

Modeling Self-Pressurization and Spray Bar Pressure Control of a Cryogenic Storage Tank in Normal Gravity

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This paper presents computational fluid dynamics (CFD) models for simulating self-pressurization and spray-bar pressure control processes in a large-scale liquid hydrogen storage tank under normal gravity conditions. For self-pressurization, the model employs the kinetics-based Schrage equation alongside the volume-of-fluid (VOF) method to account for interfacial mass transfer. The CFD predictions of pressure and temperature are compared with experimental data from the Multipurpose Hydrogen Test Bed (MHTB) experiment, and the predicted interfacial mass transfer rates are also presented. A CFD model simulating pressure control using a spray bar has also been developed. An Eulerian-Lagrangian approach models the interactions between discrete droplets and the continuous ullage (vapor) phase. The spray model is coupled with the VOF method by tracking droplets in the ullage and removing them when they reach the liquid interface. The T-sat model calculates droplet-ullage heat and mass transfer, where droplets warm up to the saturation temperature corresponding to the ullage vapor pressure before evaporating while remaining at the saturation temperature. The evolution of tank pressure, vapor temperature, and liquid temperature predicted by the CFD model is validated against data from the MHTB spray-bar mixing experiment. Overall, the CFD models agree with experimental data, demonstrating their capability to simulate self-pressurization and pressure control processes in large-scale cryogenic storage tanks. These models can be valuable tools for designing and optimizing cryogenic fluid management systems in future applications.

I. Nomenclature

A	=	Area density	p, P	=	Pressure
E	=	Energy	$\mathbf{q}$	=	Heat flux
$\mathbf{g}$	=	Gravity	$\dot{Q}$	=	Heat power
h	=	Surface curvature	R	=	Gas constant
k	=	Turbulent kinetic energy	T	=	Temperature
L	=	Latent heat	t	=	Time
M	=	Molar mass of fluid	$\mathbf{v}$	=	Velocity
$\mathbf{n}$	=	Normal vector	c_p	=	Heat capacity at constant pressure
			m	=	Mass

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<u>Greek</u>			<u>Subscripts</u>		
α	=	Cell value of volume fraction	i	=	Interface or phase
β	=	Slope limiter	il	=	Liquid side of the interface
ϕ	=	Face value of volume fraction	iv	=	Vapor side of the interface
μ	=	Dynamic viscosity	sat	=	Saturation conditions
ρ	=	Density	l	=	Liquid
τ	=	Stress tensor	v	=	Vapor
ω	=	Specific turbulence dissipation rate	p	=	Particle

II. Introduction

Efficient cryogenic fluid management (CFM) is a critical enabler for NASA's future human exploration missions. The primary challenge lies in the long-term storage of cryogenic propellants in space, where self-pressurization occurs due to heat leaks through insulation and conduction paths. Traditionally, thrusters have been used to settle the propellant and relieve tank pressure by venting during short-term operations. However, for long-duration missions, the added weight of the propellant and hardware to accommodate the increasing number of venting cycles would be prohibitively restrictive.

Maintaining the tank pressure while minimizing the boil-off loss of propellants through an active pressure control mechanism has become a significant focus area for addressing this challenge. This effort aims to overcome the limitations of traditional venting methods and enable the long-term storage of cryogenic propellants in microgravity.

Among the various pressure control strategies proposed and tested, the spray-bar thermodynamic vent system (TVS) is a promising solution for controlling tank pressure with reduced venting and without propellant resettling. The core components of a TVS include a Joule-Thomson (J-T) expansion device, a two-phase heat exchanger, and a spray-bar mixing pump system. These elements work together to reduce thermal stratification and remove heat from the tank while minimizing the loss of liquid cryogenics during pressure control [1]. For future microgravity applications, it is essential to demonstrate the effectiveness of a spray-bar TVS under unsettled conditions and to optimize this pressure control system for microgravity. In this context, CFD models, validated against ground-based test data, can be valuable design tools to extrapolate and optimize the spray-bar TVS design for successful performance in microgravity.

Various numerical models with different levels of complexity have been developed to study tank operations in both 1g and microgravity environments. However, many of these models have primarily focused on tank self-pressurization, with only a few exploring tank pressure control. The latter mainly address scenarios where an axial forced jet is used for thermal destratification via liquid mixing [2–5]. In the MHTB experiment, tank pressure control is achieved through an axial spray-bar TVS, simultaneously facilitating mixing and cooling by spraying droplets into the vapor region. Comprehensive models for gas-droplet interaction have been well-developed for applications such as thermal management of electronic equipment, evaporative mist flow heat exchangers, and combustion engines. However, their application to cryogenic storage tanks has been limited.

In previous papers, Kartuzova and Kassemi presented the results and validation of a two-phase CFD model to simulate self-pressurization and pressure control with MHTB experimental results. They conducted self-pressurization and spray-bar simulations for the MHTB tank at 50% and 90% fill levels [6–8]. Although a 25% fill level was tested experimentally, no previous CFD validation was performed for this case. This work extends the validation of the CFD model by including the 25% fill level case for the MHTB tank and different approaches to modeling self-pressurization.

This study aims to describe the development of a comprehensive two-phase CFD model for simulating the self-pressurization and pressure control of the MHTB tank at NASA Marshall Space Flight Center and its validation against MHTB ground-based test results. The MHTB tank has a volume of 18 m³ (693 ft³) and represents the size and shape of a liquid hydrogen (LH₂) propellant tank in a fully integrated space vehicle. The tank was designed to accommodate various components associated with different CFM concepts, including a spray-bar TVS [1] for active pressure control and a multilayer insulation (MLI) system for passive thermal isolation [9].

In the two-phase CFD model presented in this paper, the VOF model is used to capture the shape and evolution of the interface. A kinetics-based mass transfer submodel is employed to evaluate evaporative-condensing interfacial mass transfer. An Eulerian-Lagrangian coupled approach tracks the spray droplets and captures the interaction between droplets and the continuous vapor phase. Coupling the droplet and VOF models makes it possible to perform particle tracking in the vapor, removing particles from the vapor domain when they reach the interface. An in-house droplet-ullage

heat and mass transfer model, the T-sat model, accounts for pressure changes in the tank during the spray cycle [8]. The T-sat model calculates the evaporative mass transfer from the droplets. Droplet temperature and size changes are calculated and tracked during the simulations. Appropriate source terms are included in the governing equations to account for droplet-ullage mass, momentum, and energy transfer due to phase change.

This report validates the CFD model by comparing its predicted tank pressure and temperature evolutions with experimental results from the MHTB tank during self-pressurization. The simulation results of the spray-bar mixing process highlight how droplet vaporization contributes to changes in tank pressure during pressure control. Additionally, by comparing the CFD predictions of tank pressure and temperature evolution during the spray-bar mixing process with experimental values, we can gain further insights into the model's accuracy and the effectiveness of the pressure control mechanism.

A. Governing Equations

Fluid flow and heat transfer in the tank are described in terms of the continuity, Navier-Stokes, and energy equations for both phases:

$$\frac{\partial \rho}{\partial t} + \nabla(\rho \mathbf{v}) = 0, \quad (1)$$

$$\frac{\partial}{\partial t}(\rho \mathbf{v}) + \nabla(\rho \mathbf{v} \mathbf{v}) = -\nabla p + \nabla \left[\mu_{eff} \left(\nabla \mathbf{v} + \nabla \mathbf{v}^T \right) \right] + \rho \mathbf{g} + \mathbf{F}_{vol}, \quad (2)$$

$$\frac{\partial}{\partial t}(\rho E) + \nabla(\mathbf{v}(\rho E + p)) = \nabla(k_{eff} \nabla T) + S_h. \quad (3)$$

The present study treats the liquid phase as incompressible with variable temperature-dependent properties, except for density. The liquid density is allowed to vary linearly with temperature in the body force term of the momentum equation according to the Boussinesq approximation. The vapor is modeled as a compressible ideal gas. In this study, the movement of the interface is captured using the VOF method [10]. Interfacial energy, momentum, and mass balances are applied using source terms in the diffuse interfacial region.

B. VOF Model

In the VOF method, a volume fraction is defined in each cell such that the volume fractions of all the phases sum to unity. In the cell, the change in the interface can be tracked by solving a continuity equation for the volume fraction of the q^{th} phase:

$$\frac{1}{\rho_q} \left[\frac{\partial}{\partial t} (\alpha_q \rho_q) + \nabla \cdot (\alpha_q \rho_q \mathbf{v}_q) \right] = S_{\alpha_q}, \quad (4)$$

where the volume fraction for the primary phase is determined from:

$$\sum_{q=1}^n \alpha_q = 1. \quad (5)$$

In the VOF method, the field variables and properties are defined in terms of the volume fraction, which for a general system can be written as:

$$\rho = \sum_{q=1}^n \alpha_q \rho_q, \quad \mu_{eff} = \sum_{q=1}^n \alpha_q \mu_{eff,q}, \quad k_{eff} = \sum_{q=1}^n \alpha_q k_{eff,q}. \quad (6)$$

In this fashion, the continuity, momentum, and energy equations, as described by Eq. (1)-(3), can be solved throughout the domain for the temperatures and velocities in the two phases. In the VOF model, energy (E) and temperature (T) are treated as mass-averaged variables:

$$E = \frac{\sum_{q=1}^n \alpha_q \rho_q E_q}{\sum_{q=1}^n \alpha_q \rho_q}, \quad (7)$$

where E_q is based on the specific heat of the q^{th} phase and the shared temperature.

Evaporation and condensation at the interface are modeled as a source term in the continuity equation for the volume fraction (Eq. 4), i.e.:

$$S_{\alpha_q} = \dot{\mathbf{m}}_i \cdot \mathbf{A}_i, \quad (8)$$

where $\mathbf{A}_i$ is an interfacial area density vector, and $\dot{\mathbf{m}}_i$ is a mass flux vector, which for near equilibrium conditions can be determined based on the Schrage equation [11]:

$$|\dot{\mathbf{m}}| = \left(\frac{2\sigma}{2 - \sigma} \right) \left(\frac{M}{2\pi R} \right)^{1/2} \left(\frac{P_i}{T_i^{1/2}} - \frac{P_v}{T_v^{1/2}} \right). \quad (9)$$

Here σ is the accommodation coefficient (a value of 0.001 was used for the CFD simulations); M is the molar mass of the fluid; R is the universal gas constant; P_i and P_v are, respectively, the interfacial and vapor pressures (it was assumed that $P_i \cong P_{sat}$); T_i and T_v are, respectively, the interfacial and vapor temperatures (it was assumed that $T_i = T_v \cong T_{sat}$ at the interface). Finally, $\mathbf{A}_i$ is defined as:

$$\mathbf{A}_i = |\nabla \alpha|, \quad (10)$$

where α is the volume fraction of the primary phase.

In the present implementation, the surface tension forces at the interface are modeled via the Continuum Surface Force (CSF) model of Brackbill et al. [12]. In this model, the surface tension forces at the interface are transformed into a volume force ($\mathbf{F}_{vol}$), which is added as a source to the momentum equation:

$$\mathbf{F}_{vol} = \sum_{\text{pairs } ij, i < j} \sigma_{ij} \frac{\alpha_i \rho_i h_i \nabla \alpha_j + \alpha_j \rho_j h_j \nabla \alpha_i}{\frac{1}{2} (\rho_i + \rho_j)}, \quad (11)$$

where h_i is the surface curvature calculated from the local gradients in the surface normal at the interface:

$$h_i = \nabla \cdot \hat{\mathbf{n}}. \quad (12)$$

C. Lagrangian Spray Model

A customized Lagrangian spray model of the ANSYS Fluent CFD code [13] was utilized to simulate the MHTB tank's spray-bar mixing process. This model uses the Eulerian-Lagrangian approach, where the ullage is treated as a continuum by solving the Navier-Stokes equations. The dispersed phase is solved by tracking spray droplets through the calculated flow field. The droplets exchange mass, momentum, and energy with the ullage. In the Lagrangian spray model, the droplet trajectory is calculated by integrating the force balance on the droplet. This force balance equates the droplet inertia with the forces acting on the droplet as:

$$\frac{d\vec{u}_p}{dt} = F_D (\vec{u} - \vec{u}_p) + \frac{\vec{g} (\rho_p - \rho)}{\rho_p} + \vec{F}, \quad (13)$$

where $\vec{u}$ is the fluid phase velocity, $\vec{u}_p$ is the particle velocity, ρ is the fluid density, ρ_p is the density of the droplet, F_D is the drag force per unit droplet mass, and $\vec{F}$ is an additional acceleration. Integration of time in Eq. 13 yields the velocity of the droplet at each point along the droplet trajectory. The spherical drag law proposed by Morsi and Alexander [14] is applied for the droplet drag force calculation. The droplet energy equation is solved in the user subroutine as:

$$m_p c_{p_p} \frac{dT_p}{dt} = h \cdot A_p (T_\infty - T_p) - L \dot{m}_p, \quad (14)$$

where m_p is the droplet mass, c_{p_p} is the heat capacity of the droplet, A_p is the surface area of the droplet, T_∞ is the local temperature of the continuous phase, h is the convective heat transfer coefficient, L is the latent heat, and $\dot{m}_p$ is the rate of evaporation from the droplet obtained from the T-sat model.

The droplet mass transfer is calculated using the developed T-sat model, where the mass transfer rate is calculated from the droplet energy balance (Eq. 14). In the T-sat model, the droplet warms up to the saturation temperature corresponding to the vapor pressure. Once it reaches this temperature, it remains at saturation and uses all the energy supplied by the ullage for evaporation, such that:

$$\begin{aligned} \text{if } T_p < T_{\text{sat}}(P_v) &\Rightarrow \dot{m}_p = 0; T_p \text{ is calculated from Eq. 14,} \\ \text{if } T_p \geq T_{\text{sat}}(P_v) &\Rightarrow T_p = T_{\text{sat}}(P_v); \dot{m}_p \text{ is calculated from Eq. 14.} \end{aligned} \quad (15)$$

In this case, the evaporation rate can be evaluated directly from the droplet energy balance (Eq. 14). The correlation of Ranz and Marshall [15][16] is used to evaluate the droplet heat transfer coefficient:

$$Nu = \frac{hd_p}{k_\infty} = 2.0 + 0.6 Re_d^{1/2} Pr^{1/3}, \quad (16)$$

where d_p is the droplet diameter, k_∞ is the thermal conductivity of the continuous phase, Re_d is the Reynolds number based on the particle diameter and the relative velocity, and Pr is the Prandtl number of the continuous phase.

The relative Reynolds number is calculated as:

$$Re_d \equiv \frac{\rho d_p |\vec{u}_p - \vec{u}|}{\mu}, \quad (17)$$

where μ is the molecular viscosity of the fluid.

After the droplet energy equation is solved in the user subroutine, each droplet's mass, diameter, and temperature are updated. The mass, momentum, and energy transfer between the droplets and the continuous phase are modeled via source terms added to Eq. 1-3.

The Lagrangian Spray model is coupled with the VOF model via a user subroutine, which performs particle tracking in the ullage, removes particles from the ullage when they reach the interface, and then adds their contributions to the liquid mass, momentum, and energy equations through source terms. These source terms are added to those liquid cells near where the spray drops crossed the liquid-vapor interface. Because the VOF method produces a diffuse interface, the criteria for determining when the spray drops have crossed into the bulk liquid is defined as the liquid drop entering a fluid cell with a liquid volume fraction > 0.1 .

III. Numerical Implementation

This study is based on self-pressurization and spray-bar mixing experiments conducted using the MHTB tank under normal gravity conditions [9]. The MHTB tank consists of a cylindrical mid-section measuring 3.05 meters in diameter and height, capped at both ends by 2:1 elliptical end caps.

The formulations for interfacial mass transfer in the VOF scheme, the heat and mass transfer between droplets and ullage, and the coupling between the VOF and Lagrangian Spray models were developed and implemented as a user-defined function (UDF) in ANSYS Fluent version 24.1. The VOF model calculates interfacial mass transfer within a user subroutine, adding source terms to the momentum and relevant scalar equations. This calculation assumes that any mass “created” or “destroyed” possesses the same momentum and energy as the originating phase. This subroutine performs all two-phase calculations and is invoked once per iteration before solving the field equations.

Time-dependent conservation equations for the ullage and liquid regions were solved using a bounded second-order time-stepping scheme. The time step size was 5×10^{-2} seconds for self-pressurization cases and 1×10^{-3} seconds for spray cases. Convective fluxes in the momentum, energy, and turbulence equations were discretized using a second-order upwind scheme. However, for the scale-resolving models (IDDES, SBES, and LES simulations), only the momentum equations were discretized using a bounded central difference method instead. Pressure-velocity coupling was achieved using the Pressure-Implicit with Splitting of Operators (PISO) method.

A compressive discretization scheme was employed for the volume fraction equation, providing a second-order reconstruction based on a slope limiter [13]. In this scheme:

$$\phi_f = \phi_d + \beta \nabla \alpha_d, \quad (18)$$

where ϕ_f is the volume fraction at the cell face, ϕ_d is the volume fraction in the donor cell, β is the slope limiter, and $\nabla \alpha_d$ is the gradient of the volume fraction in the donor cell.

In the Lagrangian spray cases, cold liquid enters the liquid phase as a “tiny jet,” modeled as a source term defined in a user subroutine and added to Fluent's mass, energy, and momentum equations. For the 25% fill ratio case, ten liquid jets are placed within the liquid region, and 33 spray injections are introduced into the vapor region.

The spray-bar holes have a diameter of 1.7×10^{-3} m and a flow-through length of 0.7×10^{-3} m. The spray injection is modeled using a plain orifice atomizer with four-particle streams per injection, introducing liquid droplets at a

flow rate of 3.6×10^{-4} kg/s per injector. These values were obtained from the experimental report [1], except for the average temperature of 21.11 K, which corresponded to the liquid temperature at the end of self-pressurization and was determined based on the CFD simulation setup.

Two-way coupling between the droplets and the continuous phase is enabled. First, the subroutine calculates the mass transfer rate to model heat and mass transfer between the droplets and the ullage. The droplet energy equation is then solved to update the droplet's temperature, mass, and diameter, accounting for any evaporation. Finally, the corresponding mass and energy sources are added to the ullage phase.

The convergence criteria were set to 1×10^{-5} for all equations, except for the energy equation, which had a stricter criterion of 1×10^{-8} .

A. Self-Pressurization

To assess the impact of different turbulence models on modeling self-pressurization, various models were employed, including the laminar model; the Shear Stress Transport (SST) $k-\omega$ model [17]; Large Eddy Simulation (LES); Improved Delayed Detached Eddy Simulation (IDDES) [18, 19]; and Stress-Blended Eddy Simulation (SBES) [20]. Using these different turbulence models allowed for a comparative analysis of their effectiveness in predicting the pressure and temperature evolution within the tank during self-pressurization.

For the self-pressurization study, a two-dimensional axisymmetric model was used for all cases except for LES, which utilized a three-dimensional model representing a one-eighth slice of the entire tank. The gravitational vector was aligned with the tank's central axis in the negative axial direction. A heat flux of 1.8 W/m^2 was applied to the portions of the tank wall where the support legs are connected, while the rest of the tank wall received a uniform heat flux of 0.37 W/m^2 . These heat flux values were based on previous thermal analysis and multinode simulations. Conduction through the tank wall was not considered.

The spray bar assembly was approximated as lying along the tank centerline and was treated as an adiabatic surface. A zero velocity field was used as the initial condition for the self-pressurization simulation, and the initial tank temperature profile was set to match the experimental data. Figures 1 and 2 illustrate the location of the tank support leg connections, and the details of the self-pressurization experiment are presented in Table 1.

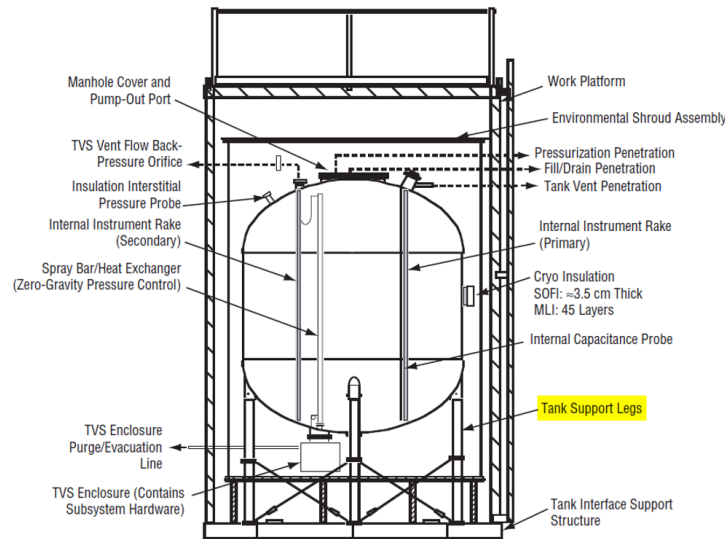


Fig. 1 Schematic overview of the MHTB tank.

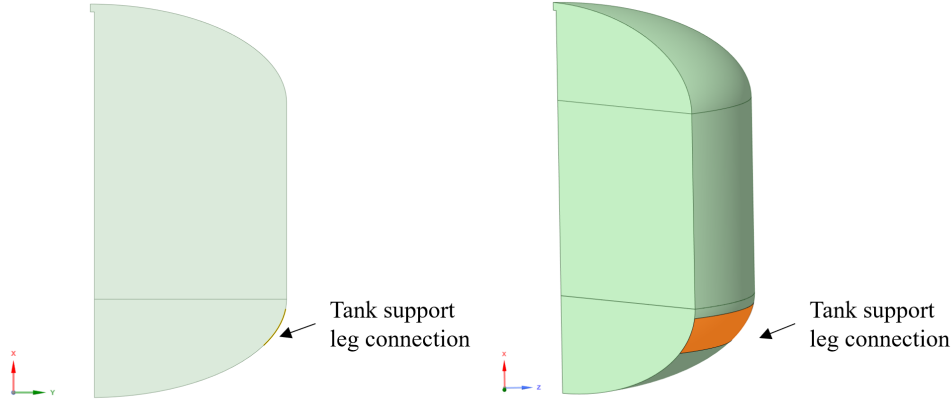


Fig. 2 2D and 3D models highlighting the locations of the tank support leg connections.

Table 1 Experimental conditions for tank self-pressurization test.

Case #	Initial Liquid Fill Level, %	Initial Pressure, kPa	Final Pressure, kPa	Test Duration, hours
1	25	122.1	135.1	18.5

B. Spray-Bar Mixing

The pressure, temperature, velocity, and phase fields at the end of self-pressurization are transformed from 2D to 3D and used as initial conditions for the spray-bar mixing case. The transformation is done by creating an interpolation file at the end of self-pressurization and using an in-house Python script to revolve the data in azimuthal slices around the central axis. A new 3D interpolation file is then created that can be read in Fluent.

The 3D spray-bar mixing case simulates a 90° sector of the full tank, utilizing two symmetry planes to represent the entire geometry. Ten submerged spray-bar holes are modeled as point sources within the liquid region, while 33 spray injections in the vapor region are represented using the discrete phase model (DPM). Each spray injection has a uniform temperature of 21.11 K and a liquid flow rate of 3.6×10^{-4} kg/s, resulting in a total spray-bar flow rate of 0.012 kg/s. This temperature represents the average liquid temperature at the end of self-pressurization. The spray injection type is a plain orifice atomizer with four-particle streams per injection. Table 2 details the spray-bar mixing experiment.

Table 2 Experimental conditions for spray-bar mixing test.

Case #	Initial Liquid Fill, %	Initial Pressure, kPa	Final Pressure, kPa	Test Duration, s
1	25	135.0	131.0	35

C. Computational Mesh

For the self-pressurization model, an initial computational mesh was generated with an average cell size of 20 mm, resulting in 15,690 cells. As shown in Figure 3, this mesh was refined near the walls and the liquid-vapor interface. The same meshing parameters were applied to the LES self-pressurization case; however, in the three-dimensional LES simulation, polyhedral cells were used instead. Additionally, the LES model represented a one-eighth sector of the entire tank, utilizing symmetry planes.

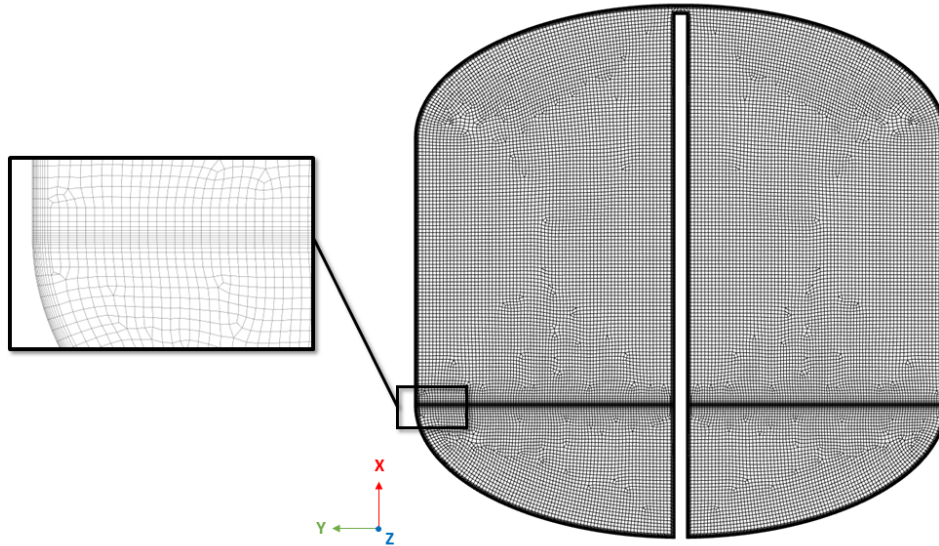


Fig. 3 Computational mesh for the 25% fill ratio self-pressurization case (15,690 cells).

The computational mesh used for the spray-bar mixing simulation is shown in Figure 4a. This model uses polyhedral cells with an average size of 20 mm, totaling 988,693 cells. Mesh refinement is applied near the tank walls, the spray-bar wall, and the interfacial area. Figure 4b shows a schematic of the tank's spray bar injectors and pump locations.

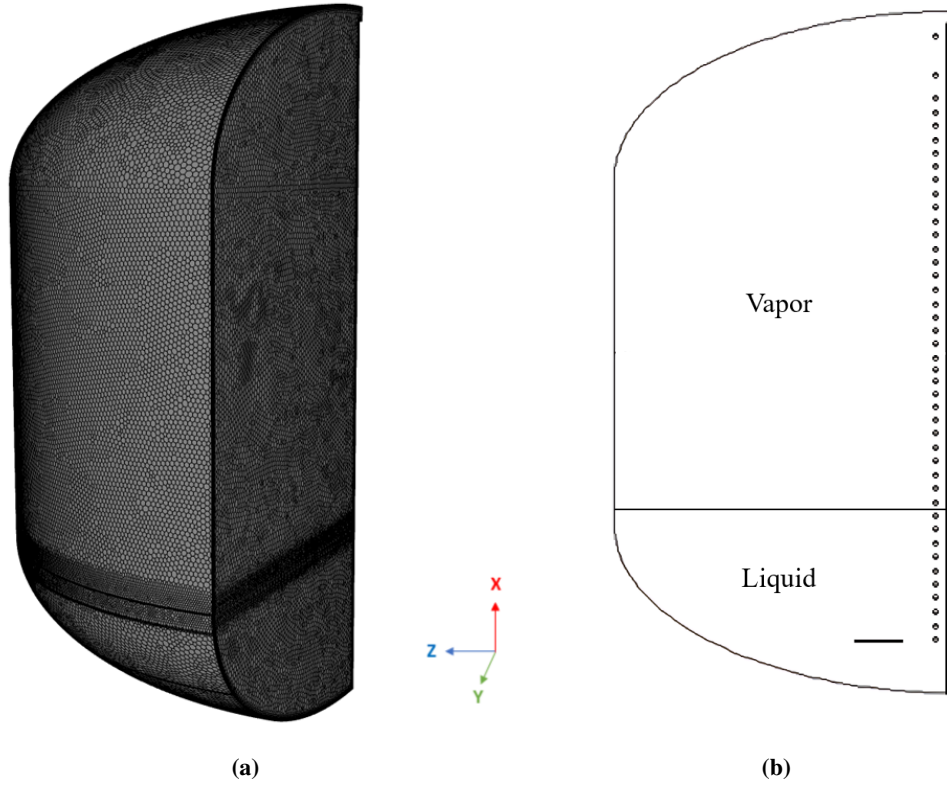


Fig. 4 (a) Computational mesh for the 25% fill ratio spray-bar mixing case (988,693 cells) and (b) schematic of spray bar injectors and pump locations at the tanks center plane.

IV. Results & Discussion

A. Self-Pressurization

Simulations were conducted to model the self-pressurization of the MHTB tank using various flow models. These included a laminar flow model and several turbulence models: the SST $k-\omega$ model, IDDES, SBES, and LES.

Figure 5 shows the evolution of tank pressure during self-pressurization, comparing the experimental data with the calculated CFD results. All models captured the general trend of increasing pressure due to self-pressurization; however, notable differences are evident in the rate and magnitude of the pressure rise. Among the models, the SBES model aligns most closely with the experimental pressure rise. The laminar, IDDES, and SST $k-\omega$ models all underpredict the pressure increase but with varying degrees of accuracy. Notably, the laminar solution is within approximately 1.5% of the experimental result at the end of self-pressurization, while the IDDES solution is within 2% and the SST $k-\omega$ solution within 8%. The LES simulation was not yet complete at the time of this writing; however, preliminary results indicate that it is tracking similarly to the IDDES solution.

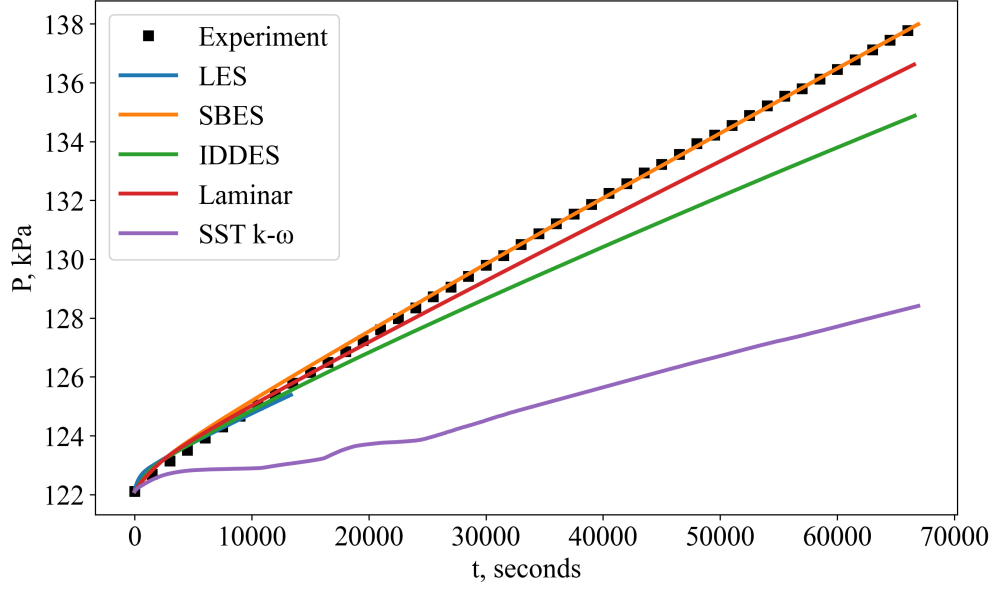


Fig. 5 Tank pressure evolutions during self-pressurization of 25% fill ratio MHTB Tank.

A mesh dependence study was conducted to determine the numerical accuracy of the simulations. Three different meshes were tested:

- A **coarse mesh** with an average cell size of 30 mm, consisting of 8,857 cells.
- The **original mesh** with an average cell size of 20 mm, consisting of 15,977 cells.
- A **finer mesh** with an average cell size of 10 mm, consisting of 50,942 cells.

Figure 6 shows the pressure evolution in the tank for each mesh configuration simulated with an IDDES turbulence model. The results indicated that the pressure evolution curves for all three meshes were nearly identical, with less than 0.3% difference in key pressure values throughout the simulation. This negligible difference suggests that refining the mesh further does not significantly improve the accuracy but does increase computational cost. Therefore, the original mesh with a 20 mm cell size was selected for its balance of accuracy and computational efficiency in the subsequent simulations.

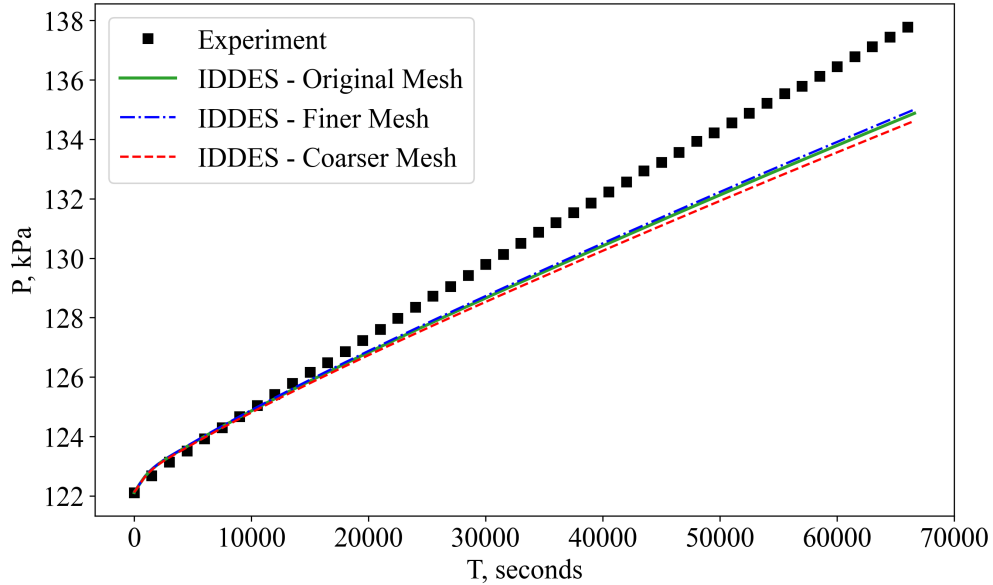
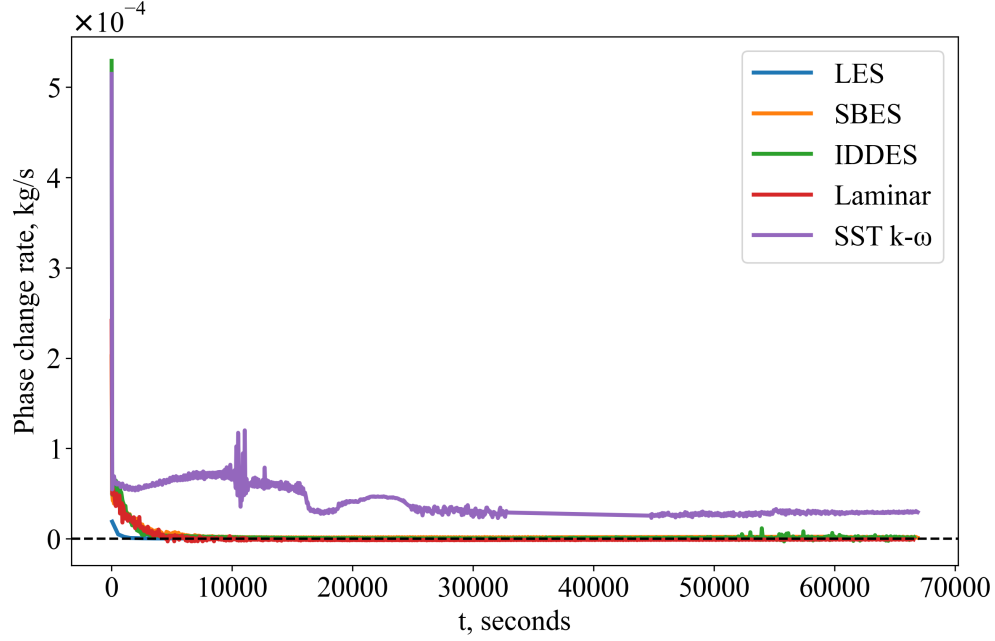
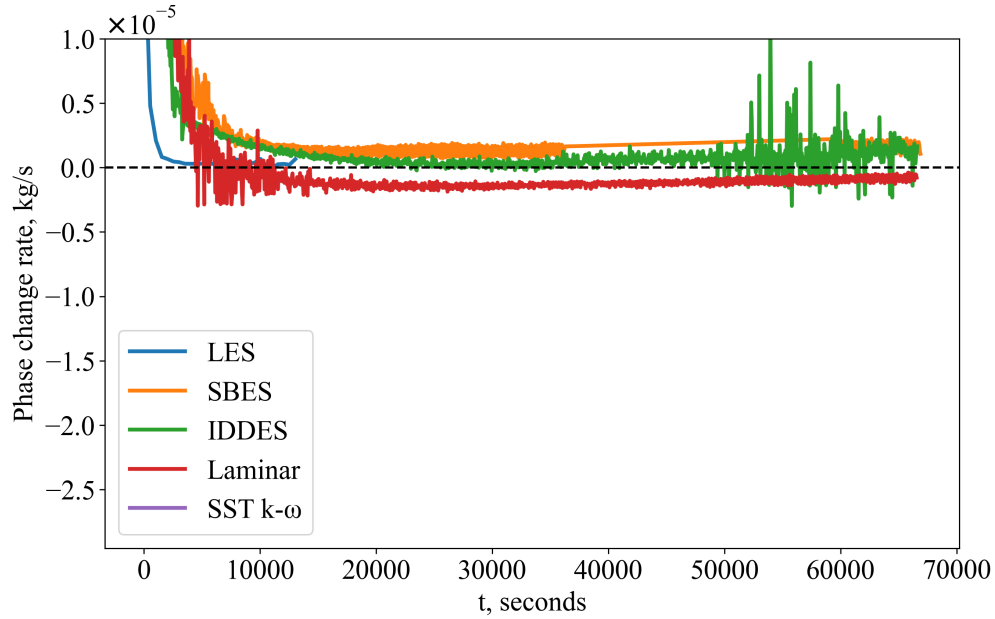


Fig. 6 Tank pressure evolutions for original, finer, and coarse meshes.

Figure 7 shows the interfacial mass transfer rate results, revealing the phase change dynamics during self-pressurization. Although experimental data for interfacial mass transfer rates is not available for direct comparison, the model's phase change rates align with the expected thermodynamic behavior under rising tank temperatures and pressures. All models initially predicted significant evaporation at the interface, driven by the tank's natural convection and the vapor temperature increase. This rate gradually decreased as the tank temperature and pressure stabilized from initial conditions, stabilizing the interfacial mass transfer.



(a)



(b)

Fig. 7 (a) Interfacial mass transfer rates during self-pressurization of a 25% fill ratio MHTB Tank. (b) Zoomed-in.

The laminar model predicts condensation at the interface through most of the self-pressurization. This outcome is likely due to the lack of turbulent mixing in the laminar model, which affects how temperature and pressure gradients develop between the liquid and vapor phases. Specifically, without turbulence to moderate the rate of pressure increase in the vapor, the vapor pressure can rise rapidly and may exceed the local saturation pressure near the interface. This imbalance between vapor pressure and interfacial temperature favors condensation rather than evaporation, even if vapor temperatures remain relatively high.

In the experiment, temperature diodes were placed along two vertical arrays, Rake 1 and Rake 2, to capture the temperature evolution within the tank. Rake 1 was positioned 0.74 m from the tank's vertical centerline, while Rake 2 was positioned 0.66 m from the centerline. Rake 1 contained temperature diodes TD-1 through TD-12, and Rake 2 contained TD-13 through TD-24. Figure 8 shows the placement of these diodes in the MHTB tank. CFD temperatures were recorded at the same positions as in the experiment. Figures 9-14 present the temperature evolution plots for selected diodes during self-pressurization, displayed as both absolute temperature and as a temperature difference ($\Delta T = T - T_0$), where T_0 is the initial temperature. The ΔT plot emphasizes changes in temperature over time and highlights differences between CFD results and experimental data. Figure 15 shows the temperature distribution along Rake 1, comparing CFD results with experimental data at the end of self-pressurization.

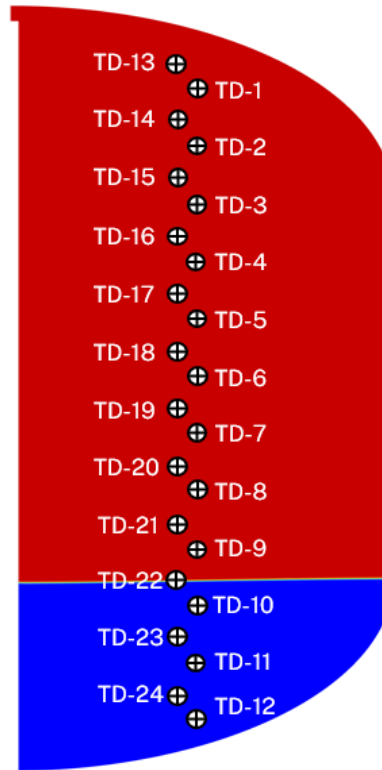
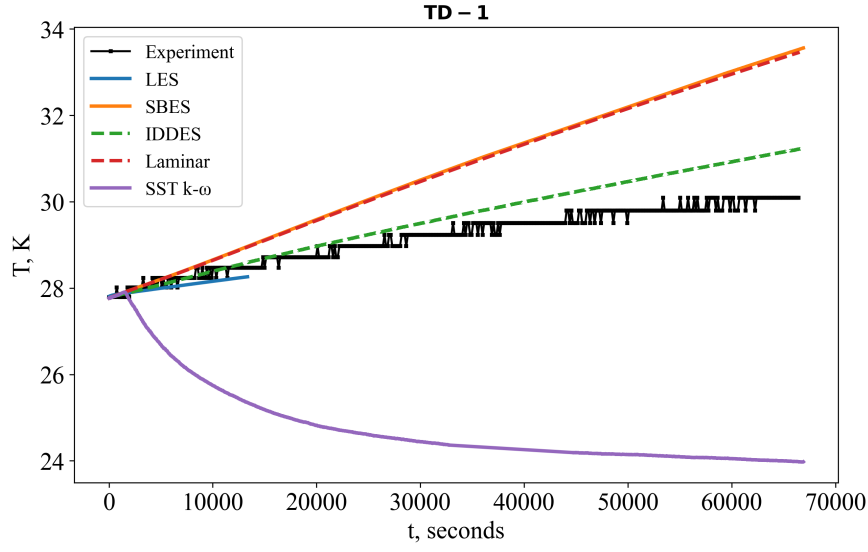
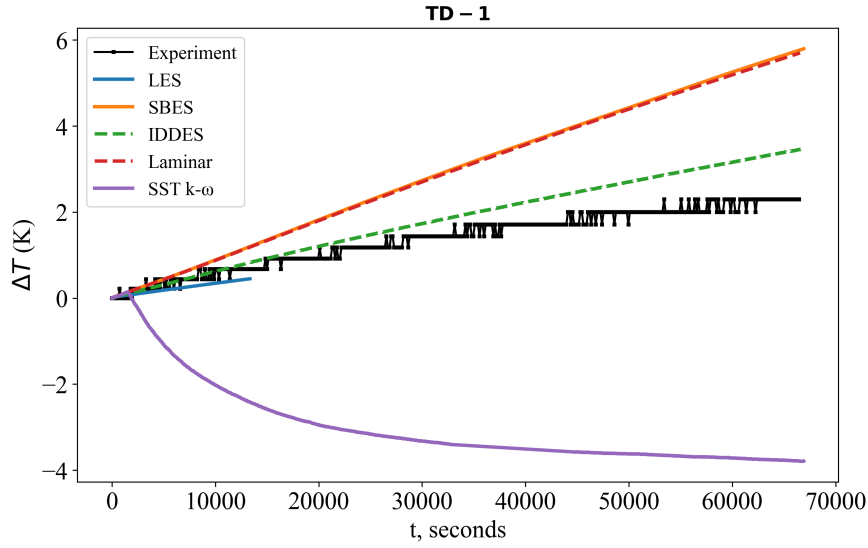


Fig. 8 Temperature diode placement in the MHTB tank showing the liquid region in blue and the vapor region in red.



(a)



(b)

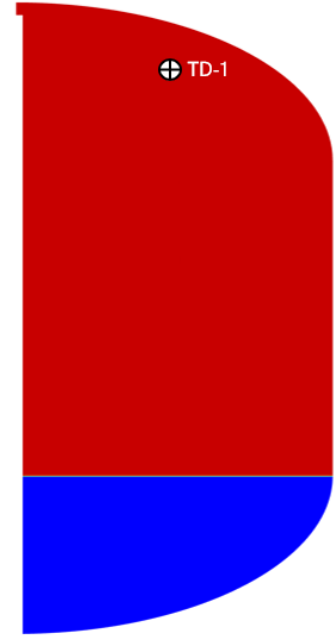
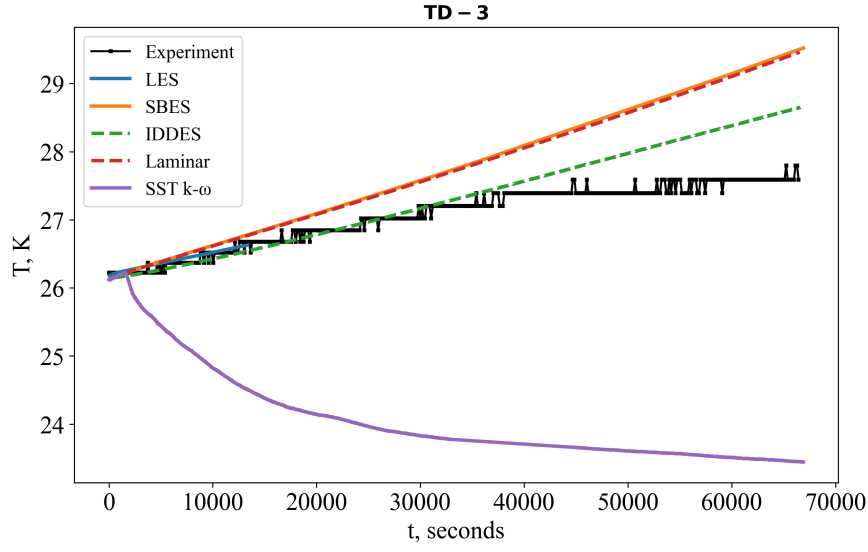
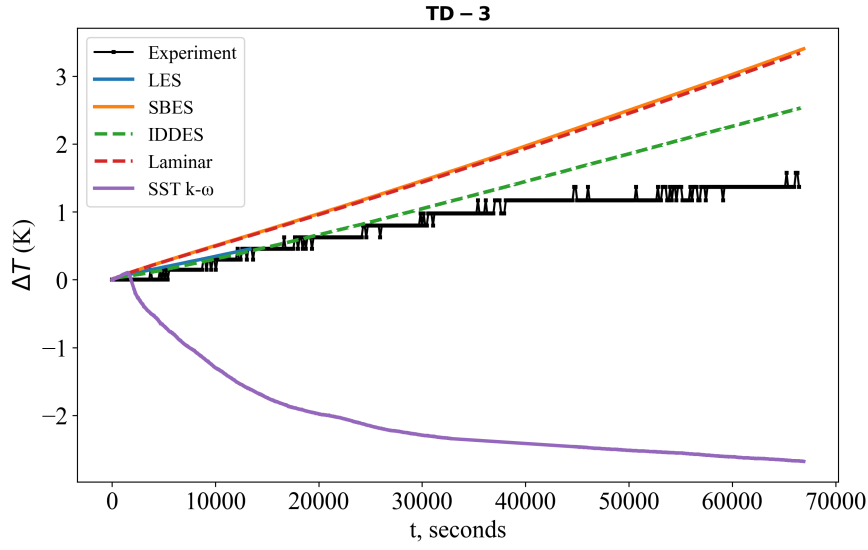


Fig. 9 (a) Temperature evolutions at TD-1 during self-pressurization, showing both the temperature and (b) the normalized temperature change (ΔT).



(a)



(b)

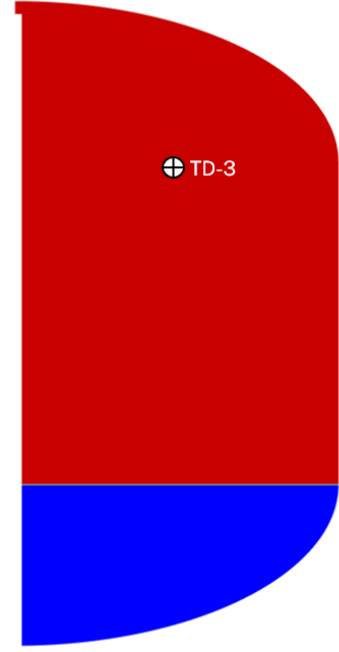
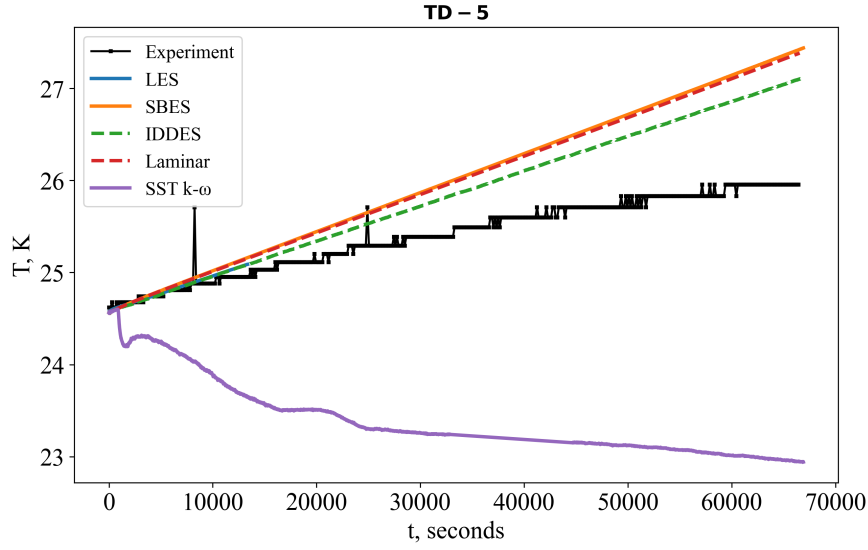
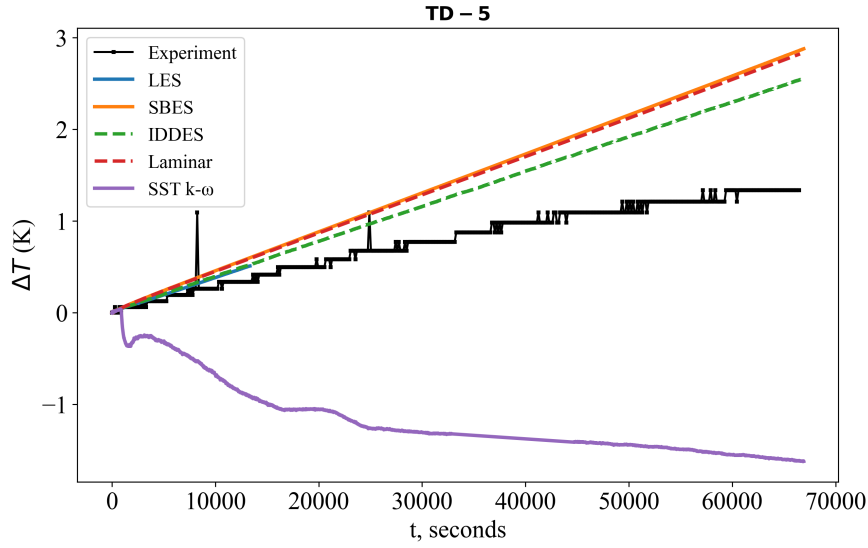


Fig. 10 (a) Temperature evolutions at TD-3 during self-pressurization, showing both the temperature and (b) the normalized temperature change (ΔT).



(a)



(b)

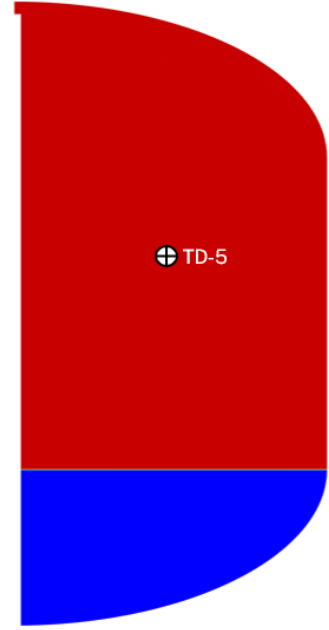
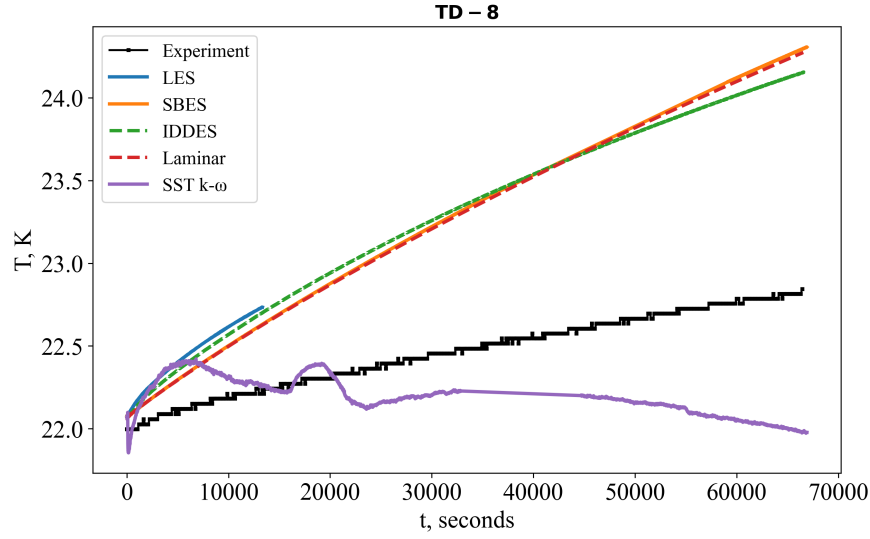
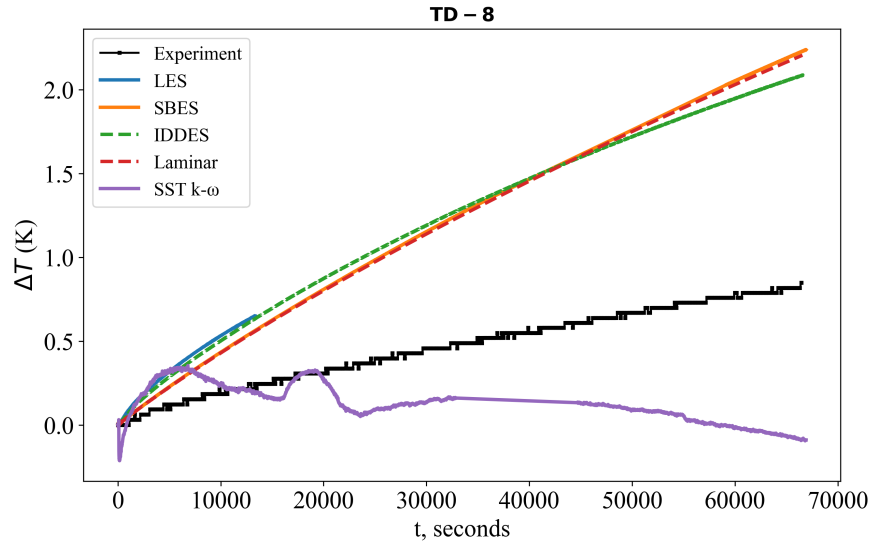


Fig. 11 (a) Temperature evolutions at TD-5 during self-pressurization, showing both the temperature and (b) the normalized temperature change (ΔT).



(a)



(b)

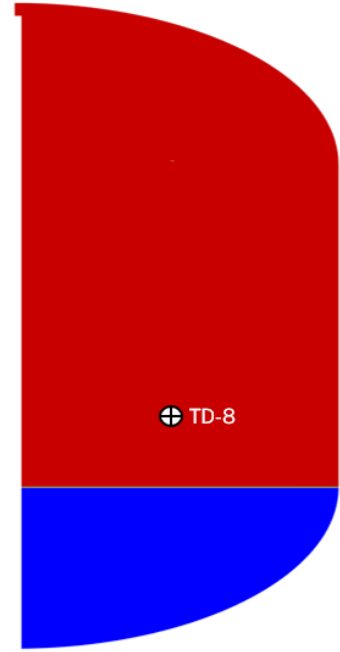


Fig. 12 (a) Temperature evolutions at TD-8 during self-pressurization, showing both the temperature and (b) the normalized temperature change (ΔT).

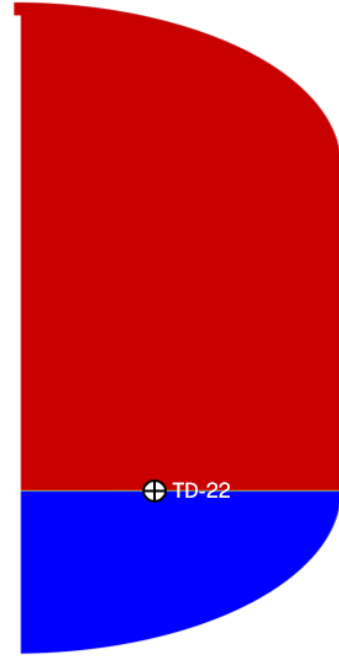
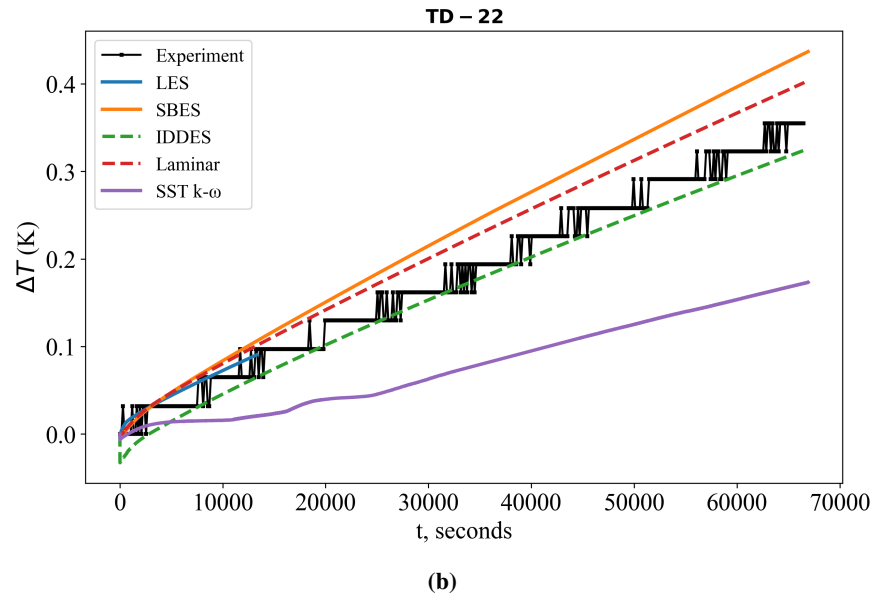
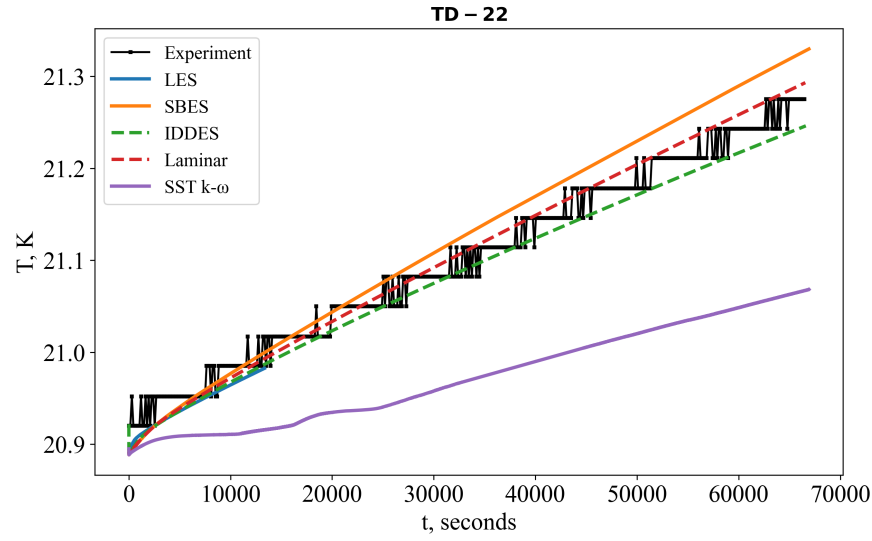


Fig. 13 (a) Temperature evolutions at TD-22 during self-pressurization, showing both the temperature and (b) the normalized temperature change (ΔT).

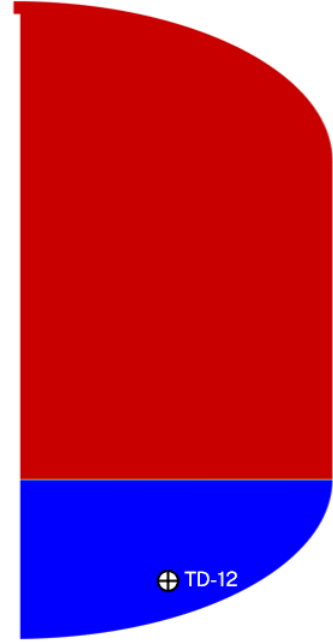
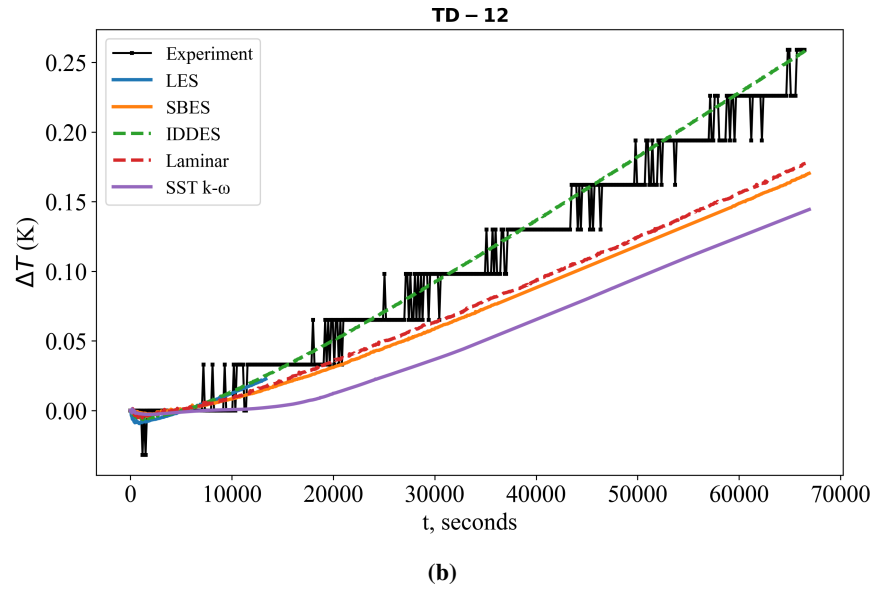
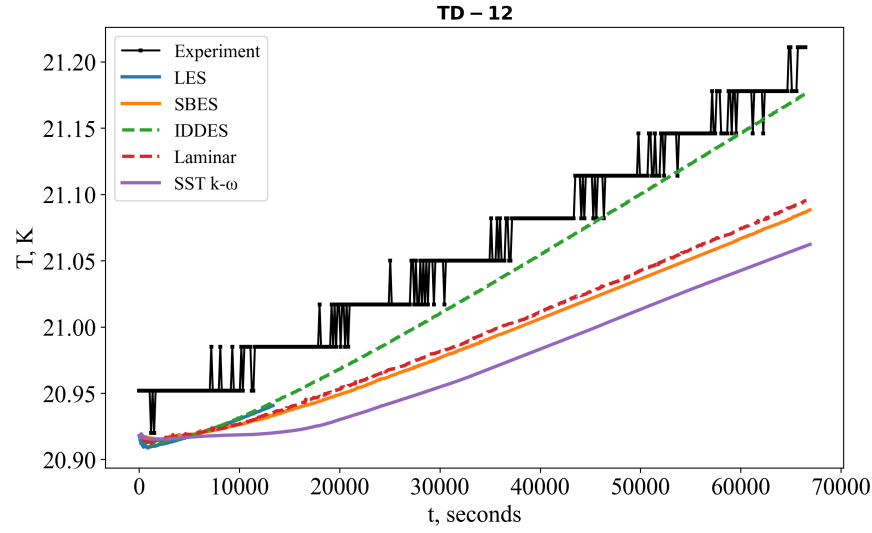


Fig. 14 (a) Temperature evolutions at TD-12 during self-pressurization, showing both the temperature and (b) the normalized temperature change (ΔT).

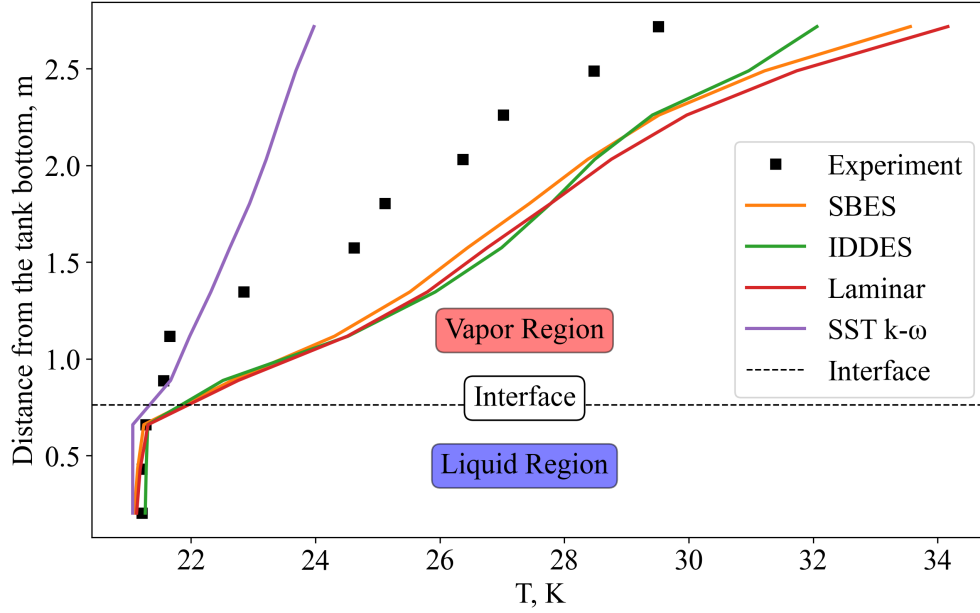


Fig. 15 Temperatures along Rake 1 at the end of self-pressurization.

When comparing tank temperature measurements, the IDDES solution closely matched experimental values, predicting temperatures within 3° , K of the experimental data in the upper ullage. Additionally, it provided accurate predictions at the interface and in the liquid region, with predicted temperatures nearly identical to the experimental data in those respective regions. However, the SBES and laminar solutions overpredicted temperatures by up to 6° , K in the upper ullage but showed progressively closer alignment with experimental values near the interface and the liquid region. The SST $k-\omega$ model showed the poorest performance in predicting tank temperatures, indicating decreased temperature in the vapor region during self-pressurization. This decrease does not occur in reality, as the experimental data show.

In two-phase flows such as this, the VOF method combined with the SST $k-\omega$ turbulence model requires careful treatment of turbulence near the vapor-liquid interface to ensure realistic flow behavior. Reynolds-Averaged Navier-Stokes (RANS) two-equation models typically predict large turbulent kinetic energy (TKE) production at the interface, increasing the turbulent viscosity levels. This excessive turbulence generation at the interface is problematic because it can lead to nonphysical mixing and numerical diffusion between the liquid and vapor phases. For the SST $k-\omega$ model, a correction is available to adjust the specific dissipation rate (ω) based on the gradient of the volume fraction, increasing the dissipation term in the TKE equation to mitigate this effect. This correction corresponds to the turbulence-damping option in Ansys Fluent [13].

The SST $k-\omega$ simulation was initially conducted with a damping factor of 100. Additional simulations assessed the impact of varying this factor, with damping values ranging from 0 to 1×10^6 . However, these adjustments did not improve the results; increasing the damping factor still led to an underprediction of the pressure rise and a decrease in ullage temperatures. Figure 16 illustrates this underprediction in pressure rise. Although a higher damping factor delays the onset of the reduced rate of pressure rise, the reduction ultimately occurs. Similarly, Figure 17 shows the effect of varying damping factors on a temperature diode in the upper ullage (TD-1). All simulation curves show a decrease in temperature, which does not occur in reality.

The damping factor is squared in the dissipation term, meaning that increasing the damping factor to 10^6 results in a dissipation term 10^{12} times greater, making the damping effect significantly stronger. Relative to a damping factor of 100, the dissipation effect is thus 10^8 larger, which can excessively suppress turbulent fluctuations near the interface. Additionally, this increased damping effect can propagate outside the interface cells due to the nature of the specific dissipation equation in the $k-\omega$ model. This propagation still results in an underprediction of the pressure rise and a decrease in temperature in the ullage, as turbulence-driven effects are overly damped and not adequately represented in regions beyond the interface.

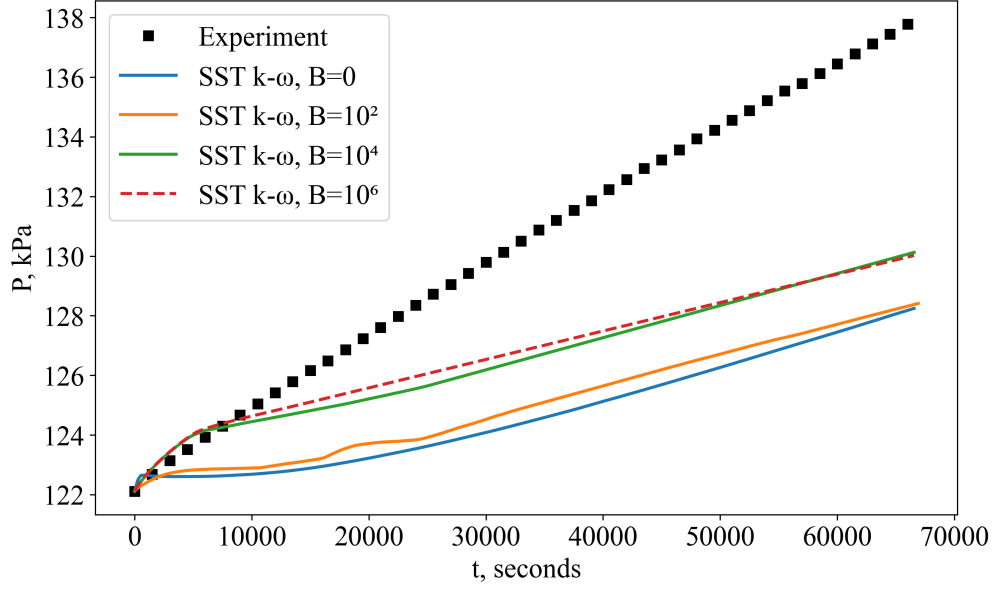


Fig. 16 Tank pressure evolution for different turbulence damping factors.

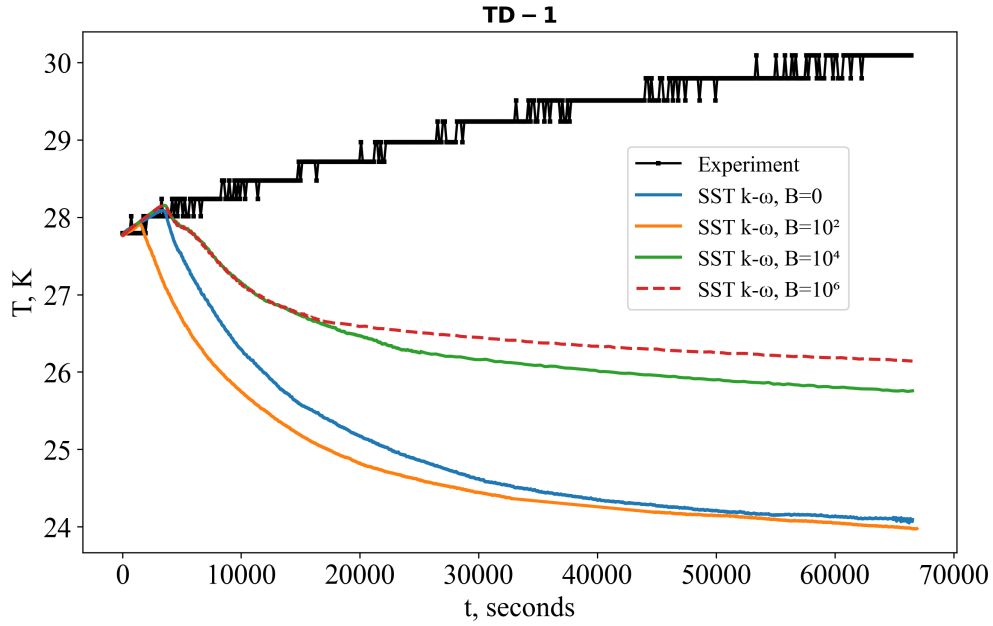


Fig. 17 Temperature evolution at TD-1 for different turbulence damping factors.

The effective turbulent conductivity, k_t , is used to assess the magnitude of turbulence and its influence on thermal energy transfer. It is defined as

$$k_t = \frac{c_p u_t}{Pr_t}, \quad (19)$$

where c_p is the specific heat, u_t is the turbulent viscosity, and Pr_t is the turbulent Prandtl number. By default, the turbulent Prandtl number in Fluent is set to 0.85 [13]. Figure 18 illustrates the effective turbulent conductivity contours at $T = 10,000$ seconds into self-pressurization for turbulence damping factors of $B = 0$, $B = 10^2$, $B = 10^4$, and $B = 10^6$. Notably, in Figure 18a, where $B = 0$, there is an elevated magnitude of turbulent conductivity above the interface.

This elevated turbulent conductivity enhances thermal mixing and heat transfer between the vapor and liquid phases, leading to a more uniform temperature distribution in the ullage. Increasing the damping factor effectively reduces the turbulent conductivity above the interface, as seen in Figures 18b through 18d. This reduction in turbulence limits heat transfer across the interface and limits thermal mixing in the ullage, which can be more representative of the physical behavior during self-pressurization. Additionally, increasing the damping factor reduces the magnitude of turbulent conductivity in the liquid region. This implies that turbulence-induced thermal transport within the liquid is also diminished. The effective turbulent conductivity values are significantly higher than the molecular thermal conductivity of liquid hydrogen, which is approximately $0.1 \text{ W}/(\text{m} \cdot \text{K})$. The SST $k-\omega$ model predicts enhanced thermal energy transfer due to turbulence. The elevated thermal conductivity leads to increased heat transfer across the interface, contributing to the underprediction of pressure rise and the decrease in ullage temperatures observed in the simulations. Overall, the damping factor in the SST $k-\omega$ model directly impacts the turbulence intensity in both the ullage and liquid regions and, thus, controls the extent of thermal mixing and energy transfer in the tank.

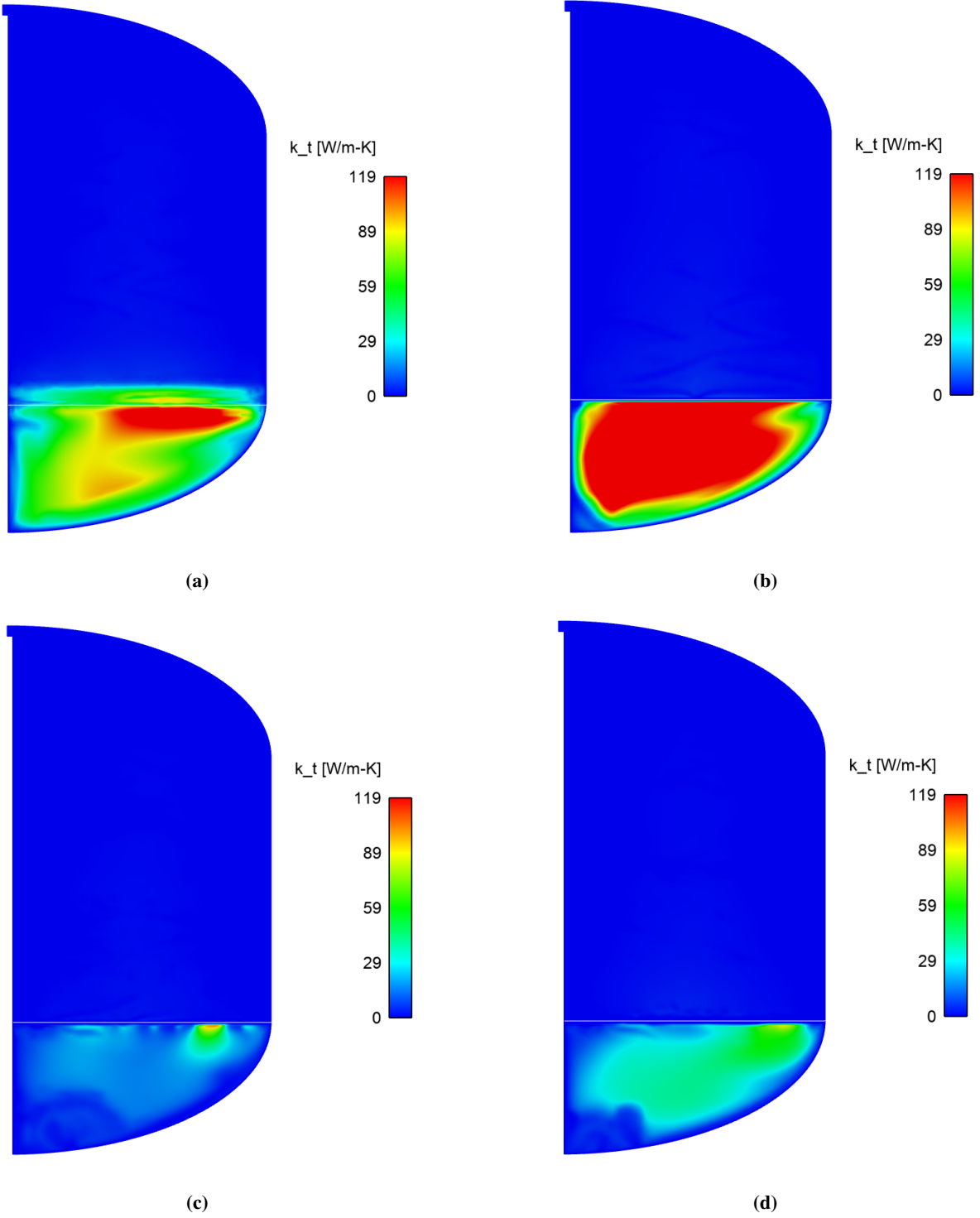


Fig. 18 Contours of effective thermal conductivity at $T = 10,000$ seconds during self-pressurization for damping factors: (a) $B = 0$, (b) $B = 10^2$, (c) $B = 10^4$, and (d) $B = 10^6$.

The laminar, SBES, and IDDES models do not suffer from artificial turbulence-damping effects. The SBES and IDDES models are hybrid turbulence modeling approaches using RANS and LES techniques. They aim to resolve large-scale turbulent structures while modeling smaller scales, offering a balance between accuracy and computational

efficiency. The SBES and IDDES models do not require a turbulence damping factor at the interface because they dynamically adjust the level of turbulence resolution based on the local flow characteristics. This adaptive approach allows them to naturally reduce TKE in near-interface regions without artificial damping. On the other hand, the laminar model assumes streamlined flow and does not introduce turbulence effects. Even though the natural convection inside the tank is in the turbulent regime (liquid $Ra = 6 \times 10^{14}$; vapor $Ra = 1.8 \times 10^{13}$), the laminar model does an adequate job of predicting the pressure and temperature evolutions inside the tank.

The LES simulation is computationally expensive because it attempts to resolve larger turbulent scales fully but offers higher numerical accuracy. Although the LES simulation is incomplete, some preliminary observations can be made. The LES results closely follow the IDDES solution curves in the pressure and temperature plots, but the LES model appears to outperform all other models in temperature prediction. This is particularly evident in Figure 9, where the slope of TD-1 aligns exceptionally well with the experimental data.

Overall, the IDDES model provided the most accurate predictions of pressure and temperature in the tank during self-pressurization, effectively balancing computational accuracy and efficiency. Its hybrid turbulence modeling approach allows it to capture large-scale turbulent structures and important small-scale effects without the excessive computational cost associated with LES. Unlike the SST $k-\omega$ model, which suffered from nonphysical turbulence generation at the interface, the IDDES model naturally adjusted turbulence levels without artificial damping.

B. Spray-Bar Mixing

To model the spray-bar mixing process, the laminar solution at the end of self-pressurization was revolved around the tank's central axis into 100 azimuthal slices, creating a 3D 90° sector. This solution was then interpolated onto a 3D 90° sector mesh, as described in Section III.B. The T-sat model, detailed in Section II.C, was used to simulate the first spray cycle following self-pressurization. In this cycle, the liquid bypasses the Joule-Thomson device, so the liquid temperature exiting the spray bar is assumed to match the average temperature of the liquid entering the pump near the bottom of the tank. For this setup, the spray-bar exit temperature is 21.11 K. It should be noted that turbulence models were not tested for the spray process in this study, as this work is still ongoing and was not completed by the time of this publication.

Figure 19 shows the tank pressure evolution during the spray process, demonstrating strong agreement between the CFD simulation and experimental data. The CFD model accurately predicted the final pressure, closely matching the experimental result. Additionally, the model effectively captures the transient behavior of the pressure drop, accurately reflecting the rate of pressure decrease during the first spray cycle. This suggests that the model reliably predicts the magnitude of the pressure change and the system's dynamic response.

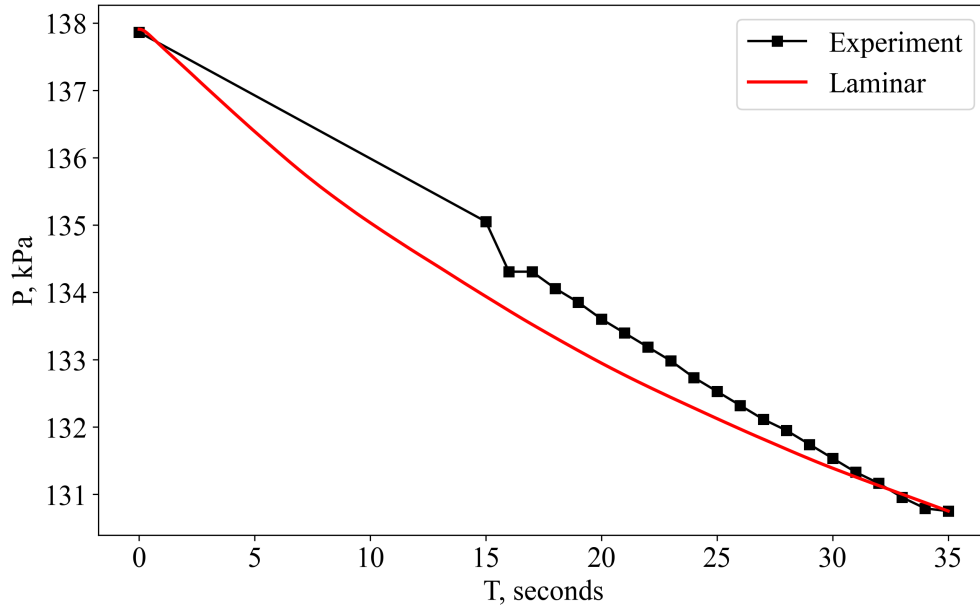


Fig. 19 Tank pressure evolution during spray cooling of 25% fill ratio MHTB Tank.

Since the CFD temperatures in the vapor region at the end of self-pressurization over-predicted experimental temperatures (Figure 15), normalized temperature change plots (ΔT) are presented in Figures 20-22 where both the experiment and CFD temperatures were normalized against their respective initial temperatures ($\Delta T = T - T_0$). This highlights temperature behavior between the CFD and experimental results. Figures 20-22 show that the temperature decrease in the ullage closely matches the experimental data, including a similar slope, indicating a consistent cooling rate. Meanwhile, the liquid temperature at TD-11 remains constant in the experiment and CFD predictions, reflecting that the spray primarily affects the vapor phase.

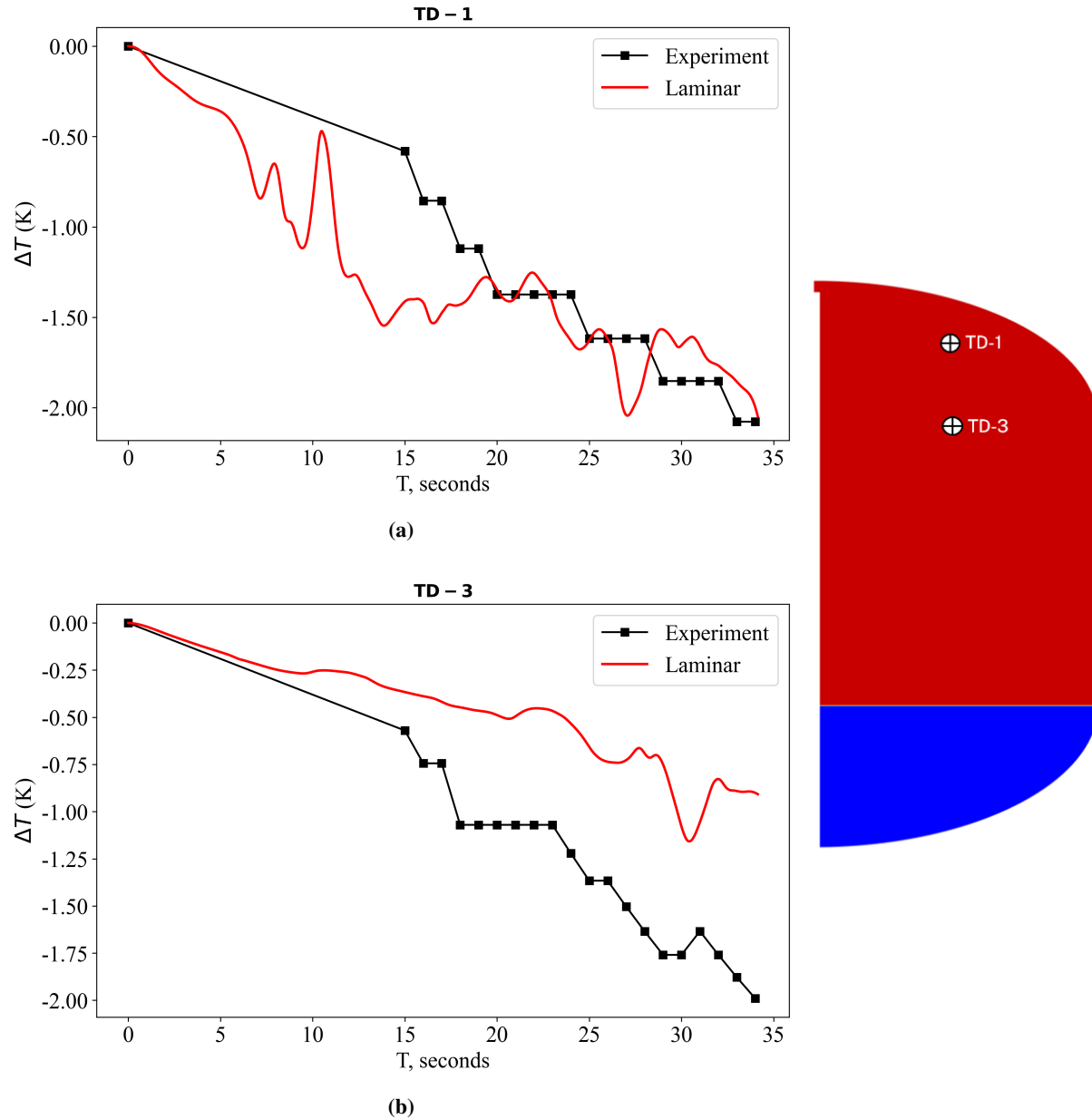


Fig. 20 Normalized temperature evolutions at (ΔT) (a) TD-1 and (b) TD-3 during the spray process.

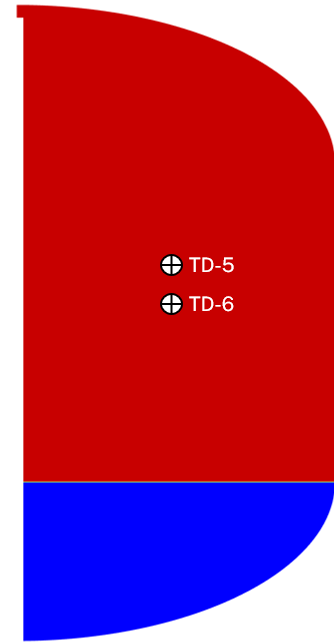
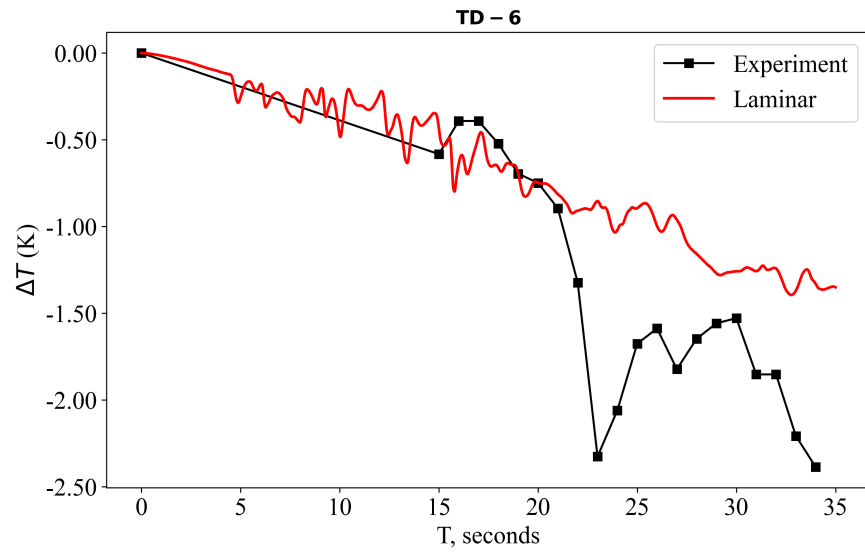
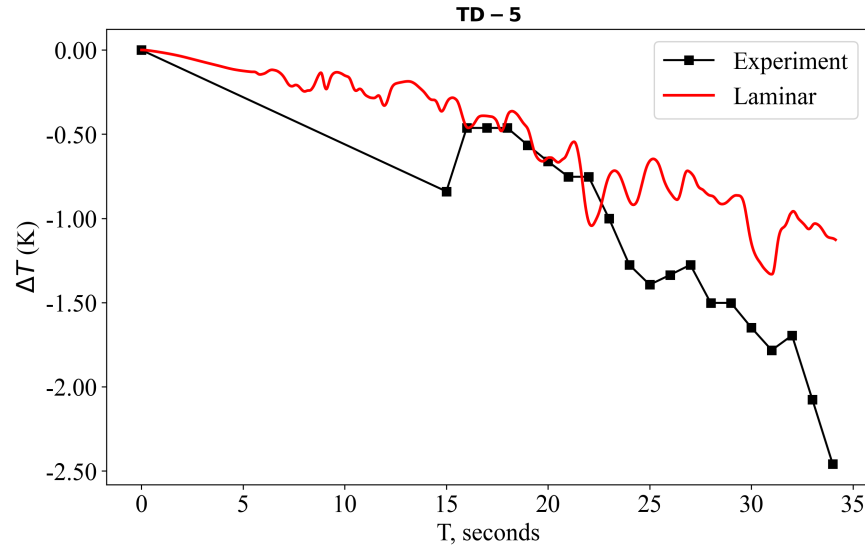


Fig. 21 Normalized temperature evolutions (ΔT) at (a) TD-5 and (b) TD-6 during the spray process.

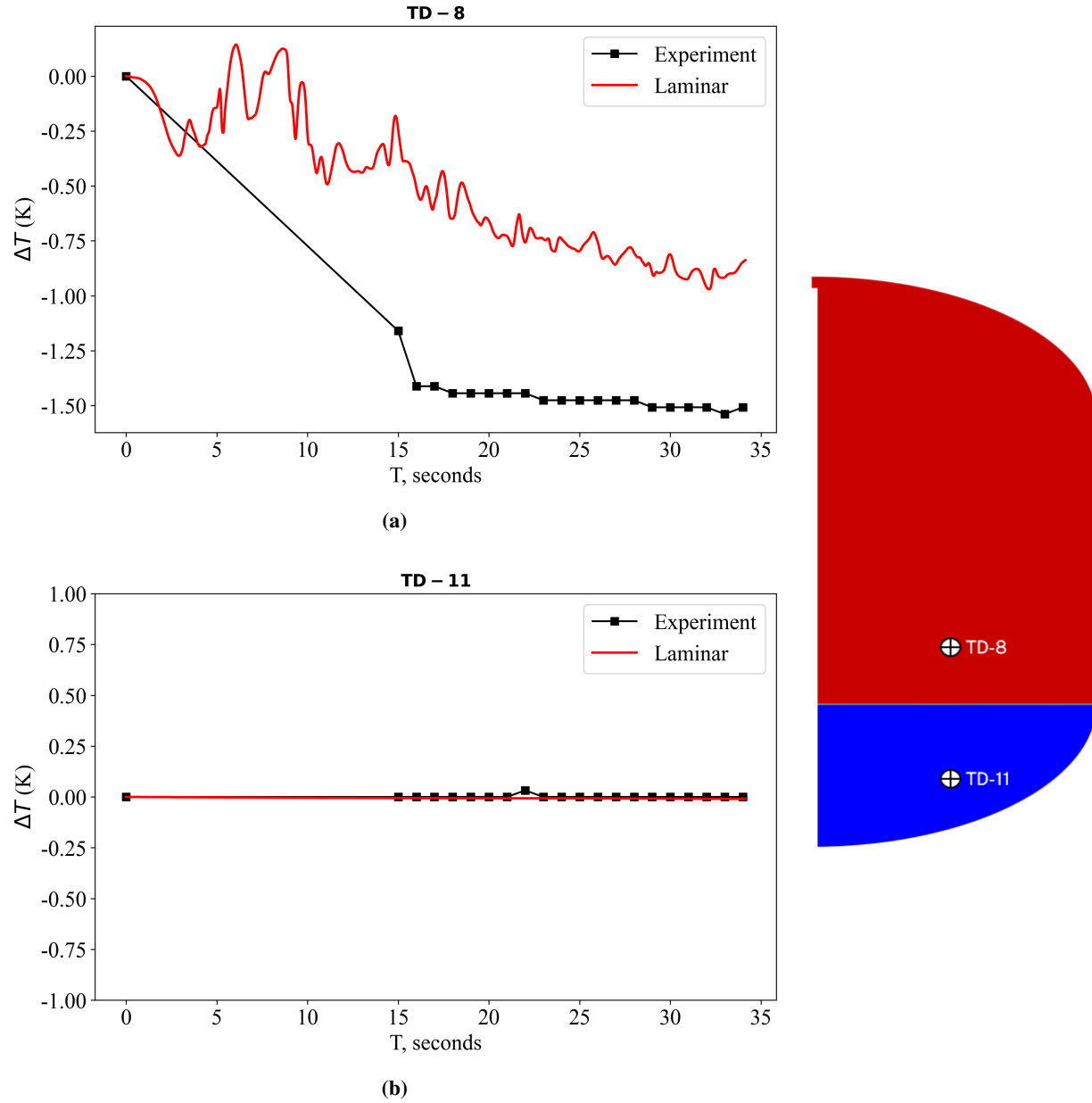


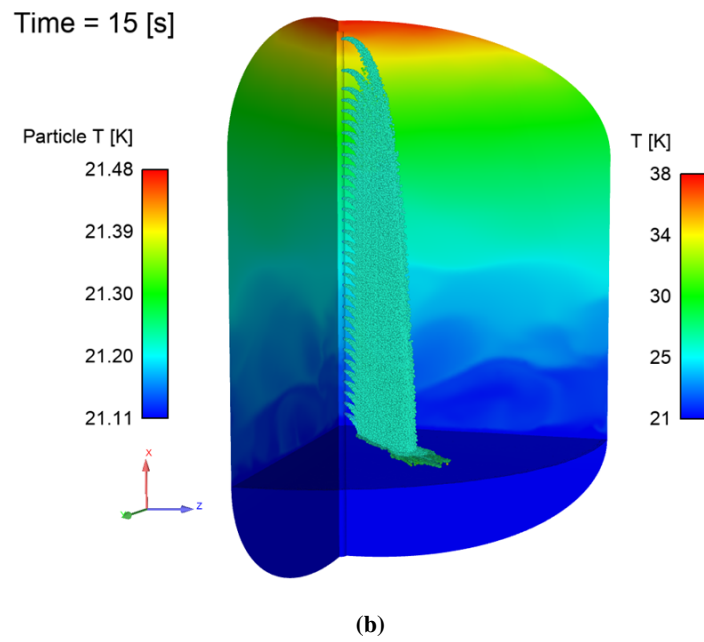
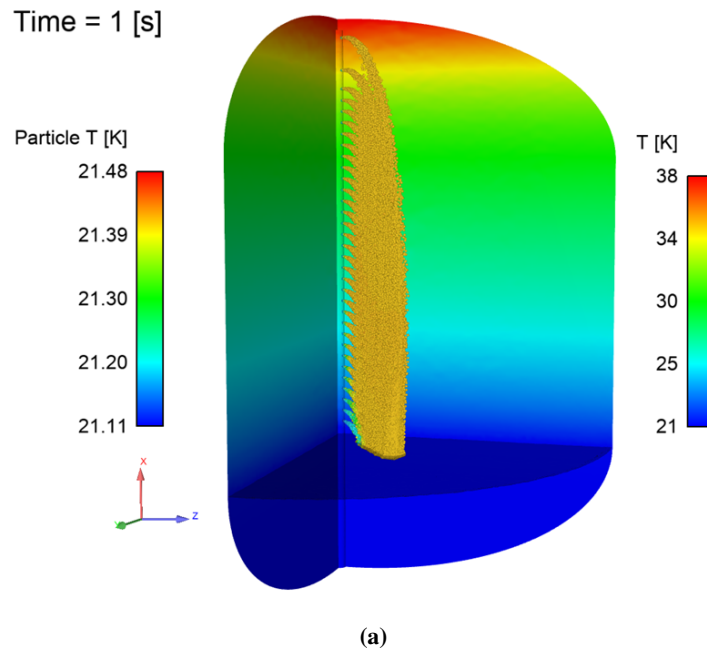
Fig. 22 Normalized temperature evolutions (ΔT) at (a) TD-8 and (b) TD-11 during the spray process.

The CFD results exhibit more pronounced vapor temperature oscillations than the experimental measurements. These oscillations may be attributed to numerical sensitivities, the model's responsiveness to transient fluctuations in the vapor phase, or the higher frequency of data collection in the CFD simulations relative to the experiments. However, these oscillations do not significantly affect the model's accuracy, as the overall trends and magnitudes of the pressure and temperature changes remain consistent with the experimental observations.

The T-sat model plays a crucial role in achieving this accuracy. By assuming that liquid droplets warm to the saturation temperature corresponding to the tank pressure before evaporating, the model ensures that all heat transferred between the vapor and droplets are utilized in the evaporation process as latent heat. This modeling approach accurately represents the spray cycle's energy exchange and phase change processes. The successful prediction of pressure and temperature drops validates the T-sat model's assumptions and demonstrates its capability to model the spray-bar mixing process effectively.

Figure 23 provides a visual representation of the T-sat model by illustrating the temperature contours of the vapor

and liquid regions, as well as the temperature contours of the droplets, at 1, 15, and 35 seconds into the spray cycle. In this figure, the legend labeled "Particle T" corresponds to the temperatures of the droplets, while the legend labeled "T" represents the temperatures of the vapor and liquid phases. The vapor-liquid interface is depicted as a semi-transparent black surface.



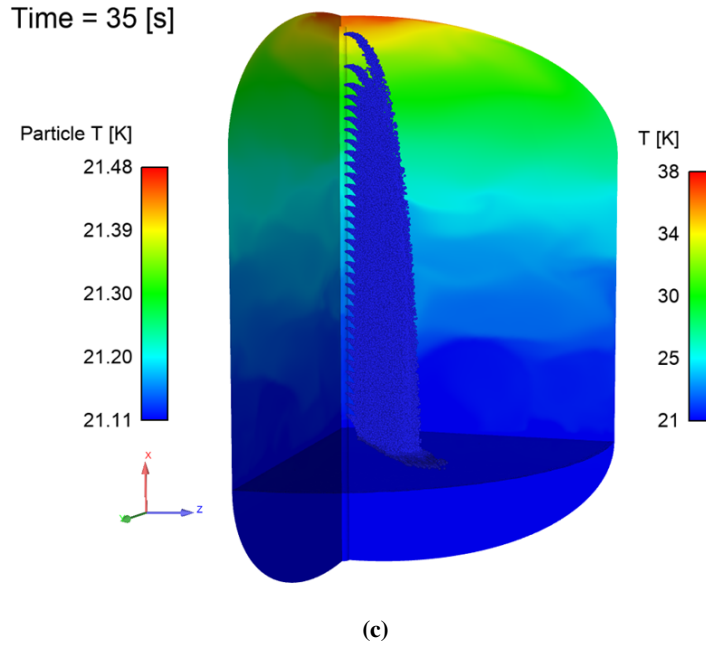


Fig. 23 Temperature contours during the spray process at different times: (a) 1 second, (b) 15 seconds, and (c) 35 seconds.

At 1 second into the spray cycle, the vapor phase remains stratified due to the conditions established at the end of self-pressurization, and the liquid droplets are warming up toward their saturation temperature. This indicates that the droplets are absorbing heat from the surrounding vapor, initiating the cooling process. By 15 seconds, the vapor phase has undergone mixing caused by convection and the droplets disrupting the stratification. The droplets continue to approach their saturation temperature; however, due to the cooling effect of the spray, the pressure in the tank has decreased, leading to a lower saturation temperature for the droplets. At 35 seconds, the overall temperature of the vapor phase has decreased further, and the droplets' temperatures are now close to the liquid temperature in the tank. This suggests that the spray cooling has effectively reduced the vapor temperature and pressure, bringing the system closer to thermal equilibrium.

Although there is no experimental data for direct comparison of mass transfer rates, the CFD model provided valuable insights into the evaporation and condensation processes at the liquid-vapor interface. Figure 24 presents the interfacial mass transfer rate throughout the spray cycle. Initially, introducing cold spray droplets leads to rapid vapor phase cooling, causing the local vapor pressure to drop below the saturation pressure of the liquid. This thermodynamic imbalance drives significant evaporation at the interface. As the spray cycle progresses, the vapor loses heat to the droplets and the surrounding liquid, causing its temperature to approach the corresponding saturation temperature. Consequently, the model predicts reduced evaporation rates and a shift towards condensation, with excess vapor condensing back into the liquid phase. This transition reflects the dynamic interplay between evaporation and condensation during the spray process and aligns with the expected physical behavior.

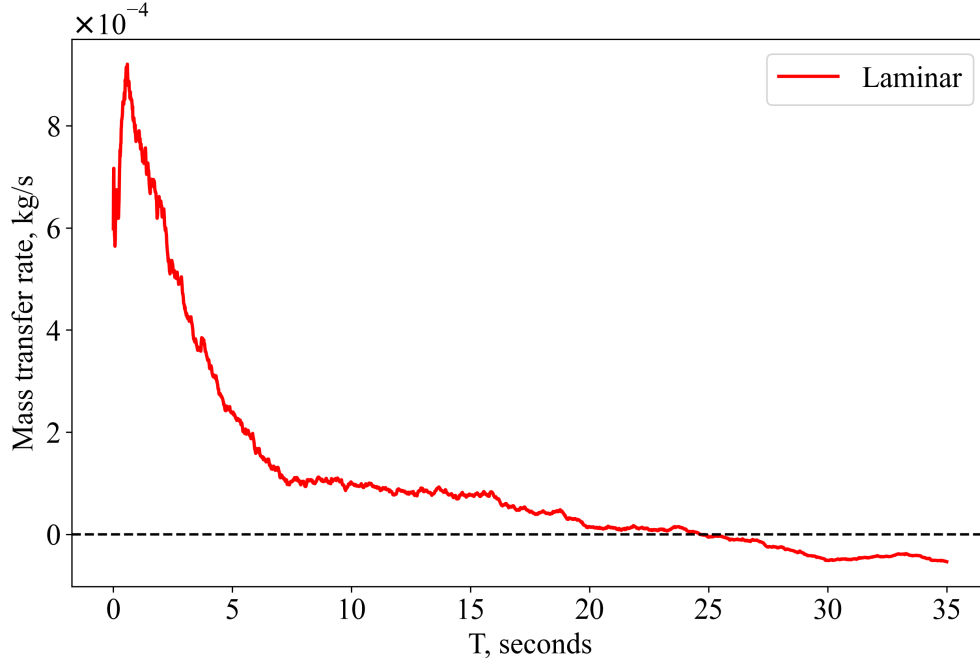


Fig. 24 Interfacial mass transfer rate, during the first spray cycle.

V. Conclusion

This study developed and validated a comprehensive two-phase CFD model to simulate the self-pressurization and spray-bar mixing processes in the MHTB tank at a 25% fill level. Various turbulence models, including LES, SBES, IDDES, SST $k-\omega$, and a laminar flow model, were employed to capture the fluid dynamics and thermal behaviors within the tank during self-pressurization. The IDDES model provided the most accurate predictions of pressure and temperature during self-pressurization, effectively balancing computational efficiency and accuracy. It successfully captured pressure and temperature changes without the excessive computational cost associated with an LES model.

The simulation results for the spray-bar mixing process demonstrated a strong agreement between the CFD model and experimental data, particularly in predicting the tank pressure evolution and ullage temperature decrease during the first spray cycle. The T-sat model proved effective in modeling the droplet-ullage interactions, accurately representing the energy exchange and phase change processes during the spray cycle.

The validated CFD model enhances our understanding of the thermodynamic and fluid dynamic mechanisms involved in cryogenic tank self-pressurization and pressure control. It is a valuable tool for optimizing spray-bar designs and operational parameters, such as droplet size, injection rate, and spray duration, to improve pressure control efficiency in cryogenic storage systems.

Future work will extend the model to simulate multiple spray cycles and investigate the effects of varying operating conditions. This will provide a more comprehensive understanding of the tank's behavior under different scenarios and contribute to optimizing pressure control strategies. Additionally, adapting the model for microgravity conditions will be essential for its application in space missions, where effective cryogenic fluid management is critical. Such adaptations will enable the model to assist in designing and optimizing cryogenic storage systems for long-duration space exploration, ultimately contributing to the success of future NASA missions.

Acknowledgments

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