CFD SIMULATIONS OF EROSION OF A STRATIFIED LAYER BY A BUOYANT JET IN A LARGE VESSEL

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ABSTRACT

One of the most important parameters in the analysis of containment safety of the light water reactors during a loss of coolant accident (LOCA) is the prediction of the hydrogen concentration. To ensure proper design of the containment and to mitigate the fire/explosive risk created by the flammable hydrogen gas, this concentration build up must be analyzed. Lumped parameter (LP) codes are the main tools used in containment thermal-hydraulic analysis; however, they are limited when it comes to scenarios which require higher fidelity analysis of local phenomena. While the use of computational fluid dynamics (CFD) allows for higher fidelity analyses, CFD requires a comprehensive validation study due to turbulence and condensation modeling.

During a LOCA accident, the leaked hydrogen from the primary circuit can form a stable stratified layer at the top of the containment building. The formation and erosion of a stratified layer is a challenging numerical problem due to the interaction mechanism of the jet flow with the stratified layer. The OECD-NEA conducted an experiment at the Paul Scherrer Institute (PSI) as part of the third International Benchmark Study (IBE-3) to investigate the erosion of the stratified layer by a vertical air-helium jet from the bottom of the large vessel (height 8 m. diameter 4 m.). During the experiment, CFD grade experimental data was generated that could be used for comparative studies.

In the present study, the experiment is simulated by using the STAR-CCM+ CFD code with various turbulence models including Reynolds-Averaged Navier-Stokes (RANS) models and Large Eddy Simulation (LES). The Realizable k-ε and k-ω SST showed good agreement with the experimental data when predicting the erosion of the stratified layer and global mixing of the gas components; specifically an anisotropic analysis with RSM showed similar behavior with the isotropic two equations model for the erosion of the stratified layer. The LES model also showed faster erosion than experimental data, while the cost of the LES simulation was much higher than RANS simulations. The current validation study contributes to the sensitivity analysis of the turbulence models for erosion behavior in the stratified layer. In addition to that, the results of this study will provide a foundation to discuss the feasibility of the CFD code usage in containment level thermal hydraulic analysis.

KEYWORDS
buoyant jet, turbulent, system level cfd, large eddy simulation

1. INTRODUCTION

The importance of hydrogen distribution is due to its explosive characteristic at certain concentration level. Specifically, during severe accident conditions in light water cooled nuclear reactors, explosive hydrogen gas may be formed due to an oxidation reaction of high temperature zirconium cladding and steam. If hydrogen gas is released into the containment building, it is then possible that a build up in concentration of the gas may lead to formation of explosive hydrogen and air mixture, which could potentially lead to a hydrogen explosion. Such a scenario may cause serious collateral result in loss of reactor safety systems.

Over the past three decades, significant knowledge has been gained with intensive research both on a national and international level. Several experimental facilities around the world have been built to investigate the hydrogen distribution such as PANDA, MISTRA, TOSQAN, THAI, PHEBUS, HDR, BMC, HYJET, etc. [1]. The results of these experiments were used as a reference for numerical code developments and validation purposes. Generally, two numerical thermal hydraulic methods are used for the analysis of hydrogen distribution in the containment vessel; the Lumped Parameter (LP) and the CFD code. LP codes are extensively validated, while CFD codes still need more validation. The most challenging computational phenomenon for the containment analysis is the formation of the stable stratified layer as a result of the hydrogen gas leakage from the primary circuit. The density of hydrogen gas is lower than air. As a result of that, buoyancy force cause the motion of hydrogen gas toward the upper side of the containment building, which results in stable stratified layer as shown in Fig. 1. The stratified layer due to different density of the gases may challenge computational models to treat strong density gradient and fluctuations of the velocity due to the pulsation of the impingement jet. The negative buoyancy effect causes deceleration on the jet flow. Hence, the erosion process occurs slowly due to negative buoyancy. In literature, several analyses of hydrogen mixing have been conducted by using CFD studies including validation of the codes by using experimental data. However, mostly generic turbulent models were used for most of them with limited number of computational volume elements. The CFD benchmark study [2] used the data of the PANDA experiment that has low momentum horizontal steam injection. The simulations turbulent models were the variations of the k-ω and k-ϵ models and the number of the mesh cells ranged from 45,000 to 1.1 million. The study showed that grid sensitivity study improved the accuracy of the results significantly. Visser et al conducted a CFD validation study [3] by using THAI (HM2) experimental data. They tried to answer the spatial and temporal discretization sensitivity for the breaking of a stable helium layer by a low momentum air injection as well as the effect of the buoyancy term in the turbulent transport equations.

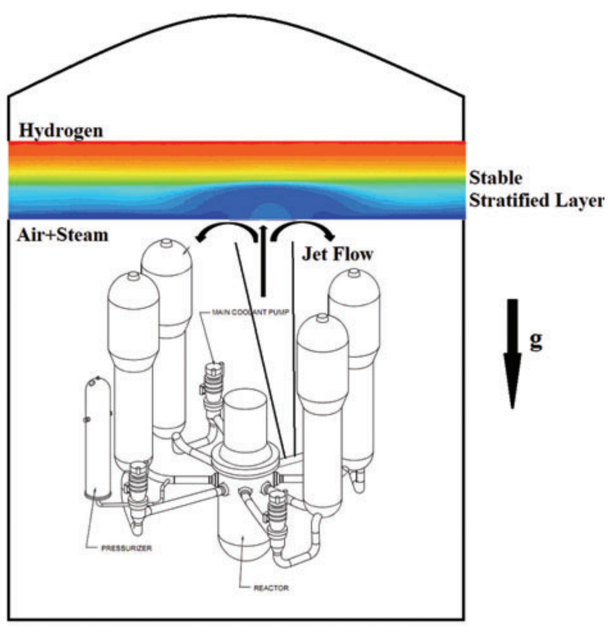


Figure 1. Stable Stratified Layer in a Containment building

2. PHYSICAL MODELS

The energy equations can be neglected depending on the flow problem such as constant isothermal flows. However, in the current analysis the energy equation must be solved due to the temperature variation of the gas mixture. The density is computed by using the ideal gas law with computed temperature from the energy equation. In addition to the energy equation, the species transport equation is solved to compute the diffusion of the gas mixture components that are helium and air for this study. The mole fraction of the air-helium gas mixtures varies in the flow domain initially due to a stable stratified layer. Buoyancy must be accounted for in the current study due to the variable density at the stratified layer.

2.1. Multi-Species Transport Equation

The transport equation for the mass fraction Y_i of species i^{th} is solved as in Eq. 1

$$\frac{\partial}{\partial \mathrm{t}} \int_{\mathrm{V}} \rho\, Y_i\, d\mathrm{V} + \oint_{\mathrm{A}} \rho\, Y_i(\mathbf{v}) \cdot d\mathbf{a} = \oint_{\mathrm{A}} \left[\rho D_{i,m} \nabla Y_i + \frac{\mu_t}{\sigma_t} \nabla Y_i\right] \cdot d\mathbf{a} \tag{1}$$

where D_m is molecular diffusivity and it was calculated by the Chapman-Enskog model Eq. 2. The diffusion coefficient used is $7\mathrm{x}10^{-5}\,\frac{m^2}{s}$ and the Turbulent Schmidt number σ_t is a default value of 0.9 , μ_t is the turbulent viscosity, ρ is the density.

$$\mathrm{D}_{1,2} = \frac{1.858\mathrm{x}10^{-3} T^{3/2}}{p {\sigma^2}_{12} \Omega} \sqrt{\frac{1}{M_1} + \frac{1}{M_2}} \tag{2}$$

where M_1, M_2 are the molecular masses of the gas components, p is the pressure, T is the temperature, σ^2 is the average collision parameter and Ω is the temperature dependent collision integral. The diffusion coefficient for helium and air mixture is $7\mathrm{x}10^{-5}\,\frac{m^2}{s}$ at T=298 K and p= 1 atm.

2.2. Turbulence Models

CFD applications have commonly been used for turbulent flow in the last three decades. Although there are numerous available turbulent models including hybrid variations, the general purpose turbulence model has not been developed yet. Each model has its own specific advantages or disadvantages according to the flow structures. Although the turbulent flow can be resolved directly by solving the Navier-Stokes equations, which is called Direct Numerical Simulation (DNS), it is not feasible for current engineering problems due to its extensive computational cost. As a compromise between accuracy and computational cost, turbulent models have been developed. Large Eddy Simulation (LES) and Reynolds-Averaged Navier-Stokes (RANS) are used extensively for most of the current engineering problems.

In the present study, the current turbulent models are used to compare their capability for a containment level safety analysis including, Realizable k-ε, k-ω SST, Reynolds Stress Model (RSM) with linear pressure strain, and LES with wall-adapting local eddy viscosity model (WALE) sub-grid model are used for turbulent sensitivity analysis. All of the listed turbulent models inherently consider buoyancy effect in the transport equations in STAR-CCM+ 9.04 [4] except the k-ω SST model. Therefore, the buoyancy term is manually implemented to the turbulent kinetic energy transport equation as a source term. The buoyancy term is given by Eq. 3

$$G_b = -\frac{\mu_t}{\rho\sigma_t} g \frac{\partial \rho}{\partial z} \tag{3}$$

3. EXPERIMENT AND CFD MODELING

3.1. Experiment

The main purpose of the experiment is investigating the erosion of a stratified layer, which is the possible LOCA post-accident scenario as a result of hydrogen leakage to the containment. Helium gas was used instead of hydrogen for safety reasons. At the beginning of the experiment, only helium was injected into the vessel to form a stable stratified layer. This process helped to create a helium-rich layer at the upper region of the vessel. The rest of the vessel is dominated by air. The stable layer means that distribution of the gases is in balance due to the balance of natural forces, which are the gravity and buoyancy forces. Axial molar fractions of gas mixture were measured before the start of the experiment as an initial condition and then they are imposed to the CFD simulation. The measured initial conditions can be seen in Fig. 2.

The erosion of the stable stratified layer occurred by injection of the low momentum gas mixture into the vessel by using a circular pipe which has a 75.3 mm inside diameter. The mass flow rate of helium-air mixture was measured as 21.94 g/s during the experiment and it was kept constant. On the other hand, the temperature of the gas mixture increased during the experiment. More details of the experiment can be found in [5].

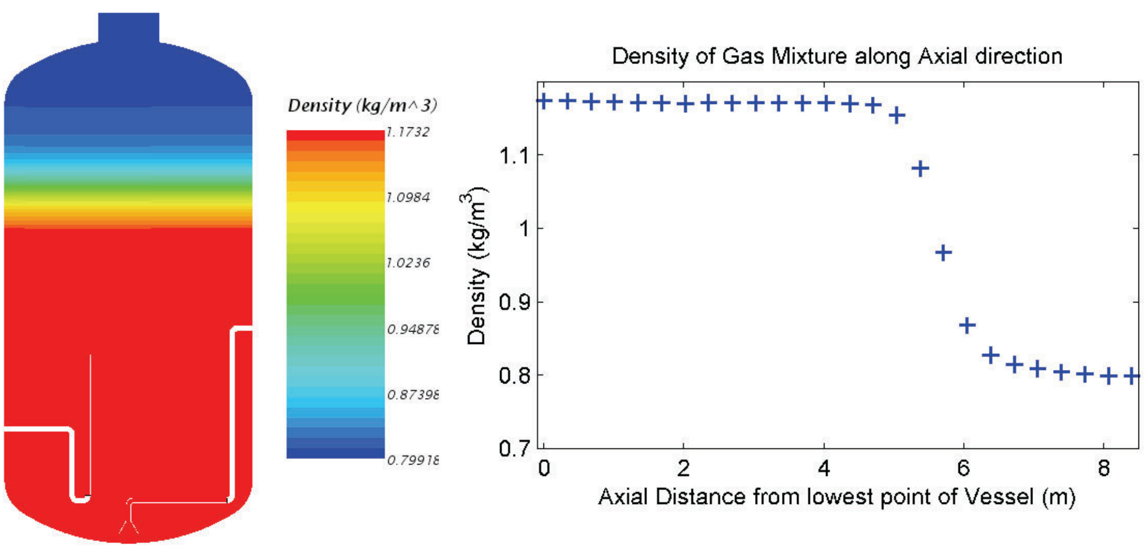


Figure 2. Initial density distribution of the gas mixture.

3.2. Boundary Conditions

The simulation followed the experimental boundary conditions exactly. An inlet boundary condition is used to inject the gas mixture vertically from the bottom of the stratified layer. The parameters at the inlet boundary is calculated by using experimental data [5]. The details of the inlet boundary conditions are given by Table I.

Table I.: Inlet Boundary Conditions

Air-Helium Mass Flow Rate	21.94 g/s (±1.1 g/s)
Air Mole Fraction	0.866
Helium Mole Fraction	0.134
Temperature	20 ^{0}C to 29.3 ^{0}C
Inlet Pipe Diameter (inner)	75.3 mm
Turbulence Intensity	7.4%
Turbulent Length Scale	3.012 mm

In the experiment, the outlet boundary condition was used to keep constant pressure in the vessel and it was placed at the bottom of the vessel. In the CFD simulation, pressure outlet can be used for the identical purpose. At the wall of the vessel, the injection pipe and the discharge pipe, the no-slip wall boundary condition was applied.

3.3. Mesh

The quality or validity of the mesh directly affects the accuracy of the numerical results. An invalid mesh contains mostly zero or negative volume cells, which do not allow to run the simulation. However, a low quality mesh can be initialized and it may not indicate any problem while the results are typically less accurate. The most important factors for the quality are: skewness angle, face validity, cell quality and volume change. In the present study, the geometry is not complex, which helps to sufficiently satisfy all quality criteria. The polyhedral meshing algorithm is used to create the volume mesh. It is chosen due to the suitability for all used turbulent models. Specifically, its convergence behavior is better than hexahedral cells for highly swirling flows that occurs due to the interaction of the jet with stratified layer.

For the current study, the near wall modeling has significant impact on the injection pipe modeling but not for the bulk region due to the location of the mixing. The variation of discretization near the wall demonstrates different outlet velocity at the outlet of the jet. Different jet velocities result in a high variation for the time of the erosion. The jet outlet velocity is diagnosed for each simulation by using experimental Particle Image Velocimetry (PIV) data, which are taken at the exit of the injection pipe. Overall, the global quality factors is assessed by a mesh independence study. The mesh refinements are applied for the injection pipe and the interaction region of the injected jet and stratified layer due to sharp gradient of velocity and density. Additionally, the main purpose is the evaluation of the erosion process with the time along the jet axis.

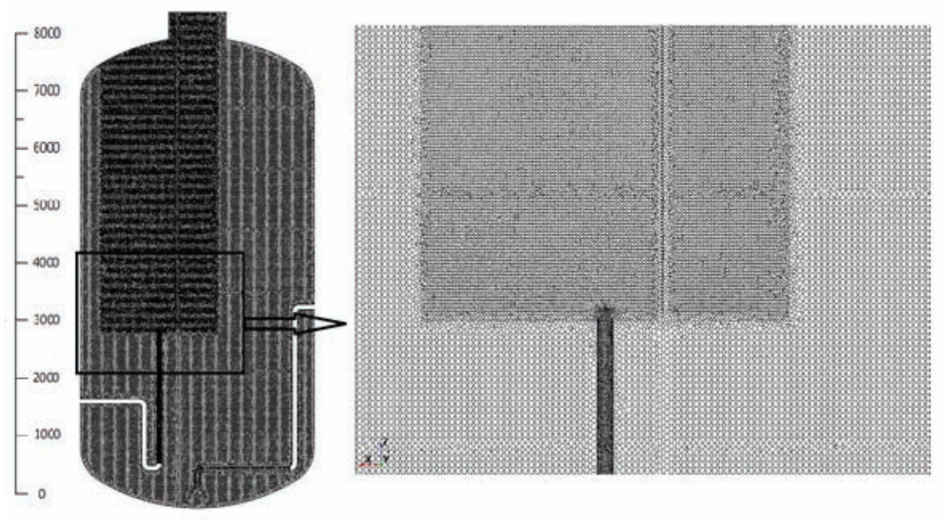


Figure 3. The dimensions and fine grid of the PANDA vessel.

Coarse and Fine grids are created for mesh and turbulence models sensitivity studies.The fine mesh can be seen in Fig. 3 and the details of the mesh is given by Table II.

Table II. Mesh details

	Coarse Grid	Fine Grid
Number of cells	4.960.166	19.052.011
Cell type	Polyhedral	Polyhedral
Base Cell size	40 mm	30 mm
Mesh refinement	Injection Pipe 7.5 mm along the jet axis 24 mm	Injection Pipe 5.5 mm along the jet axis 24 mm
y+	mostly ~ 0.1 max 30	mostly ~ 0.1 max 30

3.4. Methodology of CFD

Multi-component gas modeling is used to compute the diffusion of the air-helium gas mixture. The implicit unsteady scheme is used to prevent any stability problem due to courant number limitation of the explicit scheme. Even though the courant number is not limited the time step, the courant number is kept about 1-2 for mixing region and maximum 30-40 for whole flow domain. The time-step is kept very low at the beginning of the all simulations, then it was increased gradually. The time-step sensitivity study has been conducted for the RANS simulations by checking the monitor points in the mixing region for helium mole fraction. Fortunately, the time-step is increased up to 0.5 seconds and it allows for a significant reduction in run time of simulations that is very crucial for the containment level analysis due to the long transient time. However, the time-step strategy for the LES simulation is different than the RANS simulations. LES is a technique for direct simulation of the large eddies. It is based on Kolmogorov's theory. According to the theory, large eddies are dependent on the dimension of the flow domain while the smaller scales of turbulence flow are less dependent on the dimension of the flow domain. As a result, the smaller scale can be modeled while larger scales are solved directly. Therefore, the time step of the simulation should be small enough to capture the larger eddies. In the present study, maximum 5 milliseconds is used for the LES analysis. The CFD modeling details are given in Table III.

Table III. CFD modeling details

Solver	Segregated Pressure-based algorithm
Pressure correction scheme	SIMPLE
Spatial discretization	2nd order upwind (central scheme for LES)
Temporal discretization	2nd order implicit
Time step size	0.001-0.5
Equation of State	Ideal Gas
Multi-Component Gas	2nd order convective
Convergence Criteria	Max 10^{-5} (Max 10^{-3} for LES)
# of iterations per time step	10-20

4. RESULTS AND DISCUSSION

As a long time transient analysis, the excessive storage is required. However storage of all simulation files with 1 second interval requires 7200 simulation files for all simulations requiring about 400 Terabytes hard-drive space, which is enormous for even research level studies. In addition to that, writing of the simulation file to the hard-drive causes significant delay. As a solution, the monitor points are created to extract required data to compare at the same locations that experimental data were recorded. The selected experimental monitor points for present CFD study can be seen in Fig. 4 and Fig. 5. These figures can be used as reference for the rest of the plots in this paper. Further data-point CFD results can be found in [6].

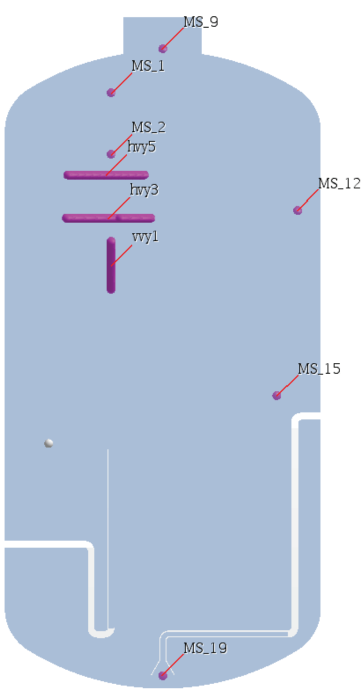


Figure 4. Monitor points and lines

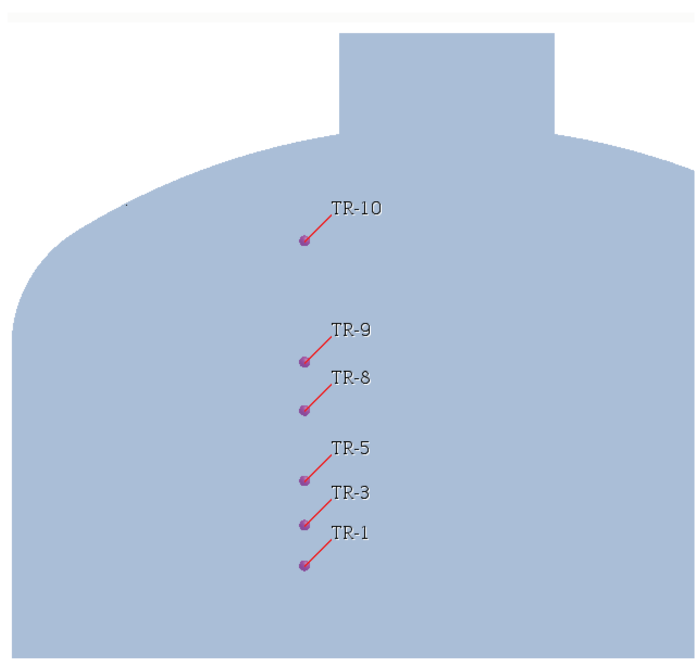
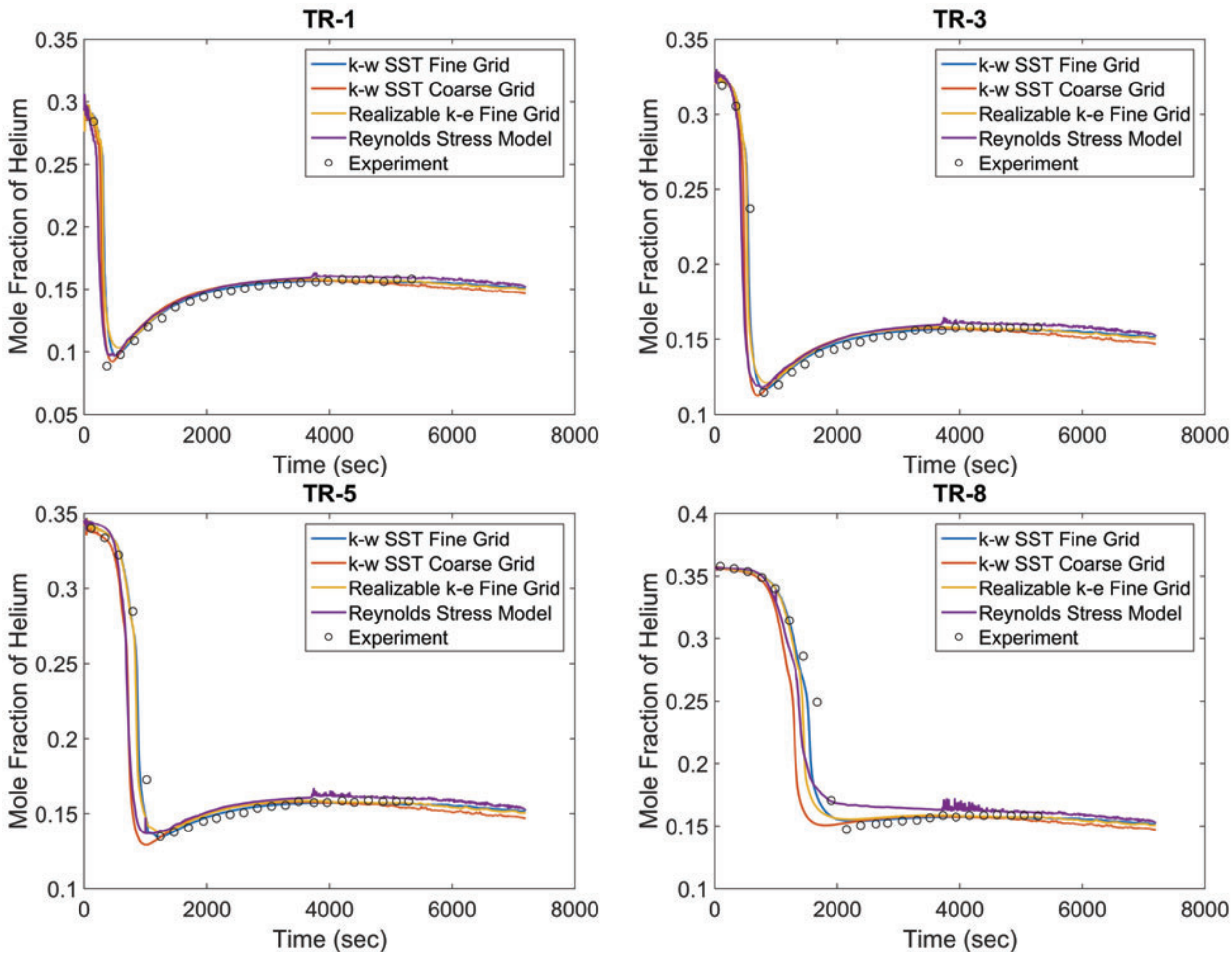


Figure 5. Monitor points for evaluation of erosion

The grid sensitivity analysis has been conducted for the k-ω SST model with a fine and a coarse grid. As show in Fig.6 and 7 the grid independence is satisfied. The outcome of the grid independent study proved that refinement in the mixing region enhances the accuracy and reduces the numerical diffusion because of the fluctuation of the velocity. The erosion rate at the upper region is more dependent on the grid resolution due to the higher density gradient at this region. This can be seen in Fig. 6. While the use of the different grids results in different erosion rate in the stratified layer, the global mixing is not significantly affected with grid resolution. After grid independence is satisfied for the k-ω SST, all other simulations run with the finer grids. Normally, grid sensitivity study has to be conducted for all individual simulation, but due to the computational cost of the study only one model is used for the grid independence study.

Overall, the RANS simulations showed good agreement with the experimental data for the erosion of the stratified layer and global mixing of the air-helium mixture, specifically, the modified k-ω SST showed good performance to predict the erosion process. The Realizable k-ϵ predicted better than k-ω SST only at the point MS-9. Above this point, the mixing is affected by the wall and the possible reason is the implementation of the all y^+ wall model. The uncertainty of the mole fraction measurement is 0.5%.



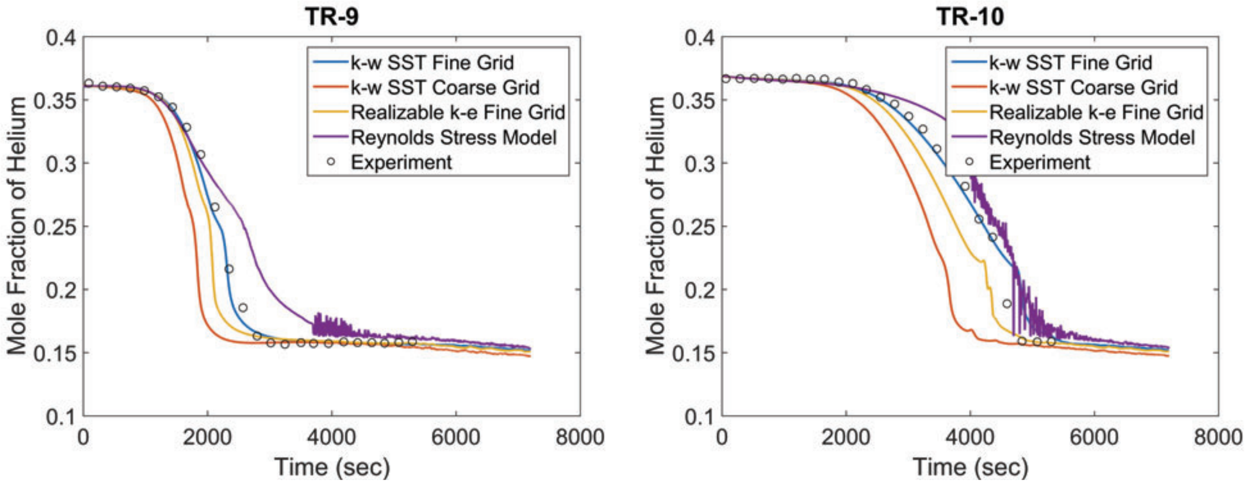
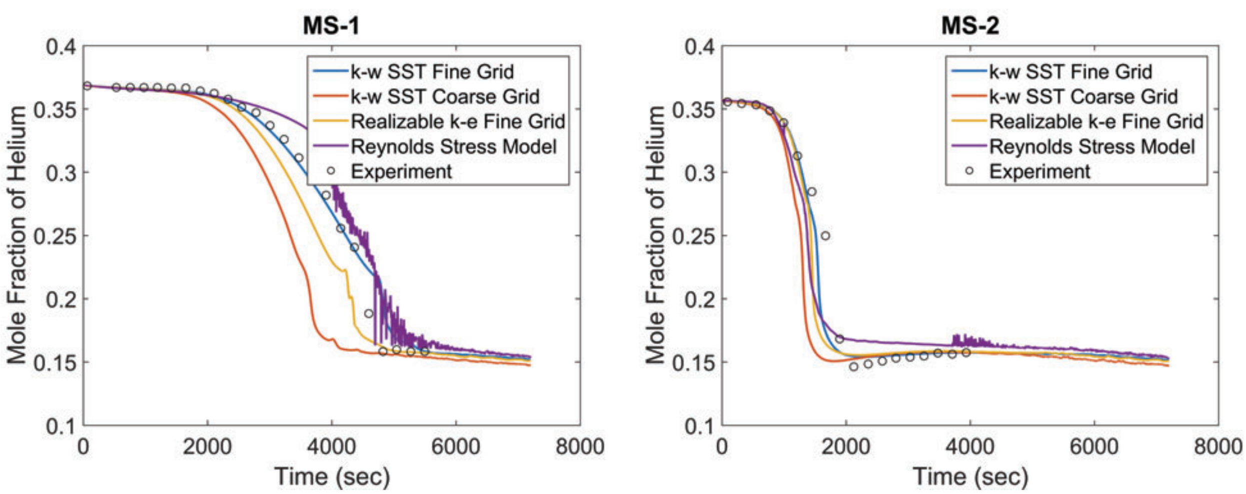


Figure 6. Mole fraction of Helium vs. Time along the jet axis for RANS models to evaluate the erosion.

The Reynolds Stress Model (RSM) is developed to account for anisotropy for the Reynolds stress tensor (RST). In general two equation models do not account for anisotropy due to the isotropic eddy viscosity assumption in the model. However, the RSM has a numerical stability problem due to the stiffness of the RST equations. In the RSM simulation, the interactions of the incoming jet and the stratified layer caused stability problems due to density gradient, specifically, at the time of the incoming jet reached at the upper level of the stratified layer. It can be seen in Fig.6 and Fig.7 (after 4000 seconds). After 4000 seconds, the sharp density gradient in the axial direction, and zero density gradient in the radial direction causes more stability problems due to the stronger anisotropy of the RST components. After this time the simulation crashed and restarted several time. Even extra cost of the solving extra five transport equations for RSM to consider anisotropy, the general erosion prediction is not better than isotropic eddy viscosity based RANS models.



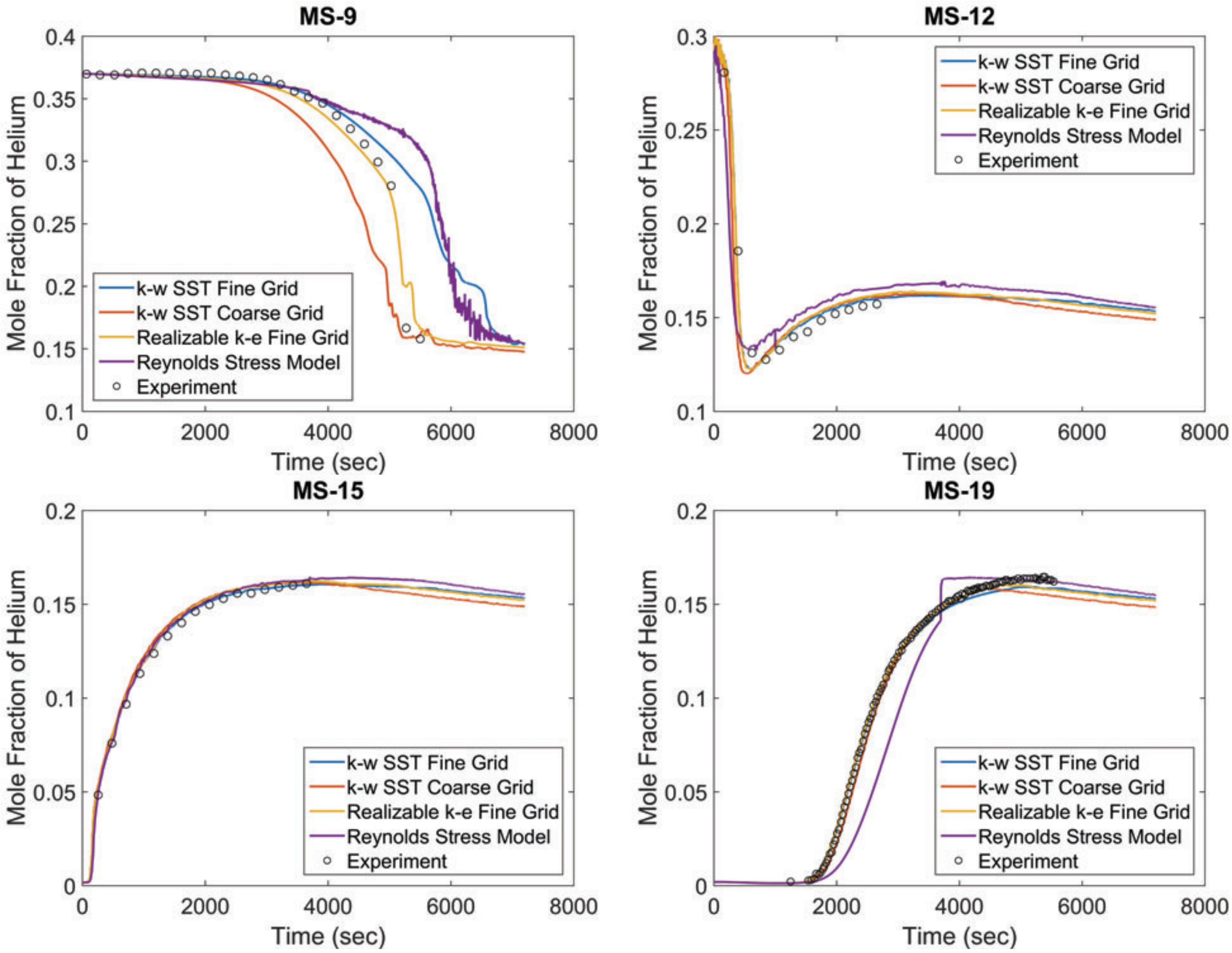


Figure 7. Mole fraction of Helium vs. Time along the jet axis for RANS models to evaluate the global mixing of the gas components.

The velocity and turbulent kinetic energy data are averaged over a time period of 204.6 s. The solution time will refer to the time in the middle of this averaging period. Solution time for HVY-3, HVY-5, VVY-1 and TKE-2 are 1213, 1795, 111, 1213 seconds respectively. As shown in Fig.8, the time averaged axial velocities are slightly under-predicted for all RANS models except the RSM. The velocities are generally overestimated for the RSM model. On the other hand, the shape of the velocity profile for the RSM model is not matched with the experimental data while the shape of the other models matched with experimental data. The averaged axial velocity on the horizontal line (HVY-3) is in better agreement with the experimental data than HVY-5. The location of the HVY-5 is higher than HVY-3 and 582 seconds late. The potential reason of the underestimation of the averaged velocity may be related with underestimation of the approaching velocity of the incoming jet and overestimation of the turbulent viscosity. Because at this time the mixing process of the gas components are predicted with good agreement. This phenomena show that the components of the multi-species equation should be investigated due to less convection diffusion and more turbulent diffusion. In TKE-2 turbulent kinetic energy distribution shows high variation for different models. It is overestimated by RSM and underestimated by the Realizable k-ϵ. The better prediction of turbulent kinetic energy for the SST k-ω resulted in also better prediction of the erosion of the stratified layer.

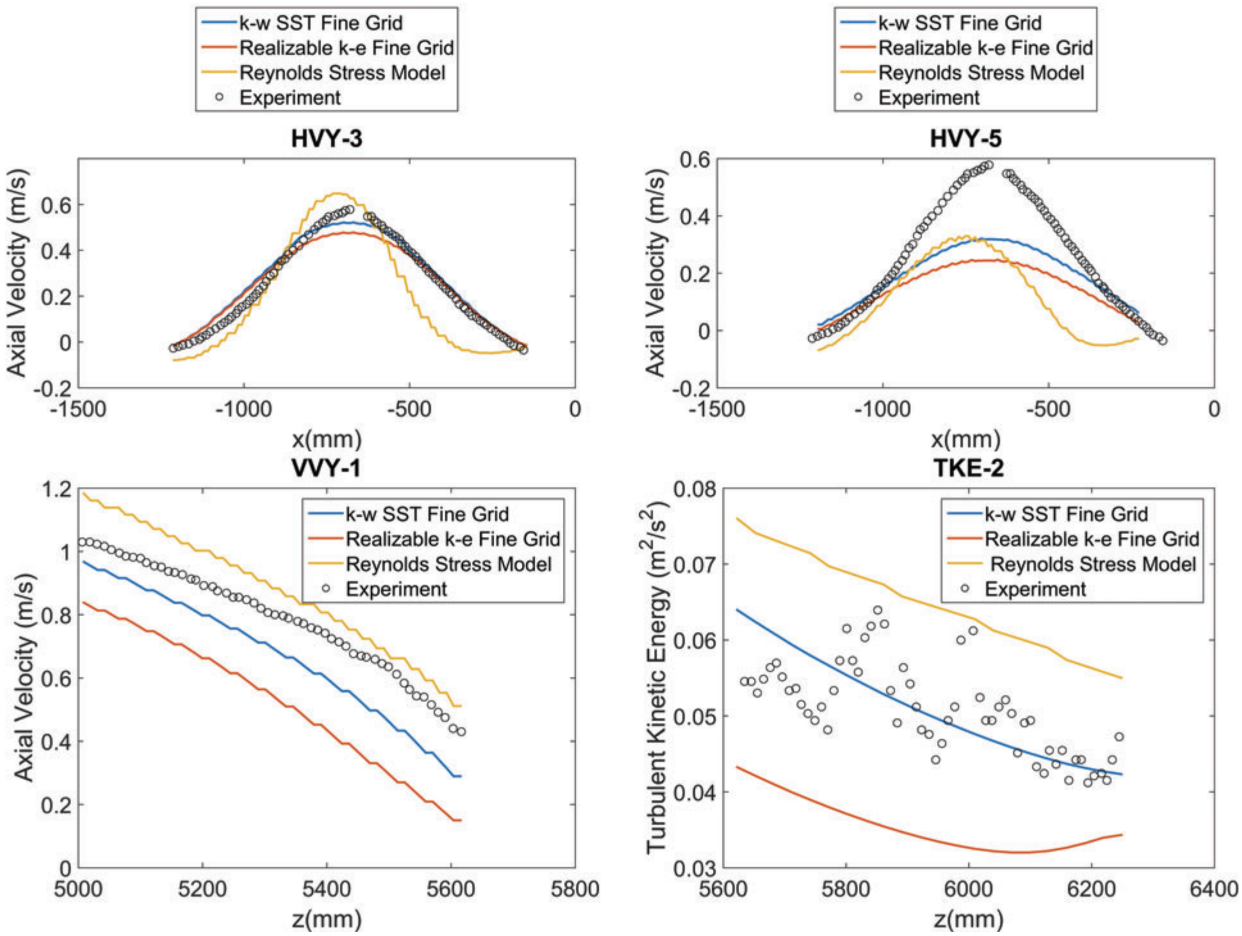


Figure 8. Mole fraction of Helium vs. Time along the jet axis for RANS turbulence models

In Fig. 9 the comparison of the LES and k-ω SST simulation are shown for the mole fraction of helium at the stratified layer along the jet axis and time-averaged axial velocity on a horizontal (HVY-3) and vertical line (VVY-1). The Large Eddy simulation is normally expected to yield results that agree more closely with experimental data due to its higher fidelity. It is resolving larger scales while modeling smaller scales. However, in the present study, the LES simulation resulted in faster erosion of the stratified layer. The reason of the faster erosion is because of the higher expansion velocity of the jet. The velocity of the jet in the centerline is higher than both experimental and numerical data from RANS simulations. Even a fully-developed boundary condition is applied at the inlet boundary, it is still overestimated. This problem could be overcome without modeling the injection pipe but due to time restriction it is not simulated for the present study. As a result of that, the rate of the erosion of the stratified layer is weakly dependent on the average of the axial velocity at the exit of the injection pipe. But it is strongly depend on the jet centerline velocity at the exit. This is also confirmed with k-ω SST simulations during this study.

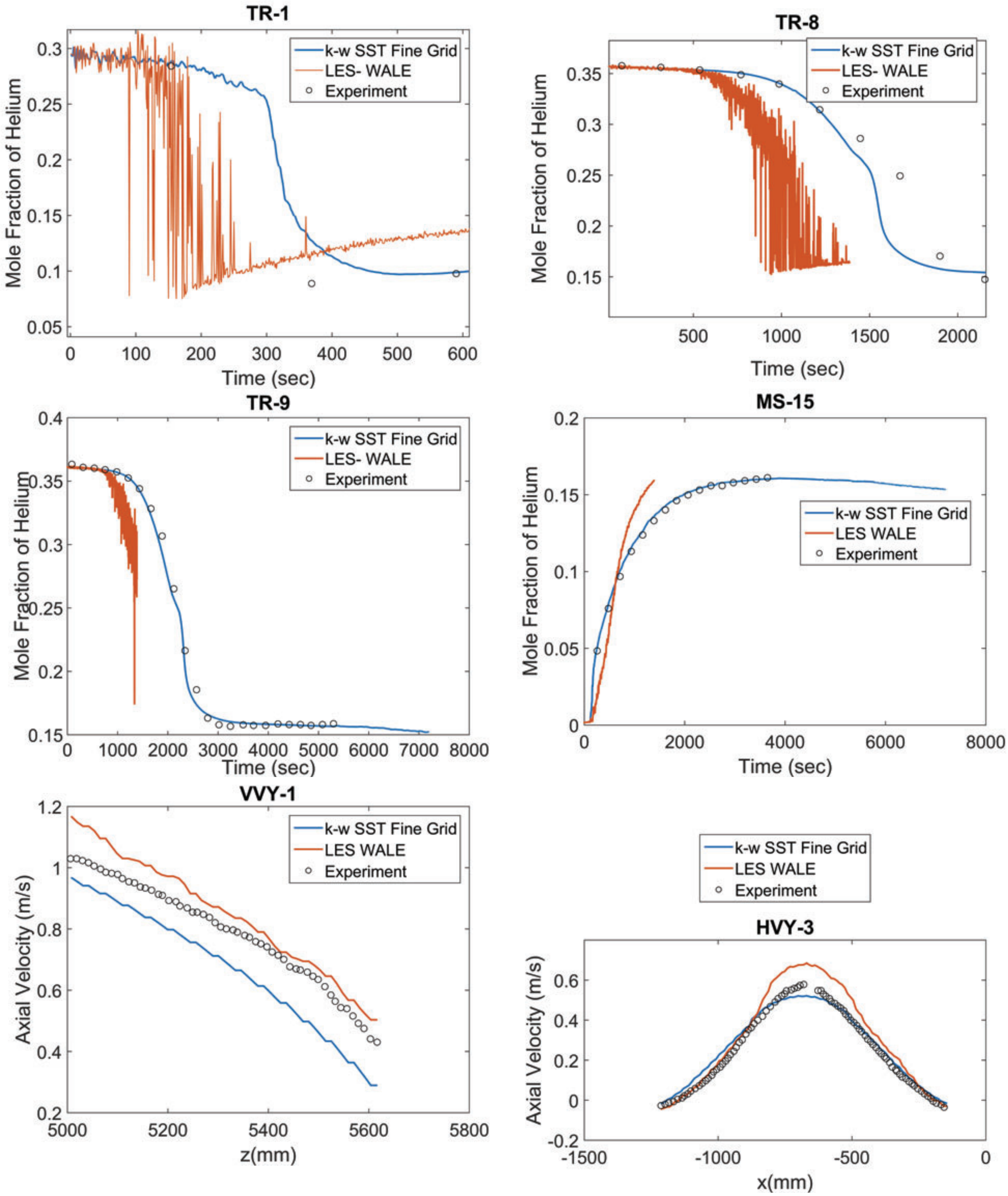


Figure 9. LES simulation comparison with k-ω SST simulation

As shown in Fig.10, the mixing and erosion characteristic for all RANS models are similar to each other, while the LES results is not. The reason of this difference is based on the jet expansion velocity. Over prediction of the jet expansion velocity caused the faster erosion and of the stratified layer. One can also note that the higher jet centerline velocity decreases the reversed flow due to buoyancy force from the stratified layer. It is well known that LES is strongly sensitive to the inlet boundary condition. The overestimation of the expansion velocity should be investigated in more detail. One of the potential reason is the numerical diffusion due to flow from small pipe into the much greater flow domain.

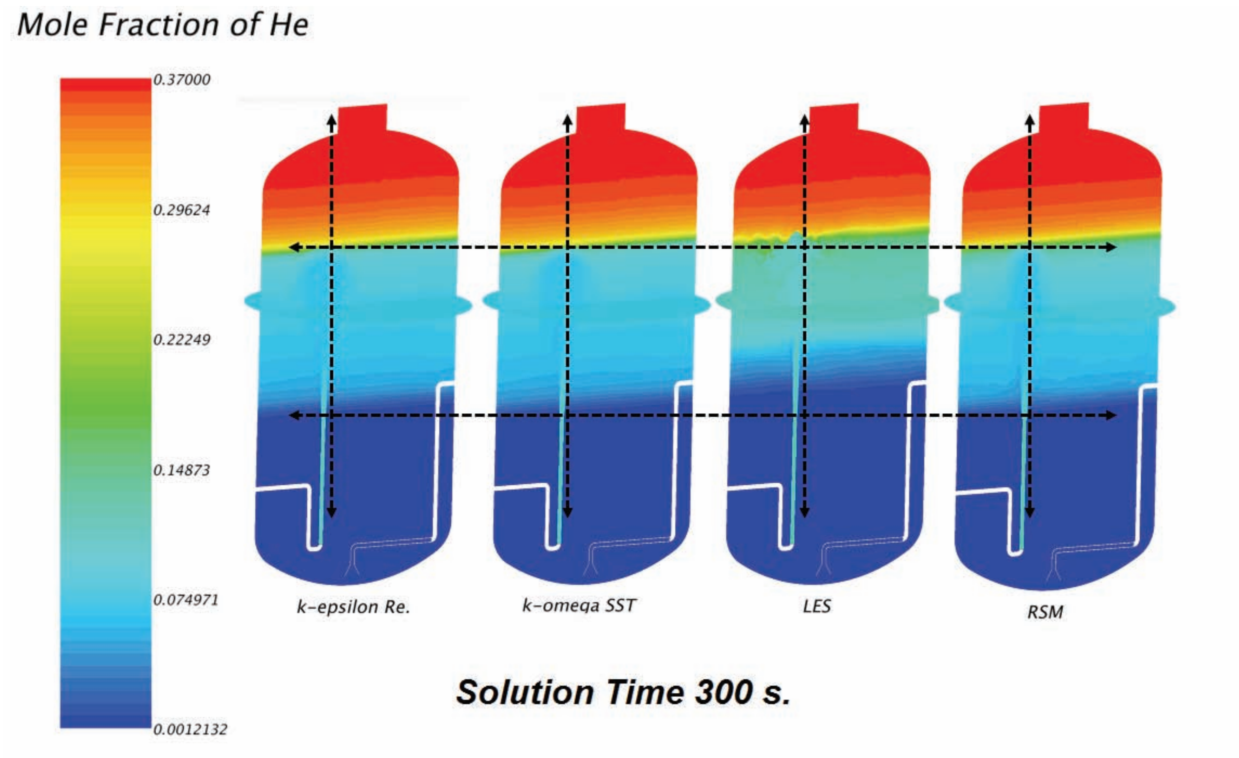


Figure 10. Qualitative comparison of the turbulent models.

Fig. 10 also shows that the two-equation models showed similar erosion and mixing prediction with RSM even with their isotropic eddy-viscosity assumption. At the same time, the computational cost of the two equations models is less than RSM. However, the RSM models may perform better than two-equation model for stronger anisotropic flow. It needs further investigation.

5. CONCLUSION

The LES simulation was conducted by using the fine grid, which was used also for the RANS simulations. The preliminary simulation results indicated that the modeling of the injection pipe must be carried out carefully due to jet velocity at the exit of the injection pipe. The exit velocity computed by the LES simulation was about 7.5% higher than k-ω SST simulation with an identical grid. The RANS simulations indicated the same problem for different turbulent models. As stated above, the injection pipe study has to be conducted before actual simulation. The results of the RANS simulation showed that the centerline velocity of the jet at the exit of the pipe significantly affected the rate of erosion of the stratified layer. A 5% increase of the jet centerline velocity resulted in the erosion of the middle region of the stratified layer to be about 1000 seconds earlier, which is very significant to predict accurate hydrogen distribution for the full scale analysis. The PANDA test specification also contains the PIV data at the exit of the injection pipe. The boundary conditions were modified to match with the experimental PIV data. The difference of the jet expansion velocity may be caused by the different implementation of the near-wall treatments.

A sensitivity study was conducted to investigate the effect of the near wall modeling on the velocity. The near-wall region was discretized below y^+ 1 to resolve the viscous sublayer instead of the using blended wall function. The Realizable k-ϵ and SST k-ω with low y^+ near wall modeling were used. The velocity results at the outlet of the pipe were compared against the experimental data. The velocity at the outlet of the pipe was higher than experimental measurements for both turbulent models. Since the outlet velocity has great effect on the evolving of the erosion process, further investigation should be conducted to check the source of over-estimation of the velocity at the exit of the injection pipe.

While, the RSM considered the anisotropic Reynolds Stresses, the isotropic eddy-viscosity based models showed better agreement with the experimental data with less computational cost. Despite the very high computational cost of the LES, it resulted in earlier erosion of the stratified layer. The reason of earlier erosion is the over-estimation of the jet centerline velocity. Overall, the two-equation RANS model showed good agreement with the experimental results. The RANS models can be used for full-containment safety analysis with a reasonable computational cost. On the other hand LES must be studied in details to investigate over-prediction of the jet centerline velocity. In addition to that, the rate of the erosion of the stratified layer is weakly dependent on the average of the axial velocity at the exit of the injection pipe. But it is strongly dependent on the jet centerline velocity. This is also confirmed with k-ω SST simulations during this study.

CFD simulation for such a large domain has been conducted successfully with reasonable amount of computational time by using a supercomputer facility. The LES simulation was performed with 1200 cores in 6 weeks, while the two-equation models with 600 cores in about 4 days. This study shows that the use of CFD for the larger scale analysis is reasonable event with LES model.

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