

Validation of Two-phase Flow Modeling Techniques in Loci-Stream using Axial Jet Pressure Control and Autogenous Pressurization Experiments

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Improvements to computational fluid dynamics modeling of cryogenic fluid management operations are presented with experimental validations. Modeling improvements includes utilizing improved delayed detaches eddy simulation to more effectively model turbulence compared to the Reynolds-averaged Navier Stokes modeling, modeling temperature dependent tank solid properties to capture large variation in thermodynamic properties at cryogenic conditions, modeling real gas equation of state for hydrogen instead of ideal gas behavior, and an on-going effort to improve interface turbulence transport for the volume of fluid method. Two flight-scale ground tests, five K-site tank axial jet pressure control experiments and an Engineering Design Unit tank autogenous pressurization experiment are validated and show the effectiveness of the improved modeling techniques. The successful validation establishes further trust in these models for flight project support and provides a pathway for maturation of in-development interface turbulence damping model for the volume of fluid method for more generalized applications.

I. Nomenclature

B	=	Damping factor in smooth wall turbulence frequency equation promulgated in Menter's SST model
f_d	=	Blending parameter in improved delayed detached eddy simulation model
t	=	Time
y	=	Interface normal distance
β	=	Constant in Menter's SST model
μ	=	Dynamic viscosity
ω	=	Turbulence dissipation rate (turbulence frequency)
ρ	=	Density

II. Introduction

NASA's near-future long-term space missions necessitate advancements in cryogenic fluid management (CFM) technologies, which is a critical technology for NASA's Artemis missions. CFM deals with safe, low cost, and reliable long-term propellant storage; pressure control and propellant location control in the tank for engine operations; as well as tank draining and filling. Consequently, NASA Space Technology Mission Directorate (STMD) has established the CFM Portfolio Project (CFMPP) to improve CFM technologies for upcoming missions. In addition to advanced hardware development and demonstration, there is a need for accurate modeling of cryogenic system behavior to support rapid, reliable, and low-cost spacecraft design and operation. CFM Modeling Portfolio within CFMPP aims to improve, develop, and validate modeling capabilities.

As part of the CFM modeling portfolio, the Propulsion Engineering Fluid Dynamics branch (ER42) at NASA Marshall Space Flight Center (MSFC) has been tasked with assessing and improving computational fluid dynamics (CFD) tools used to support future and current flight projects such as Human Lander System and Commercial Lunar Payload Services. CFD modeling is indispensable for accurately simulating and understanding these problems with high fidelity. We are engaged in improving and validating two-phase models in the Loci-STREAM CFD code to predict various CFM phenomena.

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An accurate capture of the gas-liquid interface dynamics is the primary modeling bottleneck. The interface dynamics includes altered interface turbulence transport, phase change, and thermal transport. Additionally, turbulence modeling away from the interface is another significant challenge for CFM modeling. Low speed but high Rayleigh number natural convection is often encountered in CFM problems and is difficult to model using Reynolds average Navier-Stokes (RANS) turbulence models. Moreover, CFM operations with high Rayleigh number as well as high Reynolds number flows might also pose more modeling challenges.

In this paper, previous autogenous pressurization predictions [1] are updated with an improved modeling and axial jet based pressure control test [2] is expanded to contain five tests. Implementation of turbulence transport model for volume of fluid (VOF) method is described. Utility of a hybrid RANS and implicit LES approach was also described to improve the temperature predictions of the RANS model. Validation of our modeling techniques and CFD solver Loci-Stream-VOF are demonstrated.

III. Test Descriptions

A. K-site Tank - Axial Jet Pressure Control

1. Testing Facilities

Axial jet pressure control tests were conducted at the NASA Glenn Research Center's K-site testing facility [3]. These tests provide time-transience of pressure and temperature data during the tank depressurization. An ellipsoidal tank with 2.2m major diameter and 1.83m minor diameter was insulated with multi-layer insulation (MLI) and housed inside a vacuum chamber. The Shuttle Centaur tank mixer was installed along the minor axis of the tank, which also aligns with the direction of the gravity. The nozzle diameter was 22.1mm and the nozzle outlet was located on the tank major axis 0.51m from the tank bottom. Figure 1 illustrates the configuration. A battery of sensors are places inside and on the tank for temperature, pressure and fill level measurements. Figure 2 demonstrates the locations of the temperature probes.

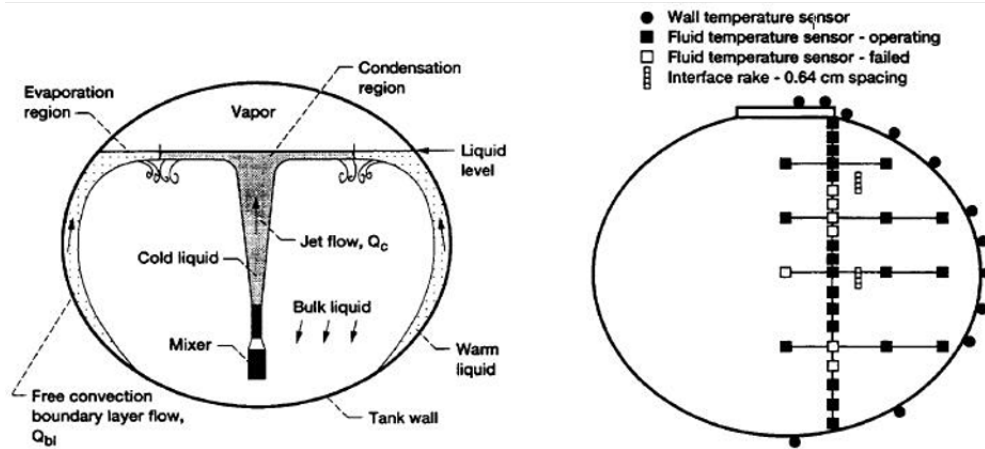


Fig. 1 Cross-sections illustrating test configuration

2. Experimental Procedure

First, the heat leakage rate of $4.2W/m^2$ was calculated by measuring the steady liquid hydrogen boil-off rate. Then the tank was filled with liquid hydrogen, the hardware was brought to saturated liquid condition, and the tank was vented until a target pressure is achieved before the tank was locked up. Wall-adjacent liquid hydrogen warms due to the heat leak to the tank and being lower density buoys up to the gas-liquid interface. A temperature gradient forms along the tank height with warmer and lighter liquid at the top. Initial temperature distribution was reconstructed from the temperature probes data. The test is initiated by turning on the mixer at a set mass flow rate. The mixer circulates the cooler liquid hydrogen from the bottom of the tank to the interface - cooling the interface. The ullage pressure drops over time as the saturation temperature and pressure drops at the interface. Depressurization stops when the liquid

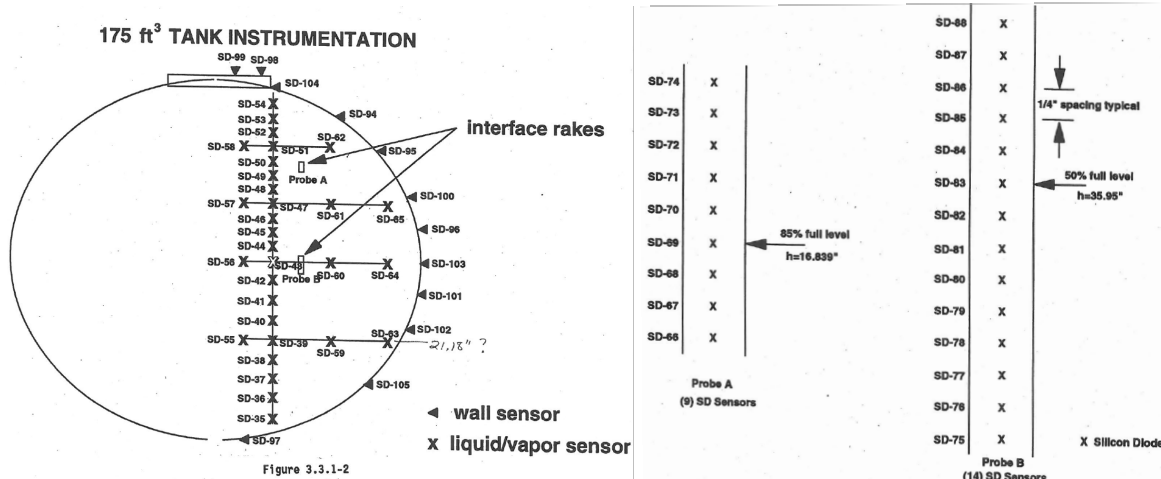


Fig. 2 Temperature sensor locations inside the K-site tank

Case	Fill Volume [%]	Fill Height [m]	Mixer Flow Rate [m^3/hr]	Initial Tank Pressure [bar]
434	86.3	1.45 (79.1%)	3.47	1.861
436	85.3	1.43 (78.0%)	1.82	1.870
449	49.1	0.93 (50.7%)	3.41	1.861
457	49.1	0.93 (50.7%)	1.82	1.865
459	49.1	0.93 (50.7%)	0.92	1.847

Table 1 K-site axial jet pressure control tests used for validation

becomes isothermal due to the continuous mixing, which ends the test. Five test cases are employed for the validation. Test conditions - fill levels, mixer flowrates and initial tank pressures are shown in Table 1.

B. EDU Tank - Autogenous Pressurization

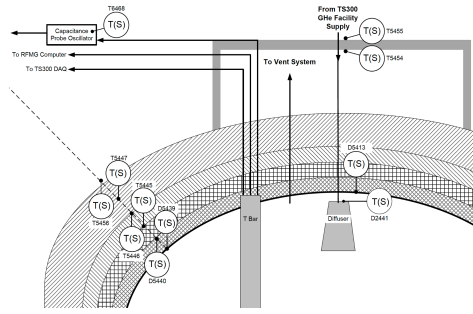
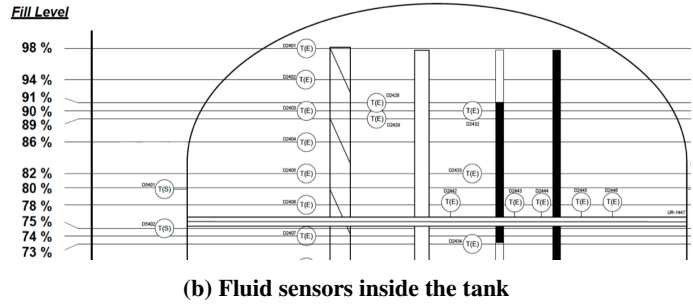
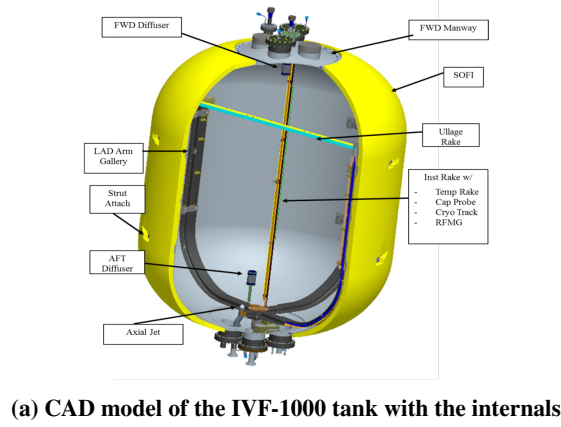
A brief background behind the EDU tank tests is provide in Patel et al [1].

1. Testing Facilities

The cylindrical double-domed tank is constructed with 2 mm thick 2219 aluminum and has an internal volume of 4.367 m^3 . The tank cylinder has a radius of 0.852 m and height of 2.334 m, and the half oblate spheroids have a minor radius of 0.615 m. The tank is insulated with spray-on foam insulation (SOFI) as well as multi-layer insulation (MLI) for insulation in vacuum conditions. The tank was mounted in vacuum chamber on a stand with struts at NASA MSFC test stand 300. A series of pressure and temperature sensors (Figure 3) were located on horizontal and vertical rakes inside the tank, on the diffuser inlet, the tank wall, and the MLI layers. [1]

2. Experimental Procedure

For this autogenous pressurization modeling test, the tank was filled with liquid hydrogen, vented at the atmospheric pressure to achieve a saturated gas-liquid interface and then locked-up at 90% fill volume. Temperature probes data show that a uniform initial temperature was achieved. All drain valves remained closed throughout the test. Gaseous hydrogen pressurant at 297 K temperature was introduced into the ullage through the diffuser for approximately 100 seconds. The measured diffuser mass flow history is shown in Figure 4 along with the corresponding ullage pressure. [1]



Fill Level (%)	Tank Station (in)	Instrumentation ID		
		Temperature Rake	Cryo Tracker	RFMG
98	85.2	D2401		
94	80.2	D2402		
91	77.3	D2428		
90	76.4	D2403	D2432	
89	75.6	D2429		
86	73.1	D2404		
82	70.0	D2405	D2433	
78	67.0	D2406		

(d) Locations of Fluid Sensors (measured from tank bottom)

Fig. 3 Temperature and pressure sensors

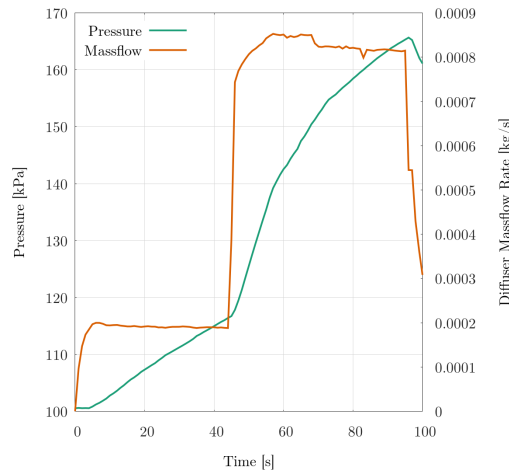


Fig. 4 Diffuser massflow and corresponding tank pressure

IV. Computational Model

The salient physics pertaining to the problem is retained and inconsequential and secondary effects are ignored for practical computational modeling.

A. Governing Equations

The governing equations for mass, momentum, and energy conservation; phase change model; two phase sharp interface model; and interface turbulence transport are already described in our previous work [1]. Since both CFM

operations involve turbulent flows, RANS equations are used.

B. Turbulence Modeling

Menter's 2003 shear stress transport (SST) model is primarily utilized for turbulence modeling [4], but improved delayed detached eddy simulation (IDDES) approach [5] is also used to address the problem of excess turbulence transport in RANS turbulence model. It is a hybrid RANS-LES model where unresolved scales - typically near-wall regions and high shear or vorticity regions where mesh refinement for LES resolution is impractical - are modeled with RANS equations and resolved scales are modeled with sub-grid scale (SGS) modeling. An implicit LES approach is used where the grid-induced dissipation provides the sub-grid scales. The blending parameter, f_d distinguishes the resolved and unresolved regions. RANS mode is indicated by $f_d = 1$ and SGS mode is indicated by $f_d = 0$.

1. Interface Turbulence Transport

Experiments like those by Fabre et al [6] show altered turbulence at the gas-liquid interface. Damped turbulence kinetic energy on the gas side of the interface and mild enhancement of turbulence kinetic energy on the liquid side of the interface was observed. Rashidi et al [7] observed streak formations at the interface that are similar to the wall. Direct numerical simulation (DNS) data from Lombardi et al [8] also show wall-like near interface characteristics on the gas side and enhanced turbulence transport on the liquid side. DNS study by Fulgosi et al [9] found gas side near-interface turbulence to be similar to a wall's viscous sub-layer, but the turbulence kinetic energy is not zero at the interface. Still, they observed similarities in the near-interface turbulence distributions which indicates that a general RANS model is plausible. Jofre et al [10] studied bubbly flow using LES and found that modeling turbulence damping on the gas side of the interface produced satisfactory comparison to DNS near the interface.

These observations are encapsulated in our simple but effective interface turbulence model for the two-phase sharp interface method [1] where gas-side of the interface is treated wall-like, and liquid side of the interface has no boundary influence.

For VOF simulations, asymmetric interface turbulence transport (ITT) model is implemented based on the work by Fan et al [11], which builds upon Egorov's approach of increasing turbulence frequency, ω in the interfacial regions where low turbulence is desired [12]. An asymmetric damping approach is implemented where the turbulence on the gas side is damped, and the liquid side is enhanced in the near-interface region.

$$\frac{D(\rho\omega)}{Dt} = \text{Production} + \text{Destruction} + \text{Dissipation} + \text{Transformation} \quad (1)$$

$$\omega \rightarrow \frac{6\mu}{\beta\rho y^2} \text{ as } y^+ \rightarrow 0 \quad (2)$$

$$\omega_{wall} = B \frac{6\mu}{\beta\rho\Delta y^2} \quad (3)$$

$$S_{ITD} = -\beta\rho\omega_{sublayer}^2 = -\beta\rho\left(B \frac{6\mu}{\beta\rho\Delta y^2}\right)^2 \quad (4)$$

The destruction term in the ω -equation (Equation 1) is $-\beta\rho\omega^2$. Based on Wilcox's asymptotic solution for ω in the viscous sublayer (Equation 2)[13], a wall ω value is specified by Menter (Equation 3)[14]. The ITT model employs Menter's wall solution as a source term (Equation 4) to the ω -equation on the gas side of the interface. A corresponding term enhances the turbulence transport on the liquid side of the interface [11].

Menter indicates that the asymptotic behavior of ω as described by Wilcox [13] is satisfied by Equation 3 as long as $y^+ < 3$ [14]. He supplies $B = 10$ for a smooth no-slip wall. The turbulence damping on the gas side of the interface due to a liquid cannot be higher than the damping caused by a wall and therefore values much higher than 10 may not be justified without a well-elucidated reasoning. Yet many studies [15][16][17] including Fan et al do so. They are likely compensating for an insufficient mesh resolution, i.e., an interface first cell height, $\Delta y > 3y^+$ and possibly other factors described in the last paragraph of this section. But such arbitrarily tuned high values could lead to non-physical damping. Indeed, while using very high B , Fan et al deviated away from the turbulence kinetic energy data from their validation experiments and also underpredicted the pressure gradients.

Author's first recommended approach is to employ a well-resolved mesh with low y^+ and not to exceed the damping factor value of 10. When such refinement is impractical, a pre-devised scaling factor as a function of an estimated interface y^+ should be used in order to avoid non-physical behaviors. The author intends to take up the problem of

developing a scaling technique in the future. Developing an interface modeling approach based on Wilcox's original method of calculating near-wall ω distribution (Equation 2) instead of Menter's simplified method of computing only the wall ω value (Equation 3) may also be particularly fruitful.

Beyond the compensation for insufficient mesh refinement by tuning B, these studies including the present one may be missing some important flow physics that arise from the gas-liquid interactions differing from a wall-fluid interaction. The author's hypothesis is that because the turbulence transport depends on the interface tangent velocity gradient, the missing flow physics may include the effects of relative gas-liquid molecular viscosities and densities, as well as the presence and degree of flow reversal (i.e., "boundary-layer" separation) at the interface. If the aforementioned modeling techniques do not provide satisfactory modeling fidelity, these hypotheses may need to be explored in the future.

C. K-site Tank - Axial Jet Pressure Control

1. Geometry

Tank internal probes rakes are unimportant to the pressurization predictions and are removed from the computational model. The tank is modeled as an axisymmetric tank because no significant circumferential velocity components are expected. A 1-degree tank sector is modeled. All the circumferential velocities are zeroed out in the governing equations. Tank solids are not modeled because they are not expected to have trivial impact on the depressurization rate. A test simulation without the heat leakage to the tank walls yielded no significant differences in the depressurization trend compared to simulations where heat leakage is modeled – indicating that small amount of heat transfer between

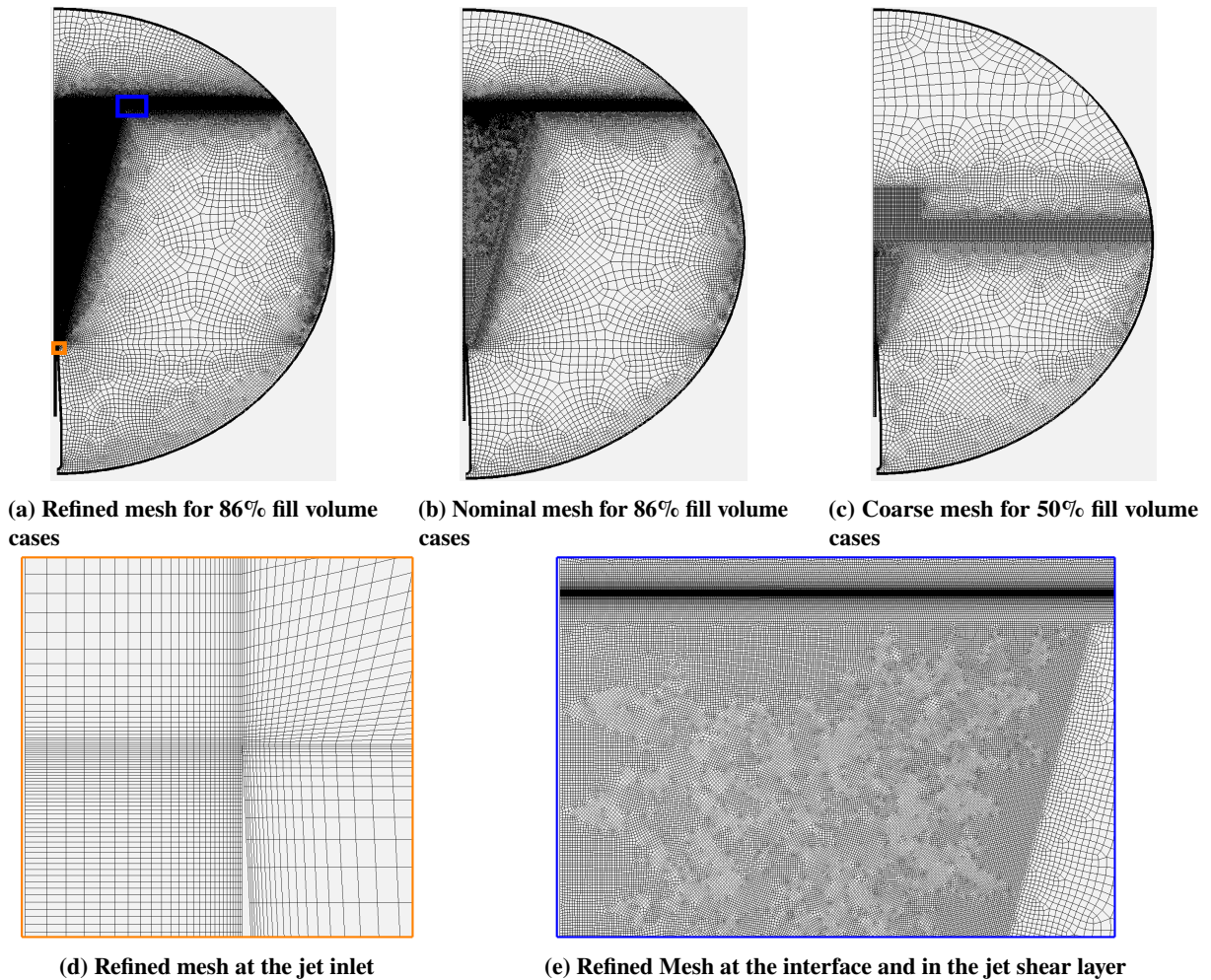


Fig. 5 Meshes for K-site tank axial jet pressure control simulations

the tank fluids and the tank walls does not significantly impact the problem.

The mixer inlet and outlet locations are known along with the jet nozzle diameter, but the precise geometry of the mixer is unknown and is approximated. The pump/mixer internals are not modeled. These approximations are expected to be inconsequential to time-accurate pressure predictions because minor flow variation near the bottom of the tank is not expected to impact either the interfacial dynamics or the convection currents - both of which are expected to primarily influence the depressurization.

2. Mesh

Six unstructured hexahedral meshes are created. Three of them are shown in the Figure 5. Each mesh has refinement in the regions of high shear, i.e., jet shear region and near the interface to sufficiently resolve the flow and thermal dynamics. The nominal mesh is 123 thousand cells for a 1-deg axisymmetric sector, which is equivalent to 44 million cells for a 3-dimensional domain. First cell wall-normal height is always 1×10^{-4} m to capture boundary layer flow with $y^+ \leq 1$. Interface normal first cell height as low as 5×10^{-5} m are tested. Largest cell edge length is restricted to 5×10^{-3} m and is refined up to 1×10^{-3} m. A mesh independent solution is obtained and discussed in V.A.3.

3. Initial Conditions

Tank conditions shown in the table 1 are used to initialize liquid fill level and ullage pressure. Axially varying temperature profile is initialized based on the temperature probe data available for each test. A typical profile has the coolest temperature at the tank bottom with a sharp thermal gradient at the interface and approximately linear temperature increase in the ullage away from the interface. Radial temperature variation is not considered owing to a lack of such data. The initial convection current and corresponding thermal gradients were expected to have negligible impact because the axial jet velocity is two to three orders of magnitude higher than the natural convection velocity and is expected to drive the pressure trends. Indeed, a test simulation initialized from a few minutes of self-pressurization simulation to set-up temperature and velocity distribution showed no noteworthy impact on the depressurization rate prediction.

4. Boundary Conditions

Tank walls were supplied with constant heat flux of 4.2 W/m^2 to simulate the heat leak. A symmetry boundary condition is applied on the sector planes of the axisymmetric model. The pump outlet is modeled in the computational domain as a constant velocity inlet boundary condition with a constant temperature, and the pump inlet is modeled as a constant volume outlet from the tank. In reality, as the test progresses, the jet-induced mixing in the liquid hydrogen warms up the inlet temperatures - reducing the efficacy of the jet to reduce the tank pressure as the test progresses. Tests were run for about 500 seconds for the test 449 to ascertain sensitivity to the warming jet. A time-varying (increasing) inlet temperature was applied by averaging outlet temperature from a previous simulation. This sensitivity tests were quantitatively non-conservative but were expected to be qualitative useful. The tests showed no impact on the

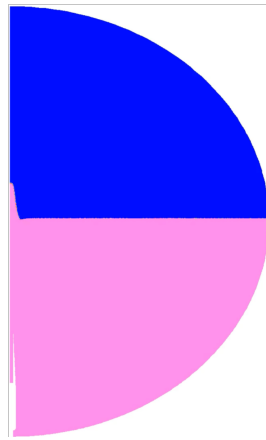


Fig. 6 Test 449 interface shape predicted by the VOF method

depressurization rate, and the cases were run with the constant temperature. Later it was found that not modeling jet warming impacts at the later part of the longer run tests with higher massflow rates, i.e., tests 449 and 457 and results in underprediction of the pressure.

For the sharp interface turbulence boundaries, gas-side is treated wall-like as usual. But the liquid side treatment deviated from the no-treatment approach (extrapolated boundary) to wall-like treatment to counterbalance the overprediction of turbulent kinetic energy arising from not modeling the non-planarity of the interface. The interface is assumed to be flat for the sharp interface solution, but the flat interface becomes non-planar when the jet impinges it (Figure 6). The change in flowfield would lower the velocities on the liquid side of the interface as well as turbulent kinetic energy than predicted by a planar interface. Wall-like turbulence modeling allows counterbalancing this modeling deficiency by lowering effective turbulent kinetic energy near the liquid side interface.

D. EDU Tank - Autogenous Pressurization

1. Geometry

Axisymmetric flow is assumed. Tank internals are removed with the exception of the forward diffuser, which is simplified (Figure 7) to have three annular cylindrical slots with same exit area as the original diffuser .

The heat transfer between the room temperature gaseous hydrogen and the tank's walls at the liquid hydrogen cryogenic temperature has significant impact on the ullage pressure. So, conjugate heat transfer analysis is conducted to model the heat transfer between the tank walls, diffuser walls, and the fluids.

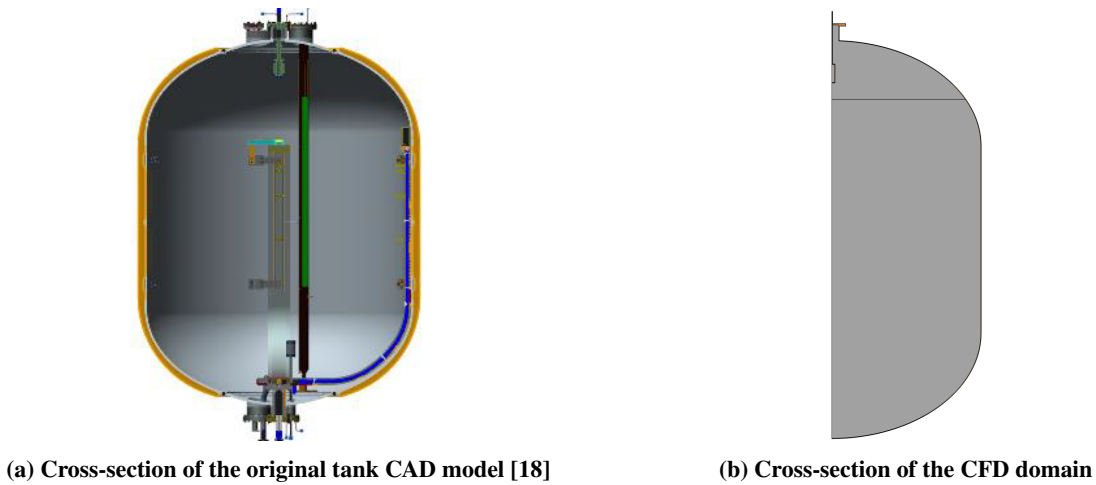


Fig. 7 Tank Model with and without Tank Internals

2. Mesh

Mesh is refined to capture the important flow features of the high-speed diffuser flow, low velocity ullage flow with convection and heat transfer between ullage gas at cryogenic temperatures and pressurant gas at room temperature, and the sharp thermal gradient at the fluid-wall boundary as well as the gas-liquid interface. Seven unstructured hexahedral meshes with varying resolution in the diffuser, ullage and interface regions are used for this validation. A representative sample is presented in the Figure 8. To accurately calculate the heat transfer between the wall and the fluid, wall integration approach was used, i.e., mesh y^+ is 1 or lower at the tank walls. The wall boundary first cell height was varied between 1×10^{-4} m and 5×10^{-5} m. The nominal cell edge length in the ullage varies between 2.5 mm and 7 mm. The first cell heights on both sides of the gas-liquid interface vary between 1×10^{-4} m and 1×10^{-6} m to accurately capture the altered turbulence characteristics, mass transfer, and heat transfer across the interface. The baseline mesh has an equivalent three dimensional cell count of 18.8 million (Figure 8b). Mesh sensitivity is presented in Section V.B.4.

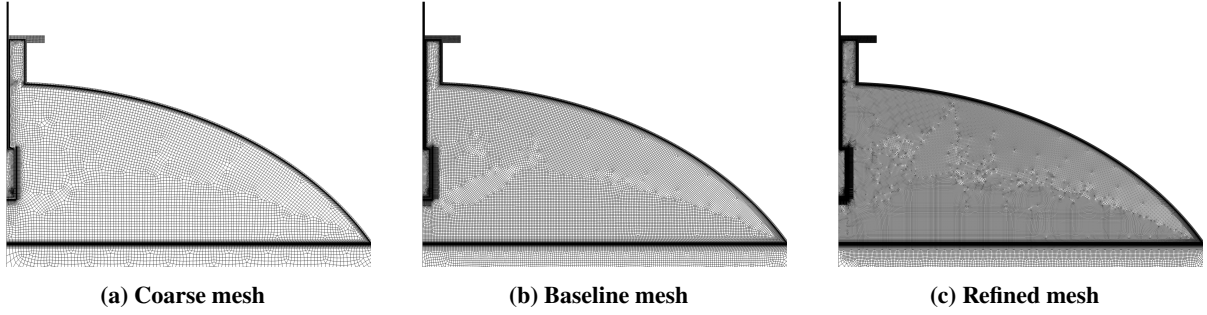


Fig. 8 Three of the mesh resolutions tested for obtaining mesh independent solutions

3. Initial Conditions

The initial temperature distribution is uniform throughout the tank fluids, and the walls and corresponds to the saturation condition for hydrogen at the initial pressure of 100 kPa.

4. Boundary Conditions

Time-varying massflow and temperatures were measured during the test and are prescribed at the diffuser inlet. The measurements across the 40 MLI temperature probes show that the tank is well-insulated in the vacuum chamber, so tank external wall is considered adiabatic.

A diffuser inlet turbulence intensity of 5% with eddy viscosity ratio of 1000 are prescribed based on the expectation of medium to high turbulence. Several simulation tests were carried out to ascertain impact of initial turbulence and diffuser inlet turbulence. They show the pressurization predictions to be insensitive to a wide range of diffuser inlet turbulence conditions.

For conjugate heat transfer analysis, a tight fit between mating solids was assumed and a small thermal contact resistance of $1e - 16$ was supplied for their contact surfaces.

E. Fluid Properties

Fluid and solid material properties were evaluated from the current National Institute of Standards and Technology (NIST) databases [19]. The liquid hydrogen converts to para-hydrogen isomeric state after sufficiently long storage. Since the flow dynamics is dominated by the liquid interactions in the K-site axial jet experiments, liquid hydrogen is assumed to be in the para-hydrogen state. For the autogenous pressurization, vapor flow dynamics dominates the pressurization and only the near interface liquid participates in the process. The newly liquefied gas converts to the ortho-hydrogen isomeric state at the interface. Owing to these reasons, the liquid is modeled in the ortho-hydrogen isomeric state for the modeling of the autogenous pressurization experiment. The liquid hydrogen is assumed to be a Boussinesq fluid to model the buoyancy effect. Since the liquid temperature does not vary considerably during the test, constant thermal and transport properties are modeled.

The vapor is modeled as an ideal gas. Sutherland's law was used to model temperature dependent vapor viscosity

Parameters	Description	Value
ρ_l	Liquid density	70.78 kg/m ³
c_{pl}	Liquid specific heat at constant pressure	9758.00 J/Kg/K
k_l	Liquid thermal conductivity	0.1008 W/m/K
μ_l	Liquid dynamic viscosity	1.3446×10^{-5} kg/m/s
α_l	Liquid volume expansion coefficient	0.016 58 K
L	Latent heat	436 480.0 J/kg
σ	Surface tension	0.001 776 N/m

Table 2 Thermodynamic properties of liquid hydrogen at 20.3450 K and 133000.0 Pa

Parameters	Description	Value
ρ	Density	Ideal gas EOS or Tabulated real gas
c_{pg}	Specific heat at constant pressure	Function of temperature
k_g	Thermal conductivity	Function of temperature
μ_g	Liquid dynamic viscosity	Function of temperature

Table 3 Thermodynamic properties of hydrogen vapor

Parameters	Description	Value
ρ_{Al}	Density of Aluminum 2219	2840.0 kg/m ³
ρ_{SS}	Density of Steel 304	7930.0 kg/m ³
c_p	Specific heat at constant pressure	Functions of temperature
k	Thermal conductivity	Functions of temperature

Table 4 Thermodynamic Properties of Aluminum 2219 and Stainless Steel 304

and conductivity. Since gaseous hydrogen deviates about 12% from the ideal gas behavior [18], real gas is also modeled using tabular equation of state, thermal properties and transport properties from the NIST database. But the choice of vapor's equation of state was found to have little influence on the pressurization prediction.

The EDU tank wall is modeled with temperature-dependent aluminum 2219 thermal properties [20], and diffuser is modeled with temperature-dependent stainless steel 304 thermal properties from NIST. The properties of ortho-hydrogen liquid (Table 2), hydrogen vapor (Table 3), tank wall, and diffuser wall (Table 4) are listed in the tables below.

F. Discretization and Solver Set-up

Spatial discretization is either first order upwind (FOU) or second order upwind (SOU) - except for the VOF equations, which are always solved using the FOU scheme. Time integration is performed using the implicit first order backward difference formula or second order backward difference formula. SIMPLEC scheme was used for pressure-velocity coupling. The second order schemes are preferred but the first order schemes are used when second order schemes are not stable. All simulations are well-converged with low residuals and 2-4 order of magnitude residual drops during Newton-Raphson iterations.

Spatial resolution is discussed in Sections IV.C.2 and IV.D.2. Temporal resolution in the range of 5e-4 seconds to 1 seconds are tested. All predictions are independent of spatial resolution, temporal resolution and mass transfer accommodation factor. The insensitivities are demonstrated in the Results section.

V. Results

Time-accurate tank pressure prediction is the primary validation goal. The probe temperature predictions are also compared and discussed as a secondary quantity of interest. The sharp interface method approach is the primary focus of the study, but the pressure prediction improvement with the VOF method owing to the ITT module is also briefly discussed.

A. K-site Tank - Axial Jet Pressure Control

1. Tank Pressurization

Across the five tests, the CFD predictions agree well with the tests, with a maximum relative error in pressure drop being -16.88% for the experiment 457 – demonstrating a reliable modeling capability. The time traces of the predicted and the actual ullage pressures are shown in Figure 9. Note: As described in Section IV.C.4, in contrast to the earlier finding, tests with higher flowrates and longer depressurization times, i.e., tests 449 and 457, were found to be affected by the jet warming effect that is not accounted for. Taking this effect into account, the maximum error is expected to be much lower than -16.88%.

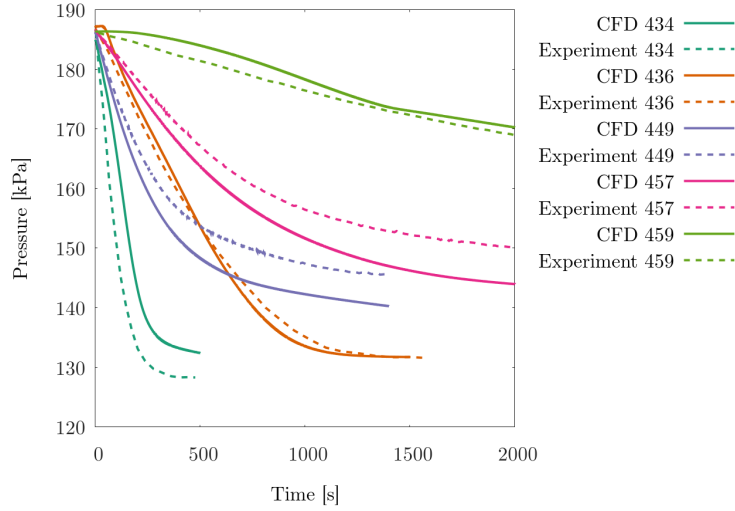


Fig. 9 Pressure prediction over time using sharp interface method compared with the test data

As the cold liquid from the tank bottom impinges the warmer interface, the interface cools due to the forced convection. A corresponding drop in the saturation temperature at the interface initiates condensation of the vapor. The vapor also cools due to the conductive and the convective cooling. Both processes lower the ullage pressure. The phase change phenomenon takes place around 1-100 micrometer length scale and the resulting latent heat exchange could produce high temperature gradient near the interface. This temperature gradient must be captured accurately because the vapor pressure is strongly affected by the interface temperature as evidenced by Antoine equation (Equation 11 in Patel et al[1]). The first cell height of at least 1×10^{-4} m normal to the interface was necessary to resolve the thermal gradient resulting from the complex interactions of the forced convection, the interfacial turbulence and the latent heat exchange.

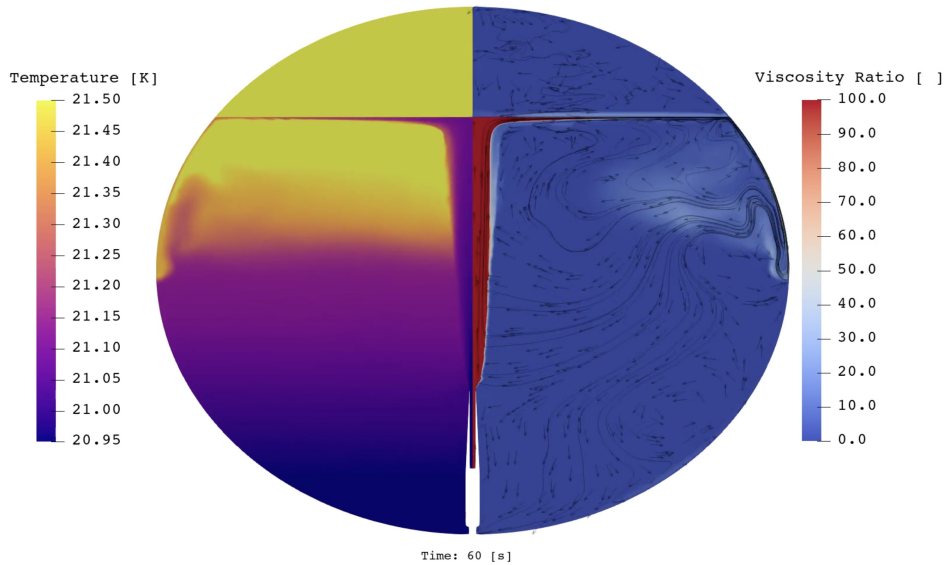


Fig. 10 Composite contour plot of Test 434 at 60 seconds shows temperature on the left side and turbulence viscosity ratio along with the streamlines and velocity vectors on the right hand side. The jet impinges the interface and depressurizes the tank through condensation and cooling of the ullage vapor. As the jet flows over the tank wall, it entrains and convects the hotter liquid which rises back up due to the buoyancy creating Rayleigh-Taylor and Kelvin-Helmholtz instabilities resulting in turbulent mixing of the liquid.

Figure 10 demonstrates the physical processes of axial jet based tank depressurization at the tank-scale through the temperature and turbulent viscosity ratio contours. The turbulent mixing induced by the mixer flow in the previously quiescent liquid governs how quickly the tank temperatures homogenizes in the liquid region of the tank. Near the gas-liquid interface, the cooling of the interface due to the jet is not uniform across the interface. The highest temperature gradient between the gas and liquid is found near the jet impingement location. This region is responsible for the maximum cooling and condensation of the vapor. After the impingement, the jet warms up downstream as it mixes with the warmer liquid, absorbs latent heat energy from condensation of the gas, and absorbs sensible heat from the warmer gas. The depressurization plateaus as the liquid temperature homogenizes over time.

The depressurization is the fastest, and the pressure drop is the largest (test 434) when the tank fill level and jet flow rate are higher because of the availability of the large amount of cooler bulk liquid to absorb thermal energy from the interfacial liquid. When the jet flow rate is low, slow and long-sustained, linear depressurization occurs (Test 459). Our CFD is able to predict depressurization at all regimes of jet flowrates, and at both high and low propellant fill levels.

The newly implemented ITT module in the Loci-Stream-VOF also drastically improves the predictions of VOF method (Figure 11). But the refined mesh resolution required at the interface to accurately capture the fluid-thermal dynamics restricts the timestep owing to the explicit time-integration requirement of the VOF advection equation where the Courant number must be maintained much lower than unity for numerical stability. More importantly, the inevitable spurious velocities and instabilities introduced at the interface by the geometrically accurate VOF method make the solution numerically unstable. More work is being done to alleviate these issues with the VOF method.

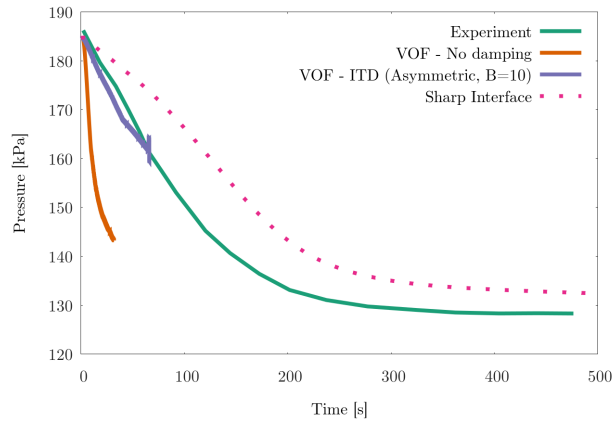


Fig. 11 ITT model significantly improves the predictions with the VOF approach, but the VOF approach is unstable at the required 0.1 mm near-interface length-scale. VOF stability enhancements are planned in the near future.

2. Tank Temperatures and Turbulence Modeling

For each of the five tests, CFD temperature data was extracted at the location where experimental temperature rake data is available. Here, we note that the probe locations (Figure 3) were extracted as accurately as possible from the available tank documentations which lacked some location information and judicious assumptions were made based on the available data and the schematics of probe locations. Small uncertainty in probe locations remain.

A related pressing problem in the CFM modeling community is that of the accurate prediction of the turbulence transport. For this particular problem, jet mixing with the quiescent liquid creates high shear stress and consequently highly turbulent flow in the mixing region, but in the rest of the tank, away from the near-wall regions, the turbulence transport is expected to be much lower. Further, the altered turbulence transport at the interface is already discussed. Here, temperature data is used as an indirect indicator for the turbulence transport to gain insight into turbulence modeling.

While Menter's SST model predicts the pressurization satisfactorily (Figure 9), the temperature comparison is less satisfactory, but IDDES model captures the temperature trends almost always better or at least as well as the SST model (Figure 12, 13, and 14). It is evident that the temperatures in the tank are more homogenized due to the overpredicted turbulence transport by the SST model. The IDDES model suppresses the SST model's overprediction 15. The switch

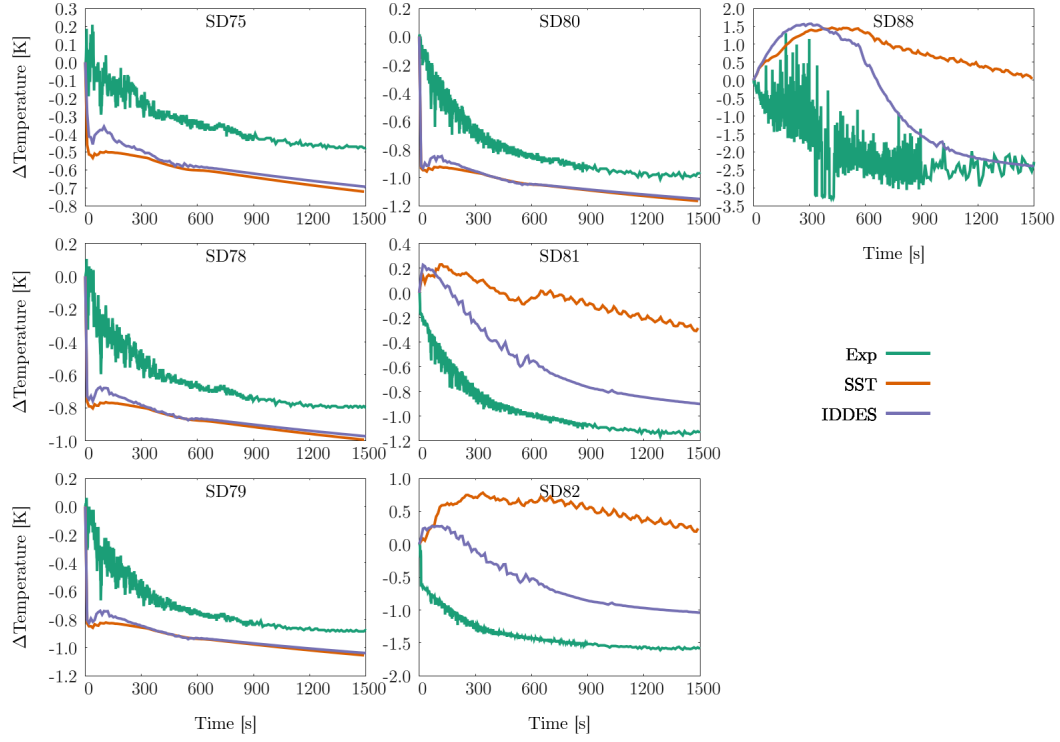


Fig. 12 Comparing SST and IDDES temperature predictions with the test data at the interface rake for Test 449

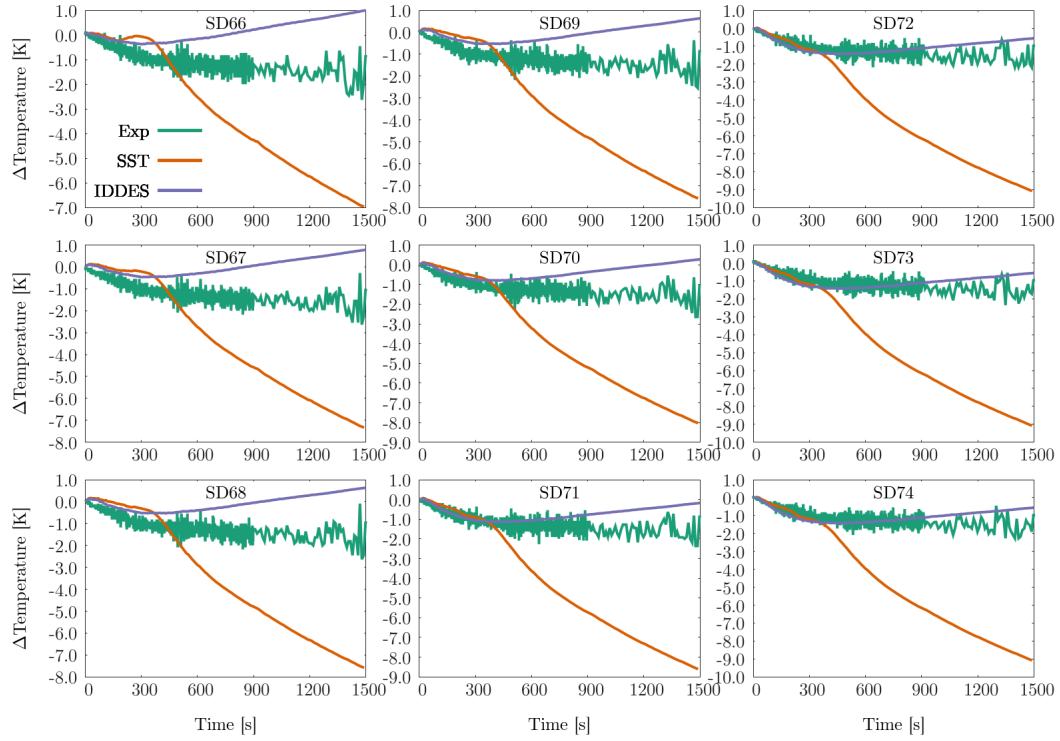


Fig. 13 Comparing SST and IDDES temperature predictions with the test data in the ullage for Test 449

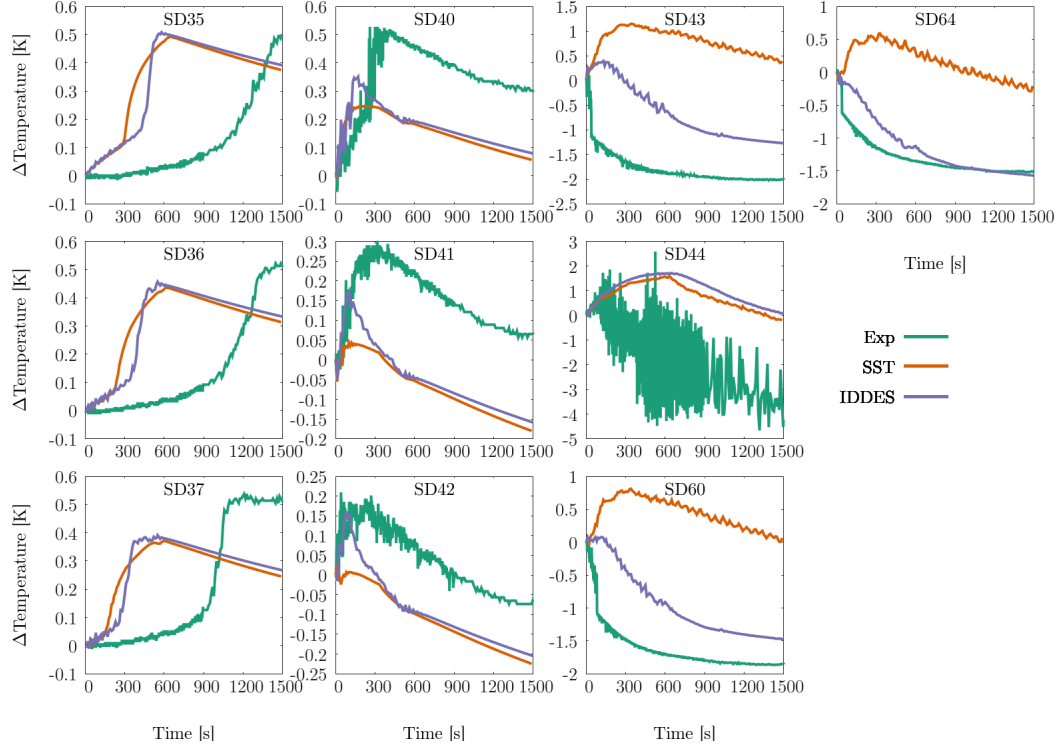
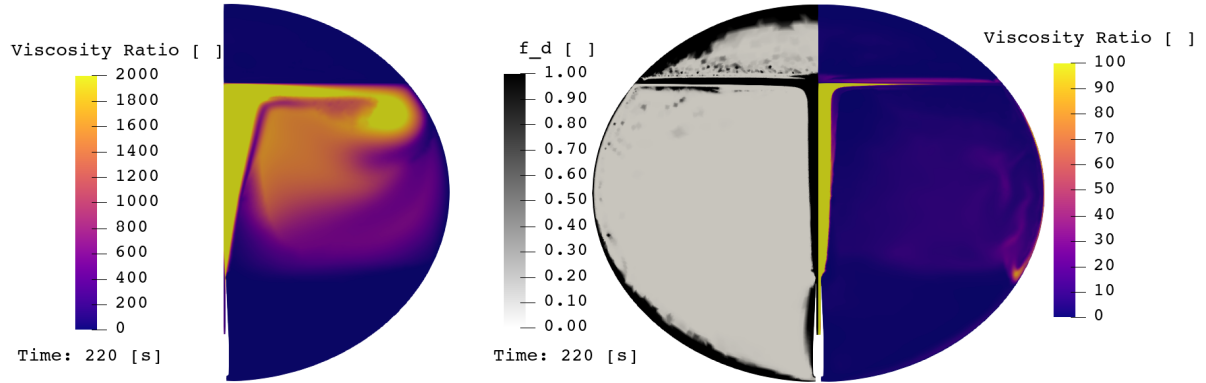


Fig. 14 Comparing SST and IDDES temperature predictions with the test data on the axial rake for Test 449



(a) Menter's SST turbulence model

(b) IDDES model: f_d and turbulence viscosity ratio

Fig. 15 Turbulent viscosity ratio comparison between Menter's SST 2003 model and IDDES 2012 model shows reduced viscosity ratio with IDDES method. Probe temperature comparisons indicate that IDDES's turbulence viscosity ratio field prediction is more accurate.

to SGS model in some flow regions avoids the excess turbulence transport observed in the SST model and improves the temperature predictions.

With turbulence modeling, there are almost always drawbacks that need to be balanced with the benefits. The two-equation RANS models are relatively simple and have been time-tested for a wide-range of engineering applications, but they fail to be satisfactory for many CFM operations. While the IDDES model improves upon the RANS models by ameliorating non-physically high turbulence mixing regions in RANS model, their mesh-dependent nature requires

careful meshing and an a priori understanding of at least some flow physics.

Current recommendation is evaluating the problem with both modeling approaches and then evaluating each against known physical processes. In our problem, the jet mixing process provides that grounding. If the mesh is too refined in the jet shear layer, it is treated with SGS turbulence instead of RANS turbulence and the mixing in the shear layer is under-predicted. Since jet mixing is a canonical and well-understood turbulence problem, the jet spreading acts as a check on the accuracy of the turbulence modeling. The solution then is to sufficiently coarsen the jet mixing regions to ensure RANS modeling in that region with the IDDES method. Note that the IDDES solution is still mesh independent in any other region. i.e., the pressure prediction is unaffected by further mesh refinement.

While this mesh-dependence is a drawback for the IDDES modeling technique, our current approach is to rely on flawed yet time-tested RANS predictions while simultaneously gaining insights from the IDDES for the problem and future turbulence modeling improvement. While the RANS approach is too diffusive, both approaches predict the pressurization of the tank well because the turbulence treatment at the gas-liquid interface drives the problem dynamics and are identically for both approaches.

3. Mesh Sensitivity

Several computational meshes were tested to achieve a mesh independent solution. For brevity, three of the meshes are shown here to demonstrate mesh independence (Figure 16).

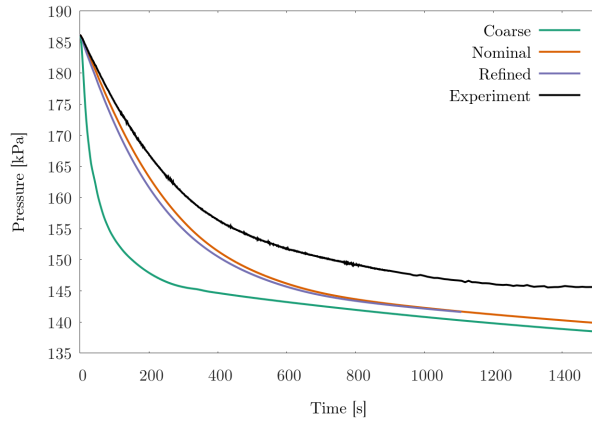


Fig. 16 Mesh Sensitivity

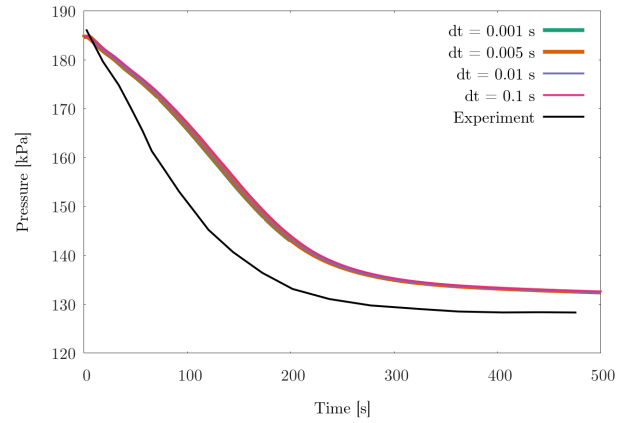


Fig. 17 Timestep Sensitivity

4. Timestep Sensitivity

Timestep independent predictions are obtained for less than or equal to 1×10^{-2} s timestep for the sharp interface predictions. In fact, little sensitivity to timesteps is shown below 0.1 s timestep (Figure 17).

5. Accommodation Factor Sensitivity

Accommodation factor in the Hertz-Knudsen-Schrage equation (Equation 11 in Patel et al [1]) is a coefficient that linearly modulates the rate of evaporation/condensation. Its value is expected to be a function of fluid property, and thermodynamic state. Some experimentally calculated values of the accommodation factor are available in literature for certain fluids but tend to vary in a wide range. This uncertainty is a more serious concern for thermodynamically open systems where mass is being added or removed from the system. But for the accommodation factor value greater than $1e-4$, the closed systems predictions seem to show almost no dependence on the accommodation factor value [21]. This feature has been observed previously in the self-pressurization tests and is now replicated in the axial jet pressure control tests (Figure 18).

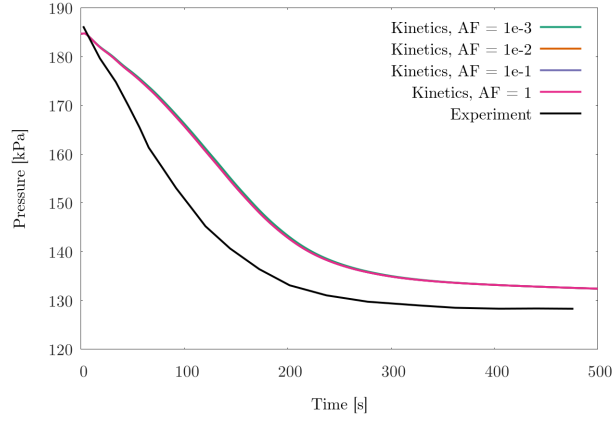
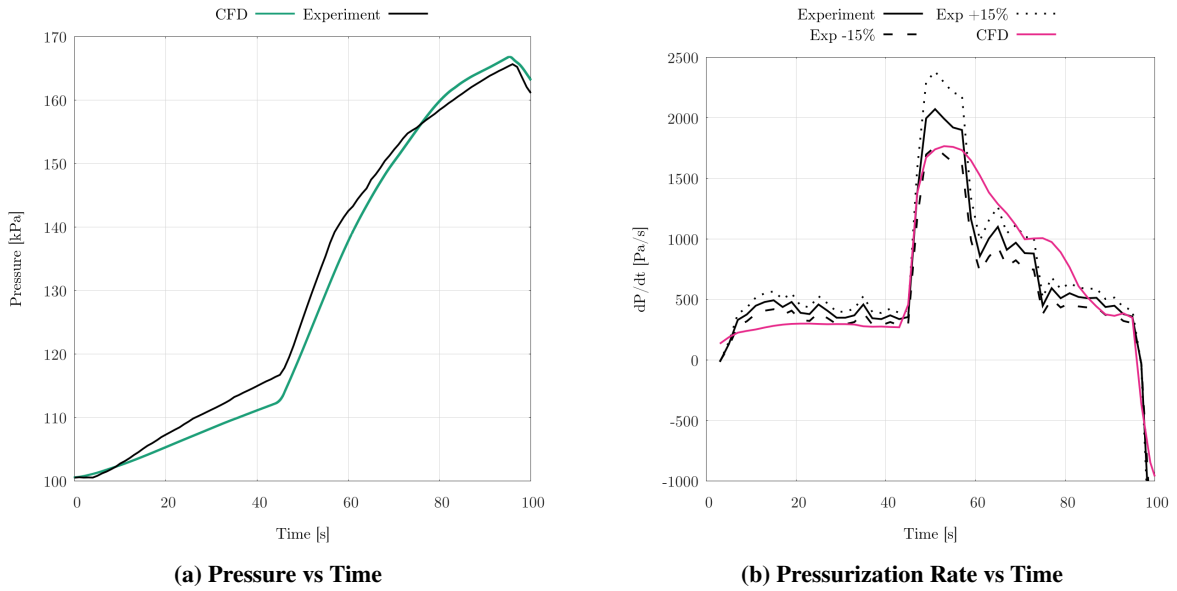


Fig. 18 Accommodation Factor Sensitivity

B. EDU Tank - Autogenous Pressurization

1. Tank Pressure



(a) Pressure vs Time

(b) Pressurization Rate vs Time

Fig. 19 Pressure and pressurization rate compared with the experiment

Pressure is predicted with a high accuracy (Figure 19a). Compared to the maximum pressure change during the test, the peak pressure is predicted with only 5.3% relative error. The pressure prediction is considerably more accurate compared to the previous prediction [1] - primarily owing to improved conjugate heat transfer modeling with temperature-dependent solid thermal properties for the tank solids as well as the improvement in the modeling of phase change energy source term.

The forward diffuser valve is partially opened from for the first 45 seconds, after which the flow rate is increased as shown in Figure 4. Pressurization rate increases sharply with the increase in the diffuser mass flow rate. This transition is also captured time-accurately by the CFD analysis. The pressurization rate is compared in the Figure 19b and also captured satisfactorily.

The peak pressurization rate in the test is 2000 Pa/s (see Figure 19b, which is three orders of magnitude higher than the rate observed in the K-site tank self-pressurization experiments [22] [21], so the interface temperature gradients and turbulence transport must be carefully modeled for a successful validation.

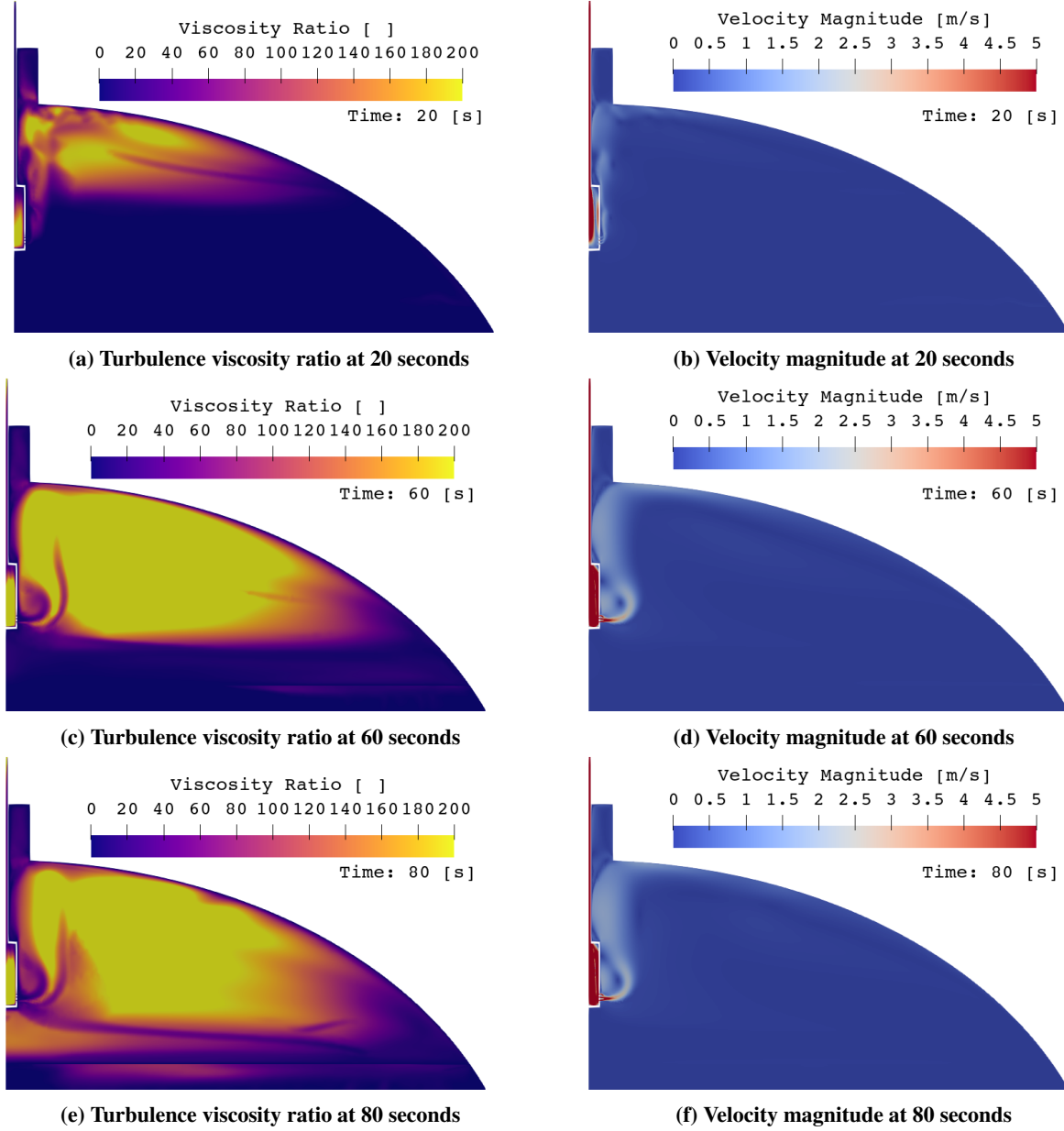


Fig. 20 Turbulent viscosity ratio and velocity magnitude shows evolution of flowfield over time

Multiple flow dynamics are interacting in the pressurization process. The compression of the cold ullage gas by the introduction of the hot gas at 298 K temperature increases the pressure and the temperature of the entire ullage through the isochoric compression process. The trickling hot diffuser inflow simply rises up (Figure 20b) in the tank due to the buoyancy effect at the low inflow rates, but as the inflow rate increases the inflow penetrates a bit further the ullage gas and increases turbulence transport. This turbulence transport also alters the ullage temperature and pressure. Further, as soon as the pressure and the temperature of the ullage increases, the interface phase equilibrium is disturbed and condensation of the ullage initiates in addition to the sensible heat transfer at the interface. The latent heat released by the vapor during the condensation increases the interface temperature. The interfacial dynamics is further affected by the near-interface turbulence characteristics, which plays a significant role in pressure prediction and discussed in the next section. Evolution of the flowfield is shown in the Figure 20.

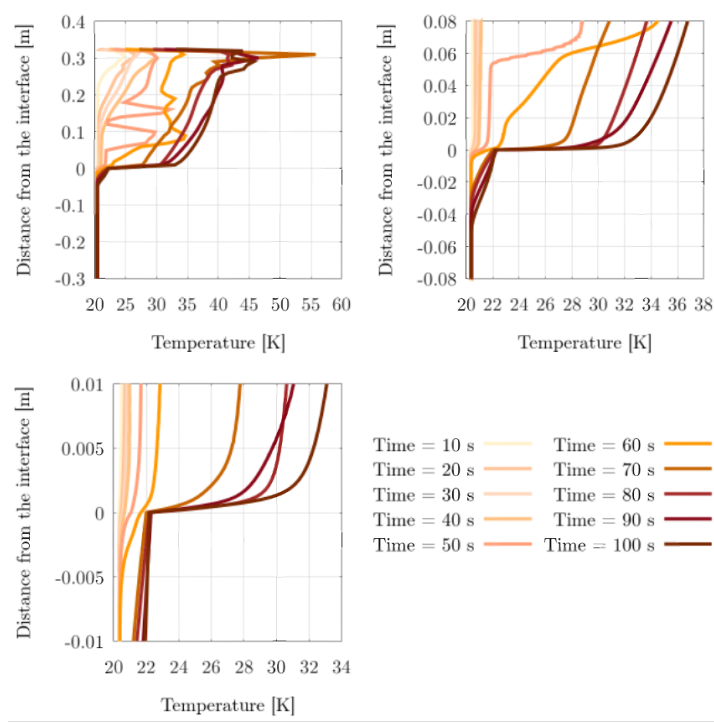


Fig. 21 Temperature across the interface over time shown on three different length scales on an increasingly refined length scale (clockwise from top left)

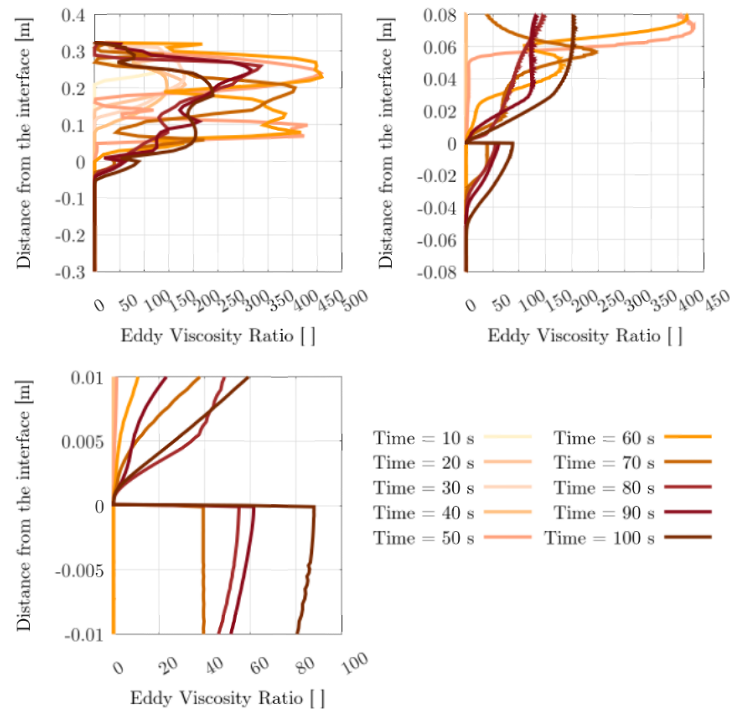


Fig. 22 Eddy viscosity ratio across the interface over time shown on three different length scales on an increasingly refined length scale (clockwise from top left)

2. Interface Temperature and Turbulence

The temperature gradient at the interface needs to be modeled and captured with high accuracy because the ullage pressure is strongly affected by the interface temperature as evidenced by the Antoine equation (Equation 11 in Patel et al[1]). A 0.2 K error in temperature prediction at the interface would result in 14% error in pressure prediction based on the saturation curve of hydrogen. Again, an interface normal first cell height of at least 0.1 mm is found to be crucial to resolve the sharp thermal gradients (Figure 21) resulting from the complex interactions of the forced convection, the altered interfacial turbulence transport and the latent heat exchange. A larger first cell height results in an incorrect thermal gradient prediction and consequently an incorrect ullage pressure prediction.

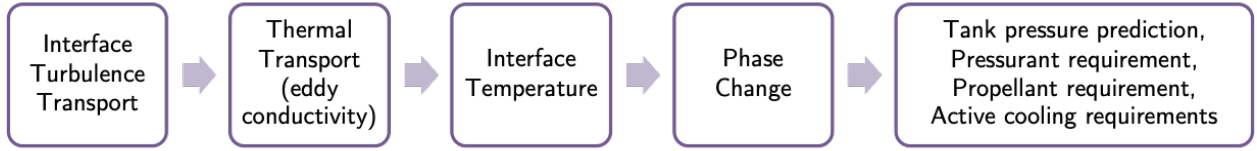


Fig. 23 Tank pressure sensitivity to the interface turbulence

Further, the interface turbulence has a large impact on the pressurization trend. The causal link is illustrated in Figure 23. Turbulence modeling is discussed in Section IV.B.1. Evolution of turbulence kinetic energy is shown in Figure 22 to demonstrate sharp change in turbulence transport across the interface. Only if this transport is modeled with sufficient accuracy, the eddy conductivity near the interface and consequently temperature of the interface can be captured accurately.

3. Fluid and Solid Temperatures

The locations of the liquid temperature probes used in the test are obtained from the tank's CAD model, but the locations of the solid temperature probes were not available in this CAD model, so they are visually approximated from a test schematic.

The diffuser temperature is predicted quite well (Figure 24b, but the tank wall temperatures at the probe D5439 is not. While the CFD captures the temperature stratification trends in the ullage well, the quantitative comparisons are unsatisfactory (Figure 24a). The reason behind these deviations is not well understood and is an active area of investigation. Turbulence modeling was initially suspected of excessive turbulent mixing (Figure 20c and 20e) which homogenizes the temperatures, but the laminar and IDDES modeling showed little improvement in the temperature prediction, so a true cause remains unidentified.

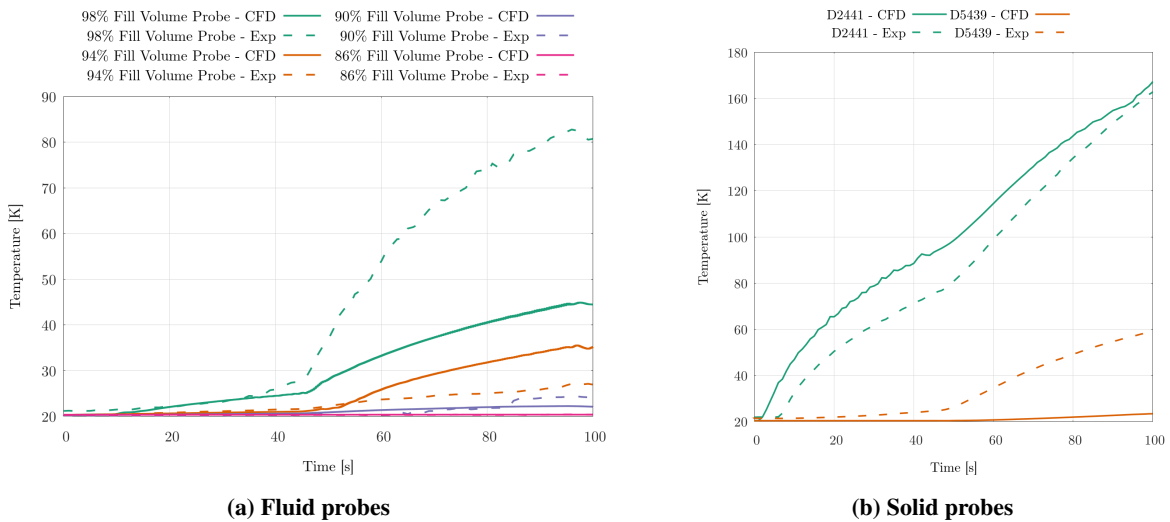


Fig. 24 Probes temperature comparison with the experiment

4. Mesh Sensitivity

Several computational meshes are tested for understanding the problem dynamics, and mesh sensitivity study. Figure 25 demonstrate the mesh independent solution. While the coarse mesh slightly underpredicts the pressure peak, all mesh are in reasonable agreement with the test data and further refinement is not justified.

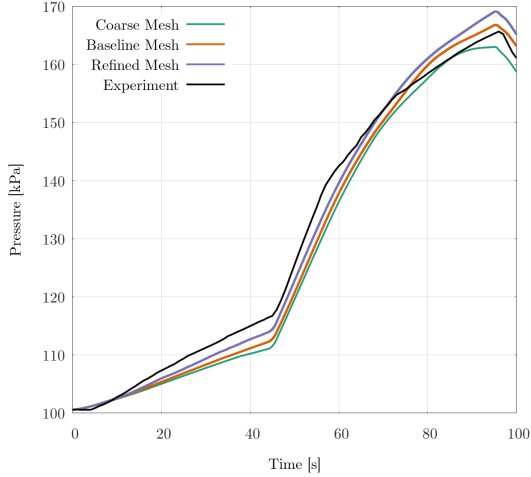


Fig. 25 Mesh Sensitivity

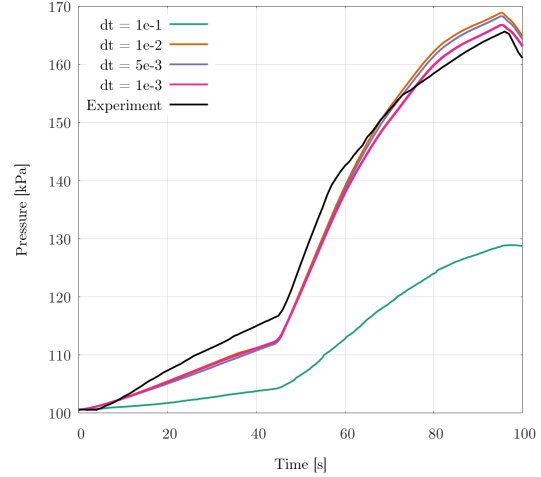


Fig. 26 Timestep Sensitivity

5. Timestep Sensitivity

The timestep independent predictions are obtained for less than or equal to 0.005 s timestep for the sharp interface predictions when using the refined mesh (Figure 26).

6. Accommodation Factor Sensitivity

See the discussion in V.A.5. For thermodynamically open system such as this autogenous pressurization problem, predictions could be sensitive to the accommodation factor. Therefore, a large range of values ranging from $1e-4$ to 1 are tested. Similar to the observations from the closed systems, the pressure predictions are found to be insensitive at or above the value of $1e-3$ (Figure 27).

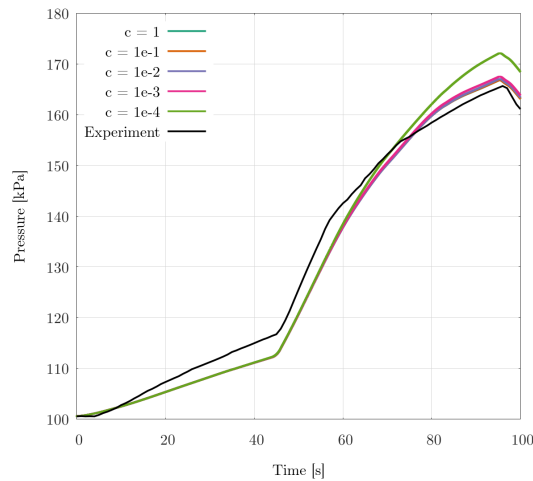


Fig. 27 Accommodation Factor Sensitivity

VI. Conclusion

Turbulence modeling plays a central role in the reliable predictions of cryogenic fluid management operations because it modulates phase change and interfacial heat transfer. Turbulence modeling approaches for the bulk fluid and gas-liquid interface are investigated to develop a reliable and practical predictive model for supporting the flight projects.

Two ground-based flight-sized CFM tests are used to validate our modeling techniques using sharp interface method. The modeling technique reliably predicts axial jet based pressure control across different jet flow rates and tank fill heights. Improving the conjugate heat transfer modeling with temperature-dependent thermal properties for the solids and an enhanced interface heat transfer modeling improved the time-accurate pressure prediction for the autogenous pressurization test. Interface turbulence transport modeling for the VOF method also shows significant improvements in predictive capabilities in the early development phase. Sensitivities to spatial resolution, temporal resolution, and phase change accommodation factor are evaluated to ensure that the validation is independent of these parameters.

For the K-site tank tests, the unsatisfactory temperatures predictions from the RANS model are improved with IDDES modeling. IDDES modeling primarily achieves this by preventing over-prediction of turbulent viscosity by the RANS model. The IDDES model's blending parameter that switches from RANS turbulence modeling to SGS turbulence modeling could be mesh sensitive, so some a priori understanding of expected flow physics is hugely beneficial. A cogent solution could be to compare the IDDES predictions with the RANS predictions to ensure elimination of the mesh-dependency. Future work may explore validation of other explicit or implicit LES approaches for better temperature predictions.

The early development of the interface turbulence damping model for the VOF approach significantly improves the predictions, but the solution is hampered by the stability issues at the required near-interface length-scale. The stability improvements and damping model improvements are planned in the near future. Once the stability issues are resolved, the modeling techniques for larger y^+ interface meshes will be explored.

The VOF approach will extend the application of the turbulence modeling techniques to the moving and morphing interface problems including the CFM operations in the micro-gravity environments.

The successful validation of our modeling techniques against these flight-scale tank experiments builds further confidence in reliability of our CFD tools for a wider range of CFM applications for supporting design of the long-term space flight missions.

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