jet and enclosure volume, to be run as two different simulations. Fig. 3 shows the division of the computational domain and where the inlet jet conditions feed into the enclosure volume. Steady state fully developed flow was computed with a periodic domain to generate fully developed velocity and turbulence profiles that can be used as an inlet condition for the transient simulation in the large enclosure. This reduced the time needed to model the physics of interest for these studies.

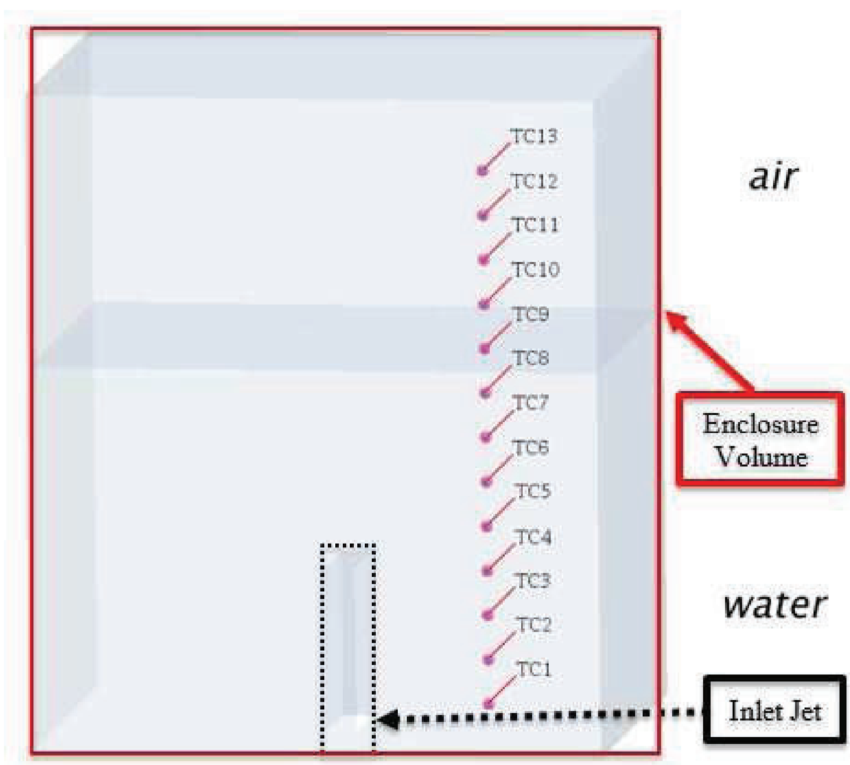

Figure 3. Division of the TJWF Computational Domain and Temperature Probe Locations

4.1.2. Enclosure volume domain and mesh

The enclosure volume is modeled using the as-built dimensions from the TJWF and meshed using the standard mesher in STAR-CCM+. The trimmer and prism layer meshers are used to develop the mesh with specific mesh controls for refinement. The base size was set to 5 mm with a maximum cell size of 0.5 m for the largest cells. There were 5 prism layers set for the walls of the domain with the total thickness of the prism layers set to 0.01 m and a 1.1 growth rate. Refinement areas are defined to resolve higher gradients near the jet outlet, jet spreading region and water level regions. The mesh and specified refinement areas are shown in Fig. 4 with the specific sizing summarized in Table II. A mesh sensitivity study was conducted utilizing the Standard Low-Reynolds κ-ε model and physical models discussed in later sections. The base size was varied for three different meshes and the temperature traces of each thermocouple were compared. The base size listed in this work was found to show sufficiently mesh independent results.

Table II. Mesh Size for each Refinement Area

Refinement Region	Size
Jet Outlet Fine	0.3 mm
Jet Outlet Coarse	1 mm
Jet Expansion	5 mm
Jet Expansion Core	3 mm
Water Level	5 mm

The boundary conditions are labeled on Fig. 4 and summarized in Table III. The initial conditions for turbulence were defined using the turbulence intensity and length scale. The turbulence intensity was set to zero for everywhere within the volume and the length scale was set to the width of the tank. The inlet turbulence conditions were defined using the precursor simulation for the inlet jet. The inlet jet and tank temperature were as measured, at 58.5 C and 20.8 C respectively.

Table III. Boundary Conditions for the Enclosure Domain

Boundary Type	Boundary Values	Surface List
Velocity Inlet	Defined by precursor simulation for velocity, temperature, and other parameters of interest	1
Pressure Outlet	Atmospheric Pressure	2
Walls	Non-slip	0

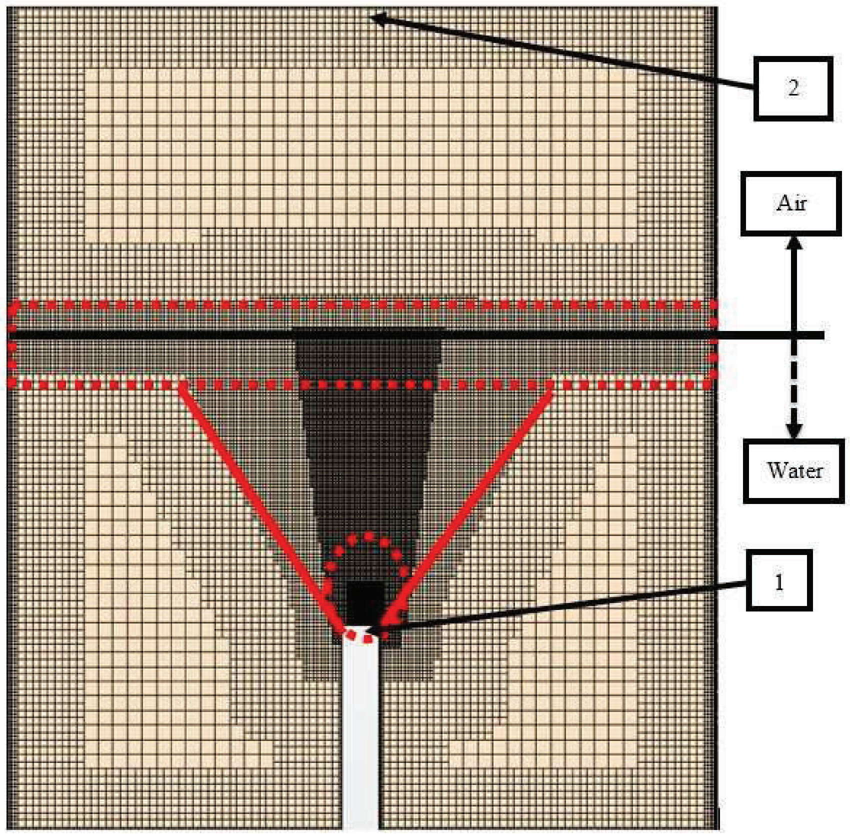

Figure 4. Mesh and Boundary Conditions for the Enclosure Volume, Jet Outlet – Dotted Oval, Jet Spreading Region – Solid Lines, Water Level Region – Dotted Rectangle

4.2. Modeling Approach

4.2.1 Physics Models

The variable density RANS equations for the water and constant density RANS equations and total energy equations are solved within a finite volume framework for each phase using the commercial package STAR-CCM+ v9.04. The SIMPLE algorithm was employed to handle the coupling of the pressure and velocity fields. The buoyancy source term for the water took into account variable density and other properties. The Eulerian multiphase mixture model using the Volume Of Fluid (VOF) approach with phase interactions was used to model the raising free surface of the water. The water properties were calculated using the International Association for the Properties of Water and Steam (IAPWS-IF97) database [13]. The air properties were set as constants as the behavior of the air is not critical for this study. The implicit unsteady formulation with a 2nd order temporal discretization is used for advancing through the simulations [14].

4.2.2 Turbulence Modeling

The turbulence modeling was conducting using the Unsteady Reynolds averaged Navier Stokes (URANS) approach, with wall functions for near-wall regions. The all-y^+ wall treatment was used for each turbulence model to account for wall effects, and the first prism layer were held within $y^+ \sim 1$. The turbulence models used were the Standard Low-Reynolds κ-ε [15], Elliptic Blending κ-ε (EBKE) [16], and Shear Stress Transport κ-ω (SST) [8] models. Due to its common use in industrial applications, its improved ability to resolve near-wall region behavior, and improved performance in low Reynolds numbers flows as seen here, the Standard Low-Reynolds κ-ε was selected as the baseline model. The common usage of κ-ε turbulence models to simulate turbulent thermal jets and plumes justified this selection. The improved near wall modeling by the introduction of additional equations and good predictions of a wide range of flows offered by the EBKE, with only a modest cost penalty, led to its inclusion in the study. Finally, the SST model was selected due its usage in previous works [7] and its good ability to model free shear flows.

4.3. Solver Definition

A sufficiently small-time step was taken to be one that caused the majority of cells to have a courant number below one, and this was achieved with a timestamp value of 1 ms. The 'iterations per time step' was set at between 200-300 for the first 0.1-0.3 seconds, to allow for system to stabilize numerically, after which the rapid reduction of the most significant residuals allowed it to be reduced to about 30.

4.4. Post Processing

The post processing was selected both to create simplified plots for comparison against experimental data, and to provide good visualization of the stratification process. The temperature within the enclosure volume was recorded at each experimental measurement point using point probes in STAR-CCM+. The probe locations within the enclosure volume are shown in Fig. 3.

5. RESULTS

The results for this study focus on the sensitivity to turbulence modeling in the enclosure volume. The turbulence modeling study provides insight into which of the three turbulence models can most closely predict the measured thermal stratification and temperature trends. For the study, only the point probes corresponding to thermocouple locations 5-9 are plotted, as it is here the most significant variations occur. The other probe locations are either outside of the area of interest due to the water level placement, or exhibit temperature variations of less than 0.1 C during the trial.

5.1. Turbulence Modeling Study

The evolution of both velocity and temperature fields for each turbulence model are shown and compared to determine performance of each model.

5.1.1 Experimental Data Comparison

The temperature traces of each point probe from both the experimental data and the simulations are shown in Fig. 5, 6 and 7. The experimental data for the thermocouples was curve fitted using the smoothing functions built-in to MATLAB. The specific model used was a local regression technique using the weighted linear least squares and a 2^{nd} degree polynomial method.

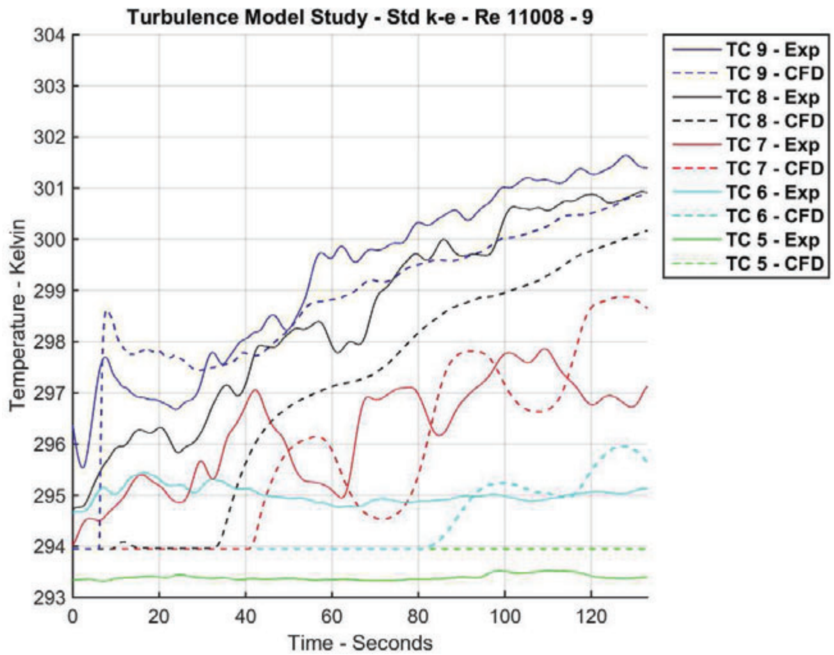

Figure 5. Comparison of Experimental and Simulation Temperature Traces Standard Low - Reynolds κ-ε.

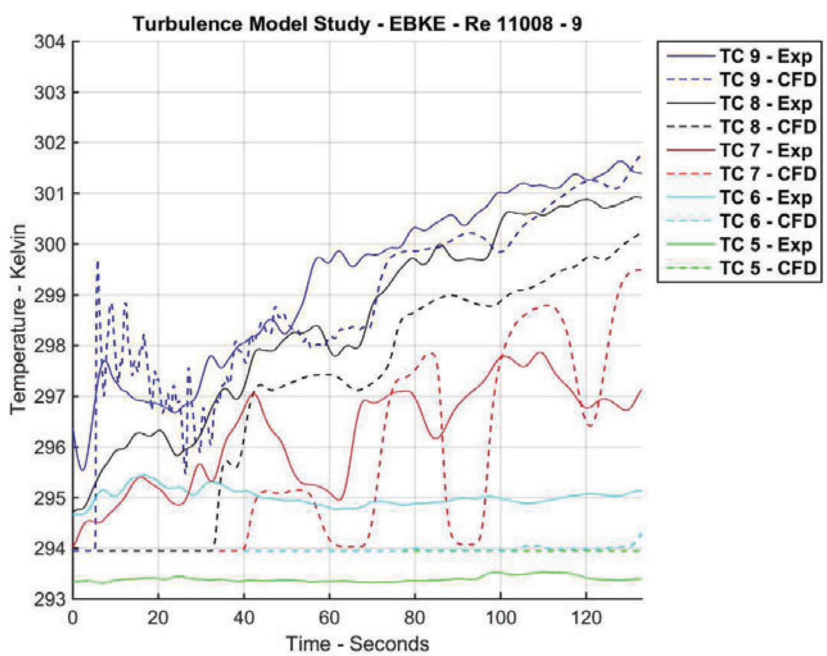

Figure 6. Comparison of Experimental and Simulation Temperature Traces - EBKE.

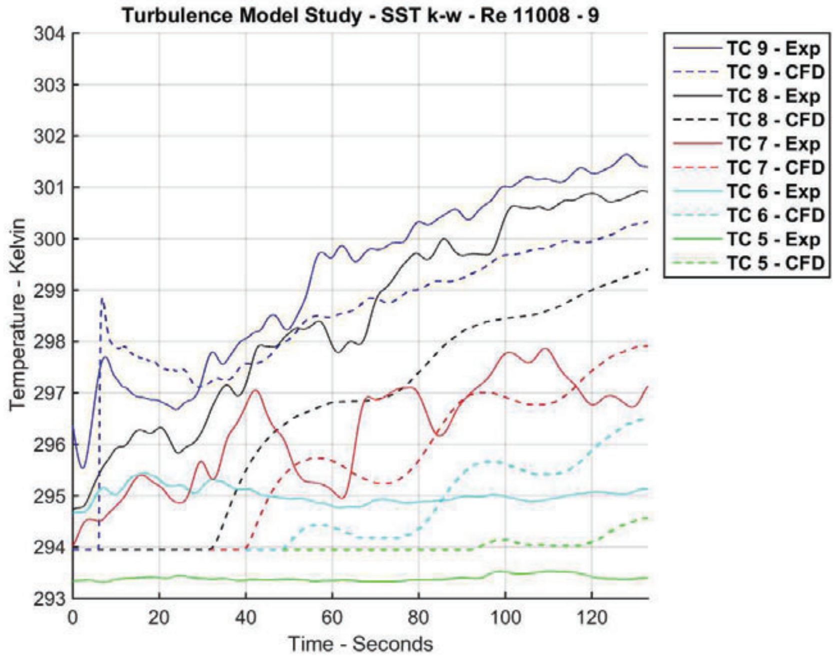

Figure 7. Comparison of Experimental and Simulation Temperature Traces - SST.

The CFD simulation results show early deviation from the experimental results within the first 20 seconds. This is observed when analyzing the TC 9 response for both the experiment and CFD simulations at ~5 seconds. Within this time, the initial temperature spike occurs but is under-predicted by the CFD simulations and does not show the earlier warm-up before the hotter water reaches TC 9. The TC 6-8 do not have a similar response within the first 40 seconds for the CFD simulations as what was observed during the experiment. Unfortunately, the TC 6 for the experiment shows a potential issue with calibration due to it predicting through the experiment a higher temperature than the original tank temperature throughout the experiment. TC 8 and 9 were observed to be in the growing thermal layer after 20 seconds into the experiment which is not captured properly by the CFD simulations. The EBKE simulation was the closest to simulating this behavior but the TC 8 temperature was under-predicted throughout the simulation. The behavior of TC 7 for the experiment has large period oscillations due to the movement of the hotter fluid. The Standard Low-Reynolds κ-ε and EBKE simulations were observed to somewhat capture these oscillations with varying success. This can be seen by how both TC 7 temperature traces oscillations are shifted in time. The EBKE has large variations of the oscillations where the magnitude increases or drops as much as 5 degrees within a very short period of time. This is much more severe than what was observed in the experiment for which TC 7 never reached the original tank temperature after heat up. For the Standard Low-Reynolds κ-ε and SST models, TC 6 heated up towards the end of the simulations which was not observed during the experiment. Additionally, the SST model's TC 5 started to heat up within the last 20 seconds of the trial which is a modeling deficiency. The EBKE simulation did not show TC 5 and 6 heat up and the heated fluid was concentrated in roughly the same regions as the experiment. Overall the EBKE simulation provided the strongest comparison to the experimental data and all three simulations showed a vast improvement over previous work [7].

5.1.2 Evolution of Velocity Fields for each Turbulence Model

The velocity fields for each turbulence model are shown at 8, 65 and 130 seconds into the trial time in Fig 8, 9 and 10. This is to show progress at the time of impingement on the free surface, half way through the trial, and the end point of the trial.

Figure 8. Evolution of Velocity Field for the Standard Low-Reynolds κ-ε Simulation at 8, 65 and 130 Seconds

Figure 9. Evolution of Velocity Field for Elliptic Blending κ-ε Simulation at 8, 65 and 130 Seconds

Figure 10. Evolution of Velocity Field for Shear Stress Transport κ-ω Simulation at 8, 65 and 130 Seconds

The Standard Low-Reynolds κ-ε and SST simulations are observed to have very similar velocity profiles within the water region of the domain. Both simulations show roughly the same jet-spreading angle and do not vary significantly after the initial impingement on the water's free surface. The EBKE simulation is observed to have a drastically different velocity profile from both the Standard Low-Reynolds κ-ε and SST simulations. The jet in the EBKE simulation is predicted to wave back and forth throughout the trial, consistent with what was seen during initial dye runs of the experiment. The overall jet spreading angle for EBKE is much larger than the Standard Low-Reynolds κ-ε and SST angles due to this wavy behavior.

5.1.3 Evolution of Temperature Fields for each Turbulence Model

The temperature fields for each turbulence model are shown at 8, 65 and 130 seconds into the trial time in Fig 11, 12 and 13.

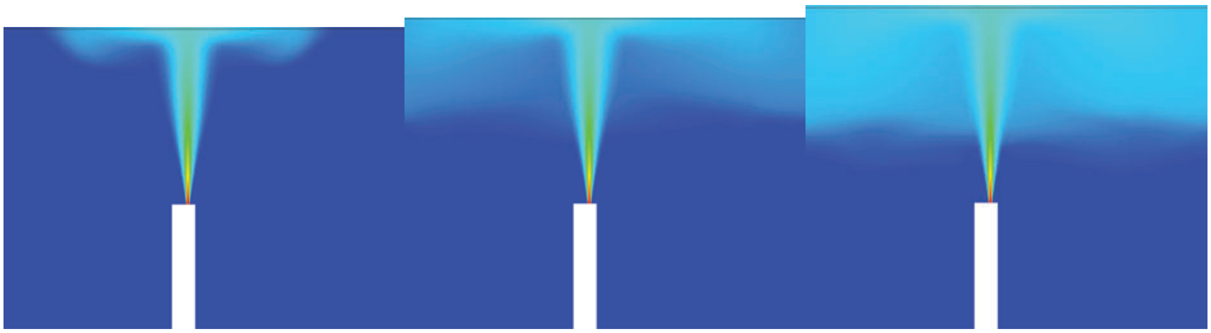

Figure 11. Evolution of Temperature Field for the Standard Low-Reynolds κ-ε Simulation at 8, 65 and 130 Seconds

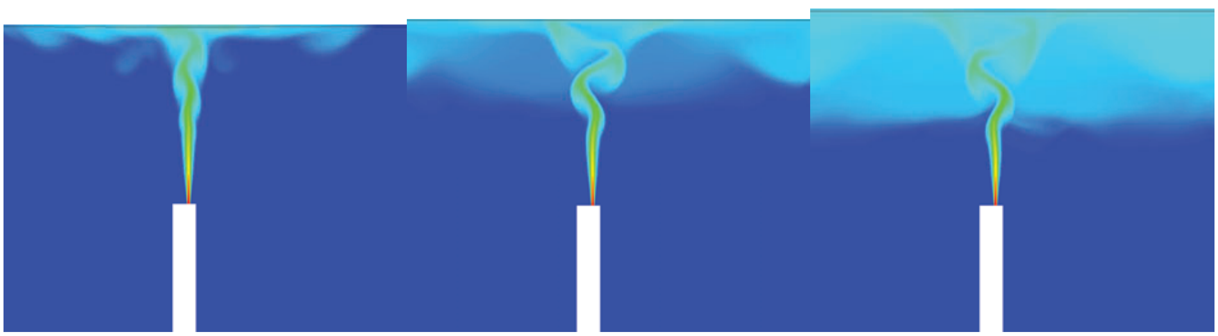

Figure 12. Evolution of Temperature Field for the Elliptic Blending κ-ε Simulation at 8, 65 and 130 Seconds

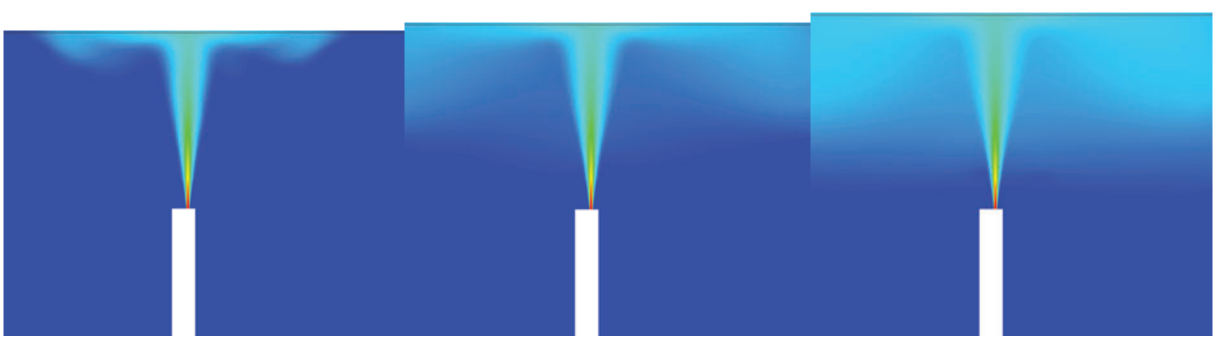

Figure 13. Evolution of Temperature Field for the Shear Stress Transport κ-ω Simulation at 8, 65 and 130 Seconds

The temperature fields for each model provide confirmation of previously seen trends in Fig. 5, 6, and7. The very complex structure of the jet and progression of the thermal layer developing for the EBKE model is shown clearly within Fig. 12. The thermal layer for each model is shown to grow “pockets” near the upper regions in each corner before expanding out into the rest of the volume. This general behavior was observed in the experiment. Different hot layers visible within the thermal layer of the EBKE model provide insight into how the hottest two traces have very similar temperatures. This is due to those traces being observed in roughly the same sublayer for the entirety of the trial. The previous result from the temperature traces in Fig. 7 where the SST simulation is shown to be much more diffusive in the water region can be observed in the Figs 11-13. For each model, thermal stratification can be clearly observed, but the temperature distribution is not predicted as expected for each turbulence model.

6. CONCLUSIONS

CFD simulations using an Eulerian multiphase mixture model and Volume of Of Fluid (VOF) approach with Standard Low-Reynolds κ-ε, Elliptic Blending κ-ε or Shear Stress Transport κ-ω turbulence models was used to attempt to simulate thermal stratification and jet behavior observed in the TJWF. In general, all three models were able to simulate the thermal stratified layer viewed in the experiments, but had more mixed results predicting the temperature traces. This work shows a strong improvement in modeling this behavior over the previous works [7] which utilized a deforming mesh approach and the SA and SST turbulence models. The EBKE model was found to provide the most accurate set of results for this trial and overall predicted the experimental results quite well. Temperature traces of the models showed the EBKE was able to capture the hotter layer recorded by the point probes and not show heat up of lower regions of the enclosure volume. The previous works did not show as strong of comparisons to experimental data or clear thermal stratification occurring based on the temperature traces. Additionally, this work suggests that the SST model is not appropriate for modeling this type of behavior. The improvement in modeling the thermal stratifying layer furthers the development of potential methods for simulating containment, spent fuel pool, and upper plenum behavior during accident scenarios.

Further work will be conducted to improve the simulation methodology and will be compared against additional experimental data sets acquired in this facility or a similar facility. Further experiments will be conducted in a similar facility [17] to the TJWF to provide a larger data set for validation. This data will include centerline velocity and temperature measurements using non-invasive experimental techniques.

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