

CFD Modeling of Tank Pressurization and Axial Jet Mixing Experiments with and without Non-Condensable Gas in the Ullage

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A two-phase CFD model for tank pressurization and following jet mixing of a cryogenic storage tank is presented using VOF approach for representing the phase boundary and the associated interfacial heat, mass and momentum transfer between the liquid and vapor regions. The CFD model was validated against pressurization and liquid jet mixing data for a 110-inch diameter tank provided by Bullard¹. Cases with like-gas and non-condensable gas pressurization are studied. The results of the cases with like-gas pressurization and following mixing are presented first, focusing on the effects of turbulence at the vapor-liquid interface on the tank pressure and phase change rates predictions. The second part of this paper is devoted to testing and validating the CFD model against non-condensable gas pressurization and following mixing. Tank pressures predicted in both cases are compared with each other and with the experimental data.

I. Nomenclature

E	= energy, J
F	= force, N
$\mathbf{g}$	= gravitational acceleration, m/s ²
h	= enthalpy, J/kg
k	= thermal conductivity, W/m·K
$\mathbf{n}$	= normal vector
p, P	= pressure, Pa
t	= time, seconds
T	= temperature, K
$\mathbf{v}$	= velocity, m/s
<i>Greek</i>	
α	= cell value of volume fraction
μ	= viscosity, Pa·s
ρ	= density, kg/m ³
σ	= surface tension, N/m
<i>Subscripts</i>	
eff	= effective
i	= interface
q	= phase

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II. Introduction

It is essential to understand the behavior of cryogenic fluids in a tank to aid in the design of the new propellant storage systems for space applications to help accomplish NASA missions. Cryogenic propellant tanks are often pressurized with helium gas, which affects condensation as well as heat transfer and phase change at the liquid-vapor interface. It is expensive to conduct microgravity experiments to study effects of non-condensable gas on the tank conditions. Therefore, developing and validating Computational Fluid Dynamics (CFD) models that include the effects of non-condensable gas helps to create a valuable tool for designing future rockets.

There is a limited number of CFD studies focusing on the effects of pressurizing cryogenic storage tanks with a non-condensable gas. Grayson et al.² used Flow3D software to model GHe pressurization of the 10 ft diameter tank known as MHTB (Multipurpose Hydrogen Test Bed) filled with LH2 and LN2, followed by depressurization using Thermodynamic Vent System (TVS) spray. In this study pressurization rates are predicted within 26% of the measured values and depressurization rates within 50%. Wang et al.³ computationally studied thermodynamic behavior of a LH2 tank in a series of successive aerospace operations using ANSYS Fluent CFD code. They observed significant influence of non-condensable helium in the tank ullage on the propellant thermodynamic behaviors; and concluded that Helium accumulation in pre-pressurization could restrain an excessive pressure decline in the following periods. However, in this study no comparison with any experimental data has been presented to demonstrate validity of the results. Kassemi et al.⁴ studied effect of non-condensable gas on pressurization and pressure control of a Zero-Boil-Off Tank in microgravity. In this study a simulant fluid with air (a non-condensable gas) in the ullage of a small-scale tank were considered. The results for tank pressure and temperatures followed experimental trends during pressurization and pressure control in 1G. Microgravity predictions were also made, but no experimental data was available for comparison.

In the current study a computational model has been developed and validated against tank pressurization and following jet mixing experiments with and without non-condensable gas, as reported by Bullard in the 1972 report¹. In the experiments performance of zero-gravity venting system was evaluated using two different tanks with 110-inch and 41.5-inch diameters. Test cases 9 and 30 conducted with the 110-inch diameter tank were selected for validating the current CFD model in this study. In the case 9 tank, initially containing liquid hydrogen and its vapor, was first pressurized with gaseous hydrogen and then liquid hydrogen was mixed with liquid jet directed vertically towards the interface in the liquid region. The case 30 is similar to case 9, except here the tank was pressurized with gaseous helium (non-condensable) instead of hydrogen. The CFD model was first validated against the case 9 without non-condensable gas and then against case 30, with non-condensable gas. To model the case with non-condensable gas our in-house developed VOF phase change model had to be modified. Details of the model modification and validation results are presented in the following sections. The results of the cases without non-condensable gas are presented first, followed by the cases with the non-condensable. Effects of turbulence modeling are discussed.

III. Mathematical Model

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:

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

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

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

In the present study, the liquid phase is treated 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 diffusely using the Volume of Fluid (VOF) method, as promulgated by Hirt and Nichols⁵. 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 Schrage⁶ equation:

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

Here σ is the accommodation coefficient; 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). Vapor pressure (P_v) in the cases with non-condensable gas is defined as a partial pressure of hydrogen vapor. 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.⁷. 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:

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

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. Turbulence modeling

In this study, the tank turbulence was modeled by utilizing the Shear Stress Transport $k-\omega$ model of Menter⁸ (kw-SST). This model is similar to the standard $k-\omega$ model of Wilcox⁹, but has the ability to account for the transport of the principal shear stress in adverse pressure gradient boundary layers. These features make the kw-SST model more accurate and reliable for a wider class of flows than the standard $k-\omega$ model.

In the VOF model, continuity of the turbulent quantities is inherently assumed since one set of equations for the turbulent kinetic energy and dissipation rate is solved for both phases throughout the domain, with properties varying according to the local volume fraction value.

IV. Numerical Implementation

Bottom mount 110-inch diameter tank, as shown in Figure 1, was considered for model validation. In the experiment gas pressurization was performed first. It was done through the tank pressurization line located at the top of the tank, as shown in Figure 2. The experimental report does not provide much information on the pressurization line geometry, but it mentions that a pressurant diffuser baffle is located approximately 1-3/4 inches (0.044 m) below the venting and pressurizing port, in the polar region of the tank. After the tank pressure reached the desired value in the experiment the pressurization was stopped, and jet mixing started. Again, very little detail is provided in the experimental report on the mixer geometry and position. From the tank schematic shown in Figure 1, the position of the mixer inlet (liquid coming into the tank) is 7.87 in (0.2 m) from the tank horizontal centerline, position of the mixer outlet (liquid leaving the tank) is approximately 14 in (0.3556 m) from the tank bottom. In the experiment the nozzle is positioned approximately 11.87 in (0.3 m) from the tank vertical centerline.

Experimental cases 9 and 30 are considered for model validation in this study. Measured tank pressures for these cases are shown in Figure 3. Both cases are similar, except in case 30 the tank is pressurized with helium gas, when in case 9 hydrogen gas is used for pressurization. Experimental steps are described in table 12 of the Bullard's report¹ for case 9 as: "Vent from final pressure of the previous run to 17 psia (117210.9 Pa) and equalize tank conditions. Then pressurize to 28 psia (193053 Pa) with GH_2 at 140°R (77.77 K) and establish pressure-time relation with mixer until $dP/dQ = 0$ ". For case 30: "repeat 9 using He as pressurant"¹. In both cases initial ullage volume is 5%, mixer flow rate is 150 L/m (0.0025 m³/s).

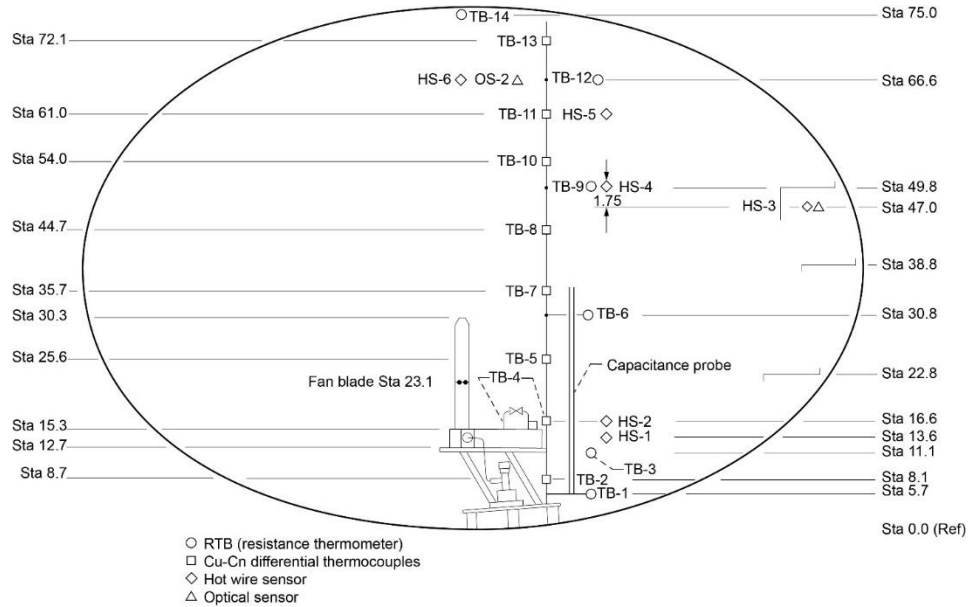


Figure 1: Schematic of the 110-inch bottom mount tank used in the experiment

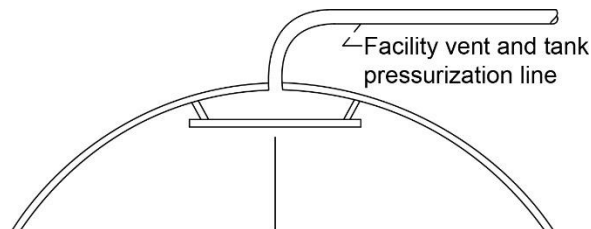


Figure 2: Schematic of the tank pressurization line

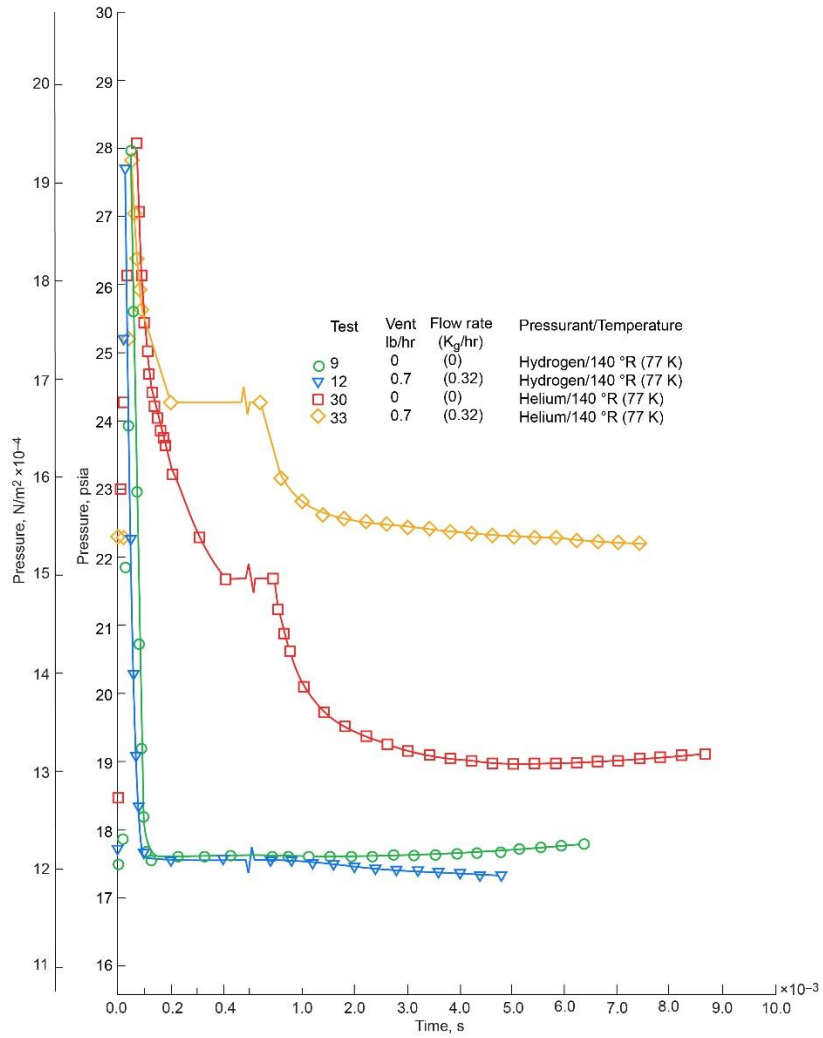


Figure 3: Experimental tank pressures - cases 9, 12, 30 and 33. (from the Figure 58 on page 118 of the Bullard report¹)

D. Tank Geometry

In this study an elliptical tank with 1.97 m minor diameter and 2.8 m major diameter, as shown in Figure 4 was considered. Axisymmetric 2D tank geometry was used in calculations.

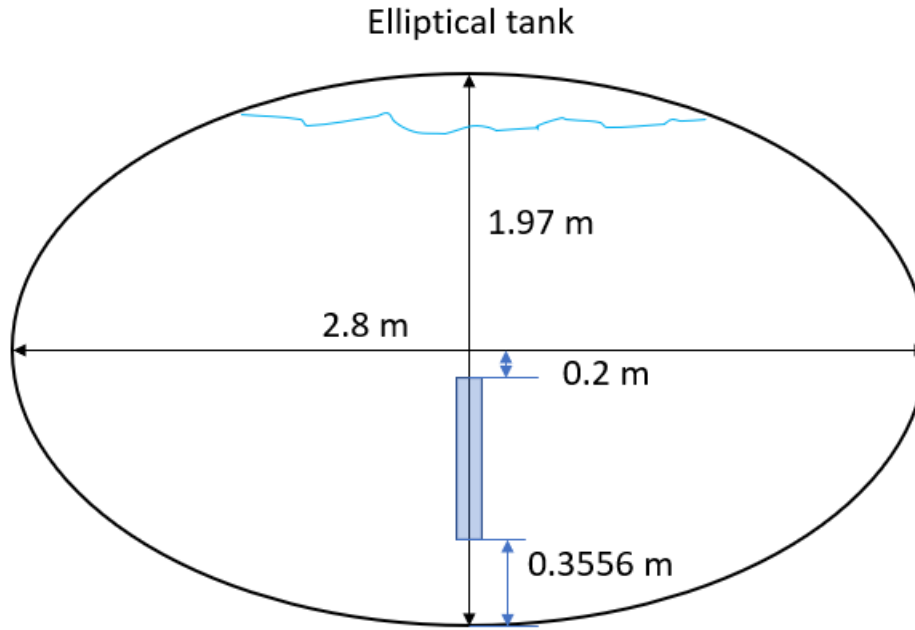


Figure 4: Tank Geometry used in CFD

E. Initial Conditions

In this case initial tank pressure was set to the initial measured value of 17.49 psia or 120590 Pa. Fluid temperatures were set to the saturation value (20.873 K) at the initial tank pressure. Initial ullage volume was set to 5%. In the cases where turbulence models were used initial values for turbulence kinetic energy and specific dissipation rate were set, respectively, to $1\text{e-}06 \text{ m}^2/\text{s}^2$ and 100 1/s.

F. Boundary Conditions

The tank wall was not included in calculations. Adiabatic boundary conditions were used at all wall boundaries. A contact angle between liquid and the tank wall was assumed to be 0 degrees. No slip boundary conditions were applied on the inside of the tank wall which is in contact with fluid. Gaseous H_2 or He is injected at the vertical line, called pressurant inlet in Figure 5. During pressurization a value of the gas mass flow rate obtained in a separate Thermal Desktop model (1.89 g/sec) is applied uniformly at the inlet surface, which was modeled as a velocity inlet. Constant gas temperature of 77 K was applied uniformly at the inlet surface. During jet mixing gas injection is turned off and liquid comes into the tank through the mixer inlet, as shown in Figure 5. Mixer outlet, located 0.3556 m from the tank bottom, as shown in Figure 5, is modeled as velocity outlet. Mass flow rates at the mixer inlet and outlet match each other and experimental value of 150 L/m ($0.0025 \text{ m}^3/\text{s}$).

G. Material Properties

The liquid hydrogen and its vapor initially fill the tank. Constant properties at saturation at the initial tank pressure of 17.49 psia or 0.1205893 MPa were used. Hydrogen properties are summarized in Table 1.

In the cases with non-condensable gaseous helium used as pressurant inlet temperature of 77 K was used. Constant helium properties at 77 K were used. Helium properties are summarized in Table 2.

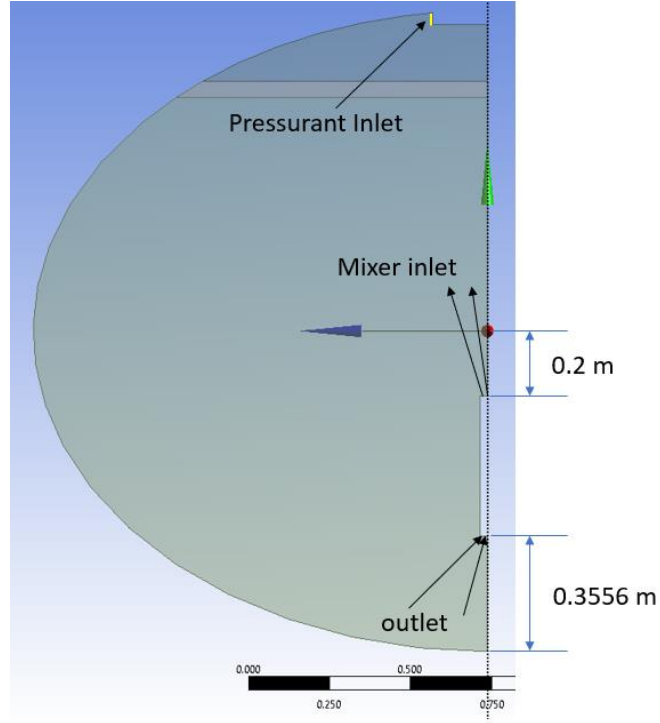


Figure 5: Computational domain and boundary conditions

Table 1: H2 properties from NIST at $T_{\text{initial}} = 20.873 \text{ K}$ and $P_{\text{initial}} = 120590 \text{ Pa}$

Property	Units	liquid	vapor
Density	kg/m ³	70.128	Ideal gas
C_p	J/kg-K	10101.0	12290.0
Thermal Conductivity	W/m-K	0.10417	0.017674
Viscosity	Pa*s	1.2706e-5	1.1108e-6
Surface Tension	N/m	0.0018282	
Thermal Expansion coeff.	1/K	0.017622	-
Molecular Weight	kg/kmol	2.0159	

Table 2: He properties from NIST at $T = 77 \text{ K}$

Property	Units	value
Density	kg/m ³	Ideal gas
C_p	J/kg-K	5196.7
Thermal Conductivity	W/m-K	0.061946
Viscosity	Pa*s	8.3066e-6
Molecular Weight	kg/kmol	4.0026

H. Computational mesh

2D axisymmetric computational grid used in the current study is shown in Figure 6. This grid is refined near the gas inlet, liquid-vapor interface and near the liquid jet inlet. It consists of 35,070 cells.

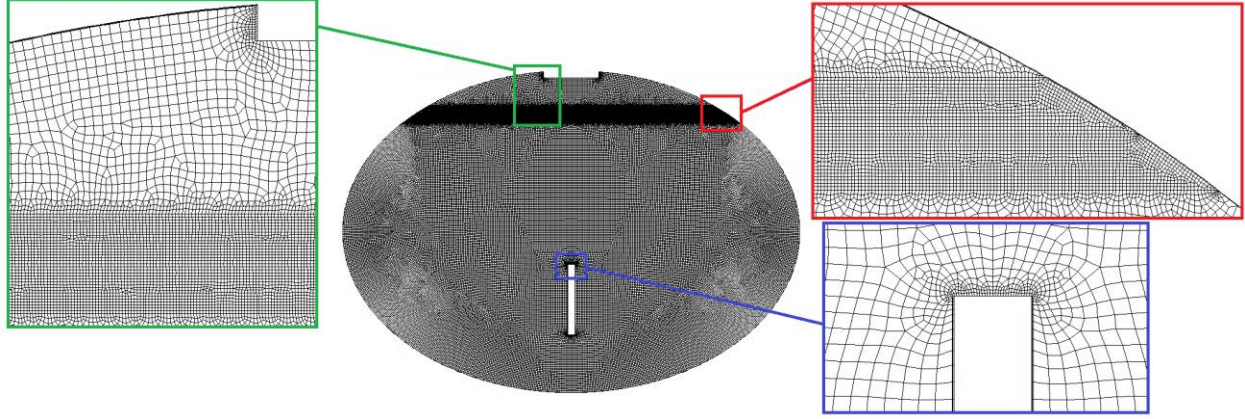


Figure 6: Computational Mesh

I. Discretization and convergence

The Second Order Upwind scheme was used to discretize the turbulence, energy, and momentum equations (cell values). The PISO scheme was used for the pressure-velocity coupling (cell values). The Least Squares Cell Based scheme was used for the gradient calculations (face values). The PRESTO! scheme was used for the pressure interpolation (face values). The Point Implicit (Gauss-Seidel) linear equation solver with the Algebraic Multi-Grid (AMG) method was used to solve the linearized systems of equations. The Second Order Implicit temporal discretization and the Compressive scheme for the VOF equation was used with the implicit VOF model. The convergence criteria are set to 1×10^{-4} for all the equations except the energy equation, for which it is set to 1×10^{-6} . Time step size value of 0.001 seconds was used.

V. Results and Discussion

CFD simulations results are presented and compared with the experimental data¹ in this section. Results of the case with like-gas tank pressurization and jet mixing are discussed first followed by the results of the case where non-condensable gas is used for tank pressurization.

J. Case 9: Like-gas tank pressurization and jet mixing

Predicted tank pressure during like-gas pressurization and following mixing is presented and compared with the experimental data in Figure 7. During pressurization the rate of the pressure increase predicted by the CFD model compares well with the experimental data. At the highest experimental tank pressure, the CFD pressurization case was stopped, as indicated by the grey dot in the figure, and the results were used as initial conditions for the following jet mixing case. The turbulent VOF case without turbulence damping (TD) at the interface predicts faster pressure drop in the tank in the beginning of mixing but matches measured pressure values after ~ 100 seconds. Three different values of turbulence damping coefficient (10, 100 and 200) were considered in this study. All cases with turbulence damping predict similar tank pressures which are higher than the ones predicted in the case without damping and measured in the experiment. Phase change rates at the interface during jet mixing predicted in the cases with and without turbulence damping are compared in Figure 8. Lower values of condensation (negative values) are predicted in the case with turbulence damping compared to the case without damping. Figure 9 shows contours of turbulence kinetic energy predicted by the VOF models with and without damping. The case without damping shows higher levels of turbulence kinetic energy on both sides of the interface in the area of jet impingement. In the case with damping higher levels of turbulence kinetic energy are present only on the liquid side of the interface but not on the vapor side.

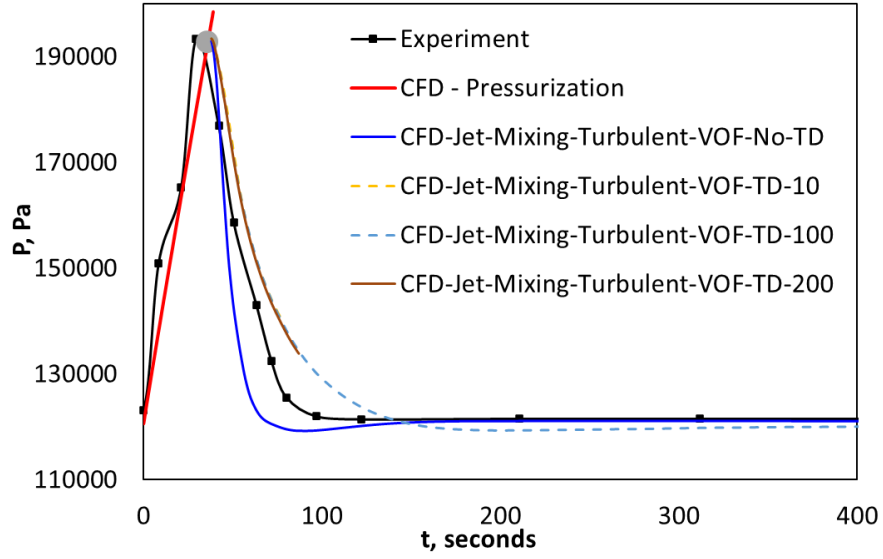


Figure 7: Tank pressure during jet mixing after like-gas pressurization: Effect of Turbulence Damping (TD) at the interface used with the VOF model

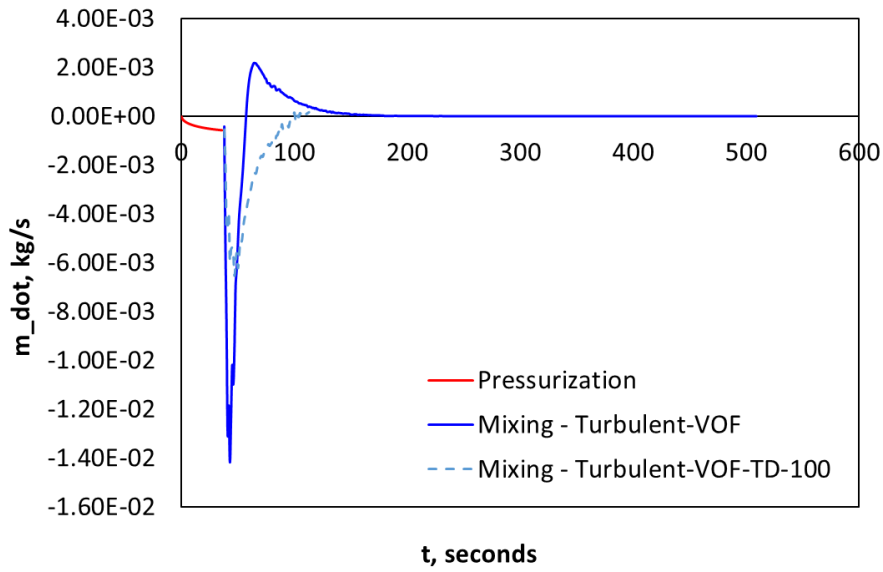


Figure 8: Effect of Turbulence Damping at the interface used with the VOF model on the phase change rate at the interface during jet mixing after like-gas pressurization

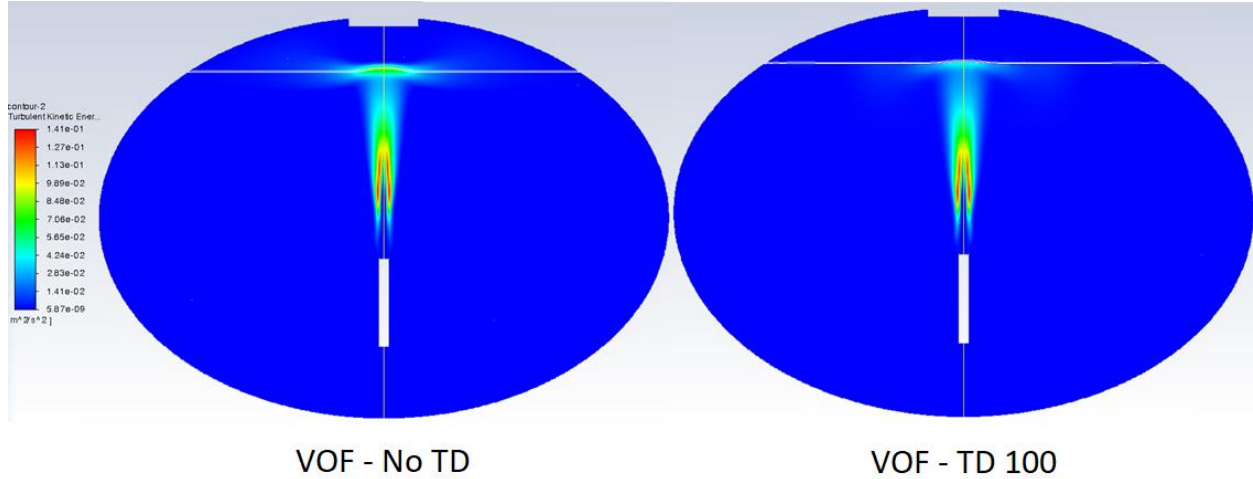


Figure 9: Contours of Turbulence Kinetic Energy in the VOF models with and without Turbulence Damping at the interface

K. Case 30: Non-condensable gas tank pressurization and jet mixing

Figure 10 compares measured and predicted pressures in the tank during jet mixing after like-gas and non-condensable gas pressurization. In Case 9, where the tank is pressurized with a like gas, pressure drop in the tank occurs very fast during jet mixing in both CFD and experiment as shown by red lines and symbols in the figure. In case 30, where tank is pressurized with a non-condensable gas, pressure drop in the tank occurs more slowly compared to case 9, as shown by blue lines and symbols in the figure. In case 9 the results of the CFD model match experimental trend of the pressure drop and the measured final pressure in the tank very closely. In case 30, with non-condensable gas, predicted tank pressure decreases faster compared to the experimental data. However, pressure in the CFD case seems to settle near the same level as in the experiment. Phase change rates at the interface during jet mixing and pressurization with and without non-condensable gas are compared in Figure 11. Condensation at the interface is significantly reduced, as expected, in the case where a non-condensable gas is present.

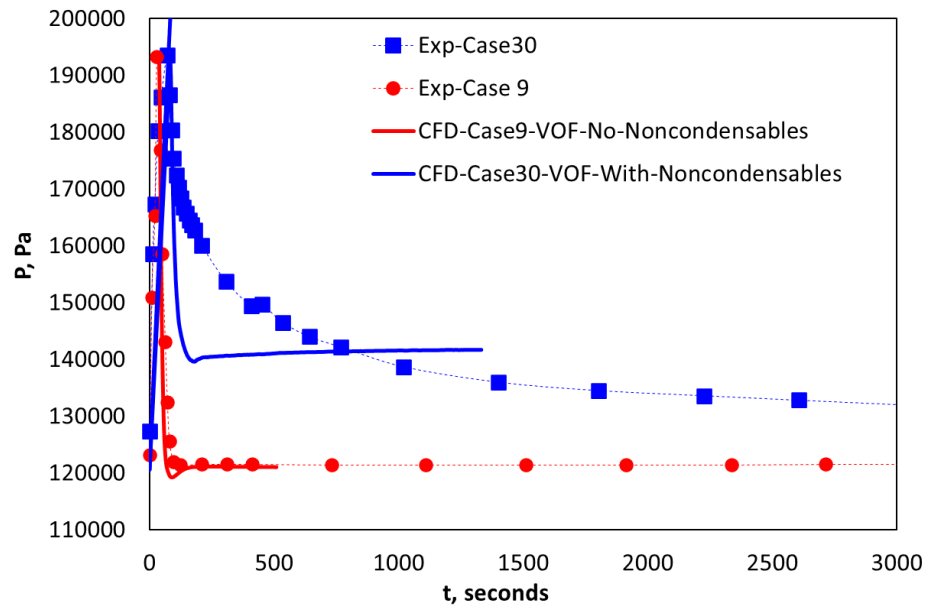


Figure 10: Tank pressure during jet mixing after like-gas and non-condensable gas pressurization: CFD vs. Experiment

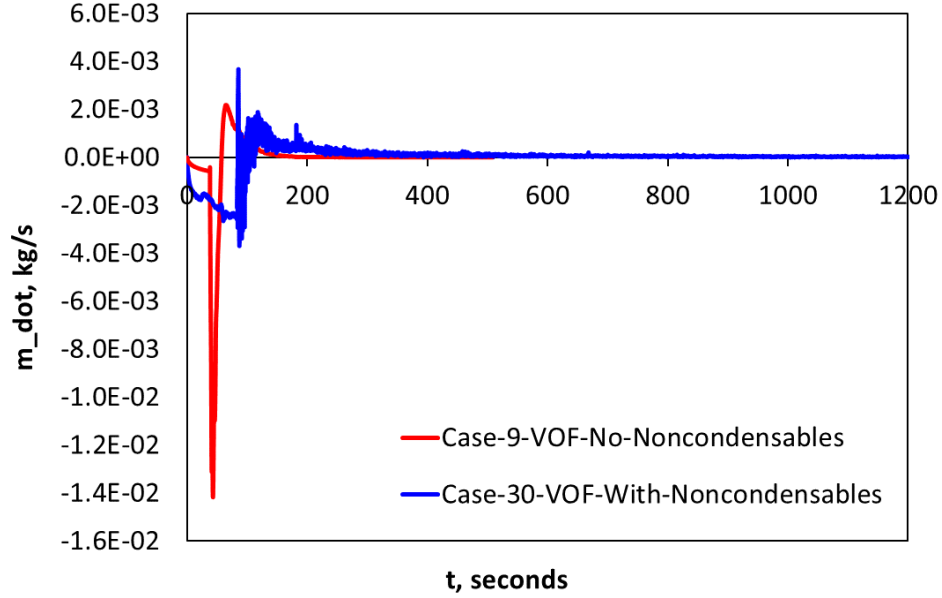


Figure 11: Phase change rate at the interface during jet mixing and pressurization with and without non-condensable gas

VI. Conclusion

A computational model of tank pressurization followed by jet mixing with and without non-condensable gas has been developed and its predictions were compared with the experimental data presented by Bullard¹. The CFD model was first applied to simulate Bullard's case 9 without the non-condensable gas and then to simulate case 30, with the non-condensable gas. To model cases with the non-condensable gas an in-house developed customized phase change VOF model was used.

For the like-gas pressurization (experimental case 9) and the following jet mixing the turbulent VOF model's predictions matched the measured pressures in the tank reasonably well. Introduction of turbulence damping at the interface in the turbulent VOF simulation resulted in a slower pressure drop in the tank during mixing, however, changing the value of the damping coefficient had limited effect. In the case with the non-condensable gas pressurization (experimental case 30), turbulent VOF model predicted a sharp initial pressure drop, in agreement with the experiment, but subsequently over-predicted the pressure drop drastically compared to the measurements. In the like-gas pressurization case the final plateaued tank pressure level after mixing was predicted well. However, in the case with the non-condensable gas pressurization final pressure level in the tank was somewhat overpredicted by the model. The VOF model predicted significantly less condensation in the presence of the non-condensable gas compared to the pure hydrogen case, thus, confirming the important trend observed in Bullard's experimental results that the non-condensable gas mitigates the interfacial condensation rate. The performance of the VOF model for predicting tank depressurization rates in presence of a non-condensable gas was affected by the limitations of its implementation. The VOF model captures the deformation of the interface by the jet, but does not perform customized calculations of the interfacial non-condensable gas concentration and the "Stefan wind". It also does not capture the dissolution of helium in liquid hydrogen.

The present validation case study against Bullard's hydrogen tank pressurization and mixing depressurization with and without the noncondensable gas, helium, has pointed out important shortcomings of the VOF CFD model in capturing the effect of the non-condensable gases with computational fidelity. The VOF model does not include a rigorous balance of species at the interface, nor does it follow Henry's Law in determining the species concentrations at the vapor and liquid side of the interface. This model must be improved to remove the mentioned short comings so that it can provide more accurate predictions of the non-condensable gas effects. It is important to develop and implement a mathematically rigorous non-condensable gas capability into the VOF scheme that has the inherent ability to handle the dynamic interface behavior encountered in future space applications.

Acknowledgments

Authors would like to thank Dan Hauser (NASA-GRC) for his help with extracting details of tank geometry, initial and boundary conditions from experimental data and for completing a Thermal Desktop case to determine pressurant mass flow rate; and the Modeling Portfolio Project within the STMD CFM Project Office for providing funding for this work.

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