Validation of a Two-Phase CFD Model for Predicting Tank Self-Pressurization in the Ground-Based K-Site Experiment

Olga Kartuzova[1] and Mohammad Kassemi[2]
National Center for Space Exploration Research (NCSER), Case Western Reserve University and NASA Glenn Research Center, Cleveland, OH 44135, USA

A two-phase CFD model for self-pressurization of a cryogenic storage tank partially filled with liquid hydrogen is presented using the Volume-Of-Fluid approach for representing the phase boundary and the associated interfacial heat, mass and momentum transfer between the liquid and the vapor regions. The CFD model is validated against self-pressurization experiment performed in the K-site flightweight hydrogen storage tank at NASA Glenn Research Center. Laminar and turbulent simulations together with conjugated heat transfer analysis are performed. Effects of turbulence, as well as tank wall conduction are presented and discussed. Predicted tank pressures and fluid temperatures are compared with the experimental data at two different heat loads for validating the CFD model.

I. Nomenclature

E	=	energy, J
F	=	force, N
g	=	gravitational acceleration, m/s^2
h	=	enthalpy, J/kg
k	=	thermal conductivity, W/m·K
n	=	normal vector
p, P	=	pressure, Pa
t	=	time, seconds
T	=	temperature, K
v	=	velocity, m/s

Greek

α	=	cell value of volume fraction
μ	=	Pa·s
ρ	=	density, kg/m^3
σ	=	surface tension, N/m

Subscripts

eff	=	effective
i	=	interface
q	=	phase

II. Introduction

A computational model has been developed and validated against tank self-pressurization experiment, as reported by Hasan et al. in the 1991 paper[1]. In the experiments a tank (known as K-Site tank) filled with liquid hydrogen and its vapor was used. Test cases with 49% fill level and two different values of heat flux entering through the tank wall (2 W/m^2 and 3.5 W/m^2) were selected for model validation.

Details of the CFD model and validation results are presented in this paper. Predicted tank pressures are compared with the experimental data. Effects of turbulence modeling as well as conjugate heat transfer calculations are discussed. Predicted fluid temperatures will be compared with the experimental values in the final paper.

[1] Research Assistant Professor, Department of Mechanical & Aerospace Engineering, and AIAA Member.
[2] Research Professor, Department of Mechanical & Aerospace Engineering, AIAA Associate Fellow.

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:

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

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

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

In the present study, the liquid phase is treated as incompressible with constant 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 promogulated by Hirt and Nichols[2]. 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:

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

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

$$\sum_{q=1}^{n} \alpha_q = 1. \tag{5}$$

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:

$$\rho = \sum_{q=1}^{n} \alpha_q \rho_q, \qquad \mu_{eff} = \sum_{q=1}^{n} \alpha_q \mu_{eff_q}, \qquad k_{eff} = \sum_{q=1}^{n} \alpha_q k_{eff_q}. \tag{6}$$

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:

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

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.:

$$S_{\alpha_q} = \dot{\mathbf{m}}_i \cdot \mathbf{A}_i\,, \tag{8}$$

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[3] equation:

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

Here σ is the accommodation coefficient (value of 0.001 was used); 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:

$$\mathbf{A}_i = |\nabla \alpha|, \tag{10}$$

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.[4]. 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:

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

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

$$h_i = \nabla \cdot \hat{\mathbf{n}}. \tag{12}$$

C. Turbulence Modeling

In this study, two different turbulence models were used and compared against each other in the VOF model. The first is the Shear Stress Transport k-ω model of Menter[5] (kw-SST), and the second is the Realizable k-ε model of Shih et al.[6] (RKE).

Shear Stress Transport k-ω model of Menter[5] (kw-SST) is similar to the standard k-ω model of Wilcox,[7] 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-ω model.

Realizable k-ε model (RKE), proposed by Shih et al.,[6] uses an improved dissipation rate equation and "realizable" eddy viscosity formulation. The equation for the model dissipation rate is based on the dynamic equation of the mean-square vorticity fluctuation at large turbulent Reynolds number. In this model eddy viscosity formulation is based on the "realizability" constraints (under certain conditions[6] normal Reynolds stresses may become negative, which is unphysical or unrealizable).

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

A flightweight hydrogen storage tank, also known as K-Site, was considered for model validation. The tank is an ellipsoidal volume of revolution with major diameter of 2.2 m and major-to-minor axis ratio equal to 1.2. Tank geometry and computational mesh are shown in Figure 1. Liquid Hydrogen and its vapor fill the tank at a 49% liquid fill level. Heat fluxes, uniformly distributed along tank wall, of 2 and 3.5 W/m^2 are considered. The effect of modeling conjugate heat transfer between the fluid and solid tank wall is discussed in the paper.

D. Initial Conditions

In this case measured initial ullage temperature profile reported by Hasan et al.[1] was applied. Initial liquid fill level was set to 49% by volume. In the cases where turbulence models were used initial values for turbulence kinetic energy and specific dissipation rate were set, respectively, to 1e-06, m^2 /s^2 and 100, 1/s.

E. Boundary Conditions

The tank wall, made of 2219 aluminum, is included in calculations in most cases. The tank wall material is modeled with constant density and temperature dependent properties for thermal conductivity and specific heat. Tank wall thickness is 2.2e-03 m. Simulations are performed with and without tank wall. In the cases without the tank wall included in calculations heat flux is applied uniformly at the inner tank wall location. In the cases with conjugate heat transfer a uniform heat flux is applied at the outer tank wall location and coupled heat transfer is modeled at the inner tank wall location. A contact angle between liquid and the tank wall is assumed to be 0 degrees. No slip boundary conditions are applied on the inside of the tank wall which is in contact with fluid. Uniform heat fluxes of 2 or 3.5 W/m^2 are applied at the outside wall boundary to match experimental conditions.

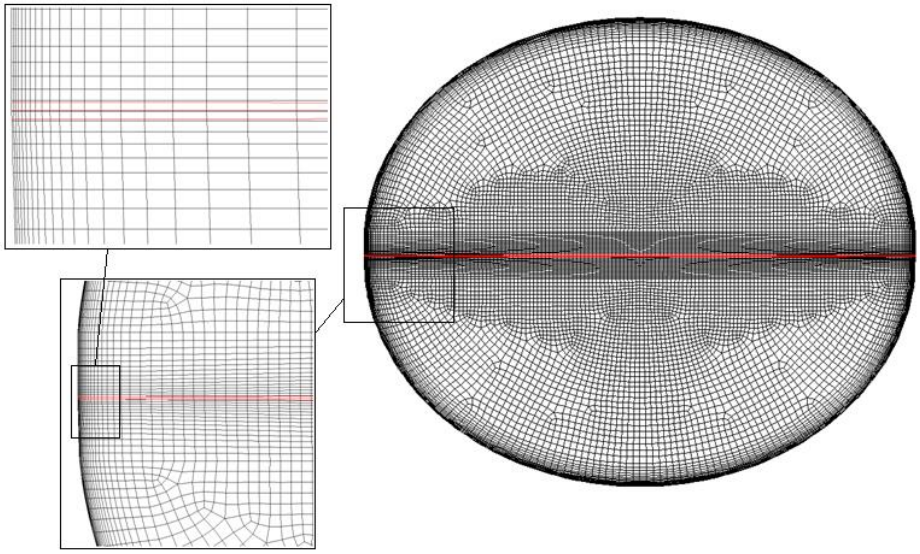

Figure 1: Tank geometry and computational mesh

F. Material Properties

The liquid hydrogen and its vapor fill the tank. Parahydrogen properties from NIST REFPROP database are used. Constant properties at saturation at the initial tank pressure are applied.

G. Discretization and Convergence

The Second Order Upwind scheme is used to discretize the turbulence, energy, and momentum equations (cell values). The PISO scheme is used for the pressure-velocity coupling (cell values). The Least Squares Cell Based scheme is used for the gradient calculations (face values). The Body Force Weighted scheme is used for the pressure interpolation (face values). The Point Implicit (Gauss-Seidel) linear equation solver with the Algebraic Multi-Grid (AMG) method is used to solve the linearized systems of equations. The Bounded Second Order Implicit temporal discretization and the Compressive scheme for the VOF equation is used with the implicit VOF model. The convergence criteria are set to $1x10^{-4}$ for all the equations except the energy equation, for which it is set to $1x10^{-6}$. Time step size value of 0.05 seconds is used.

H. Computational mesh

2D axisymmetric computational grid used in the current study is shown in **Error! Reference source not found.**1. The mesh is refined near the tank walls to keep the y^+ value less than 5 and near the liquid-vapor interface to resolve interfacial heat and mass transfer. The grid size used in this study is 7682 cells.

V. Results and Discussion

Preliminary CFD simulations results are presented and compared with the experiemntal data obtained in the experiment[1] in this section.

I. 3.5 W/m^2 Heat Flux

Predicted tank pressure during pressurization is presented and compared with the experimental data in Figure 2. Here, despite natural convection in the tank being turbulent in both liquid and vapor regions, the conjugate Laminar model is best at predicting tank pressure during pressurization (within 7% of the measured values). Laminar model without tank wall overpredicted tank pressure. Both turbulence models tested result in similar tank pressures, which are much lower than measured values. Including tank wall in calculations with the turbulence model had little effect and didn't improve predicted tank pressures significantly. Temperature contours during pressurization, as predicted by the laminar and turbulent (k-w-SST) models, are shown in Figure 3 at the beginning, middle and end of simulation. Both models predict stratification in the vapor region with gradually increasing temperatures. However, the turbulent

model predicts significantly lower vapor temperatures, compared to the results of the laminar model, indicating increased mixing in the tank.

Fluid temperatures will be compared with the experimental data in the final paper.

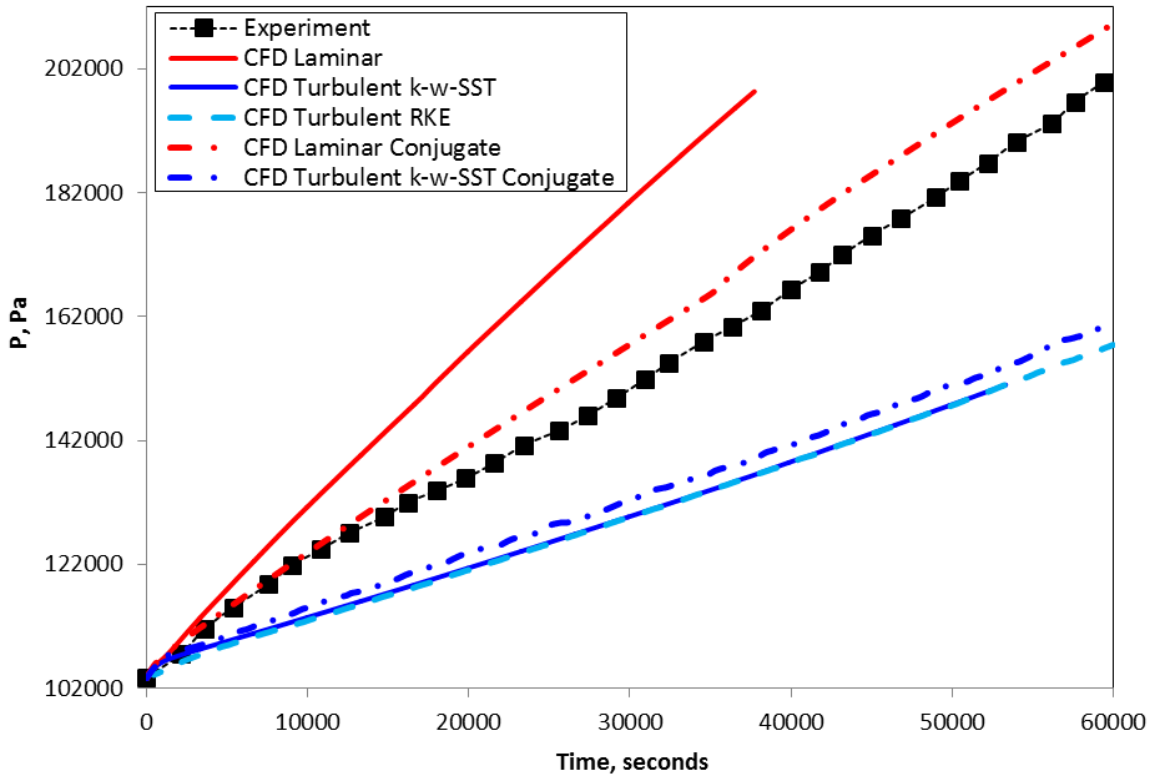

Figure 2: Tank pressure during tank pressurization with 3.5 W/m^2: CFD vs. Experiment

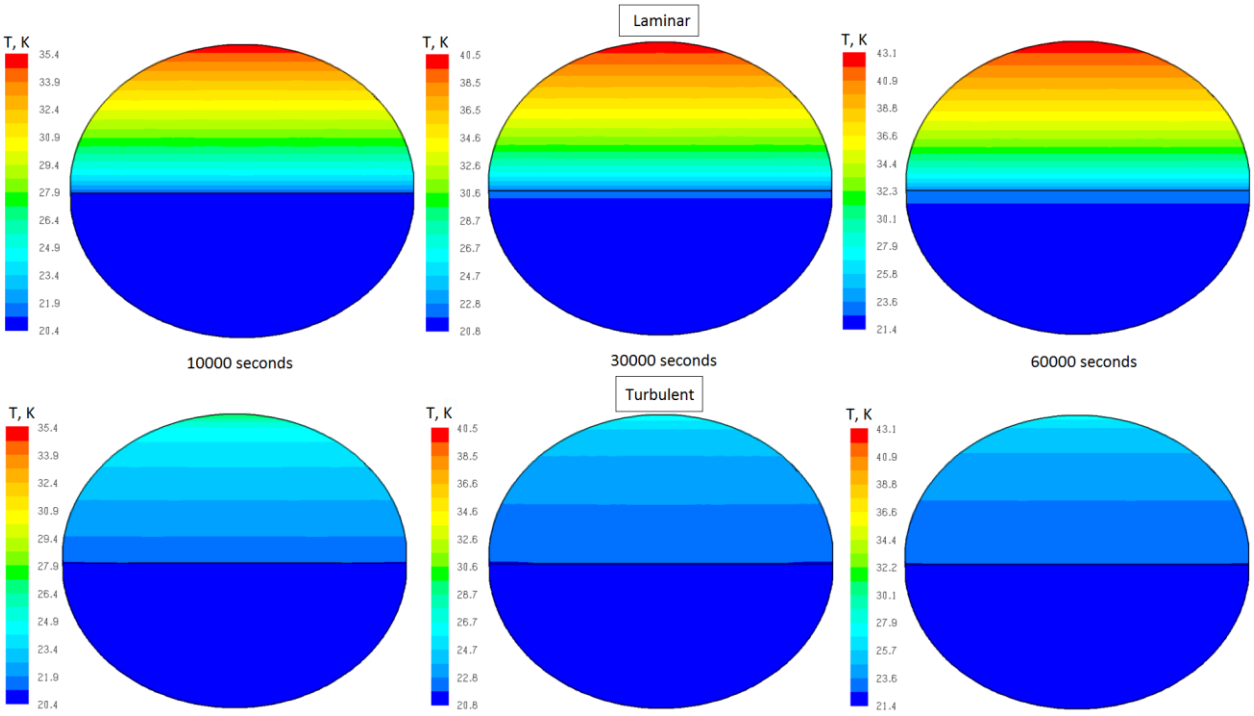

Figure 3: Temperature contours during pressurization with 3.5 W/m^2: Laminar vs. Turbulent model

J. 2 W/m^2 Heat Flux

Predicted tank pressures during pressurization with 2 W/m^2 heat flux value are presented and compared with the experimental data in Figure 4. Here, just like in the case with the 3.5 W/m^2 heat flux value, the laminar model predictions are a lot closer to measured values (within 3%), compared to the results of the turbulent (k-w-SST) model, which underpredicts measured tank pressure during pressurization (by 16%).

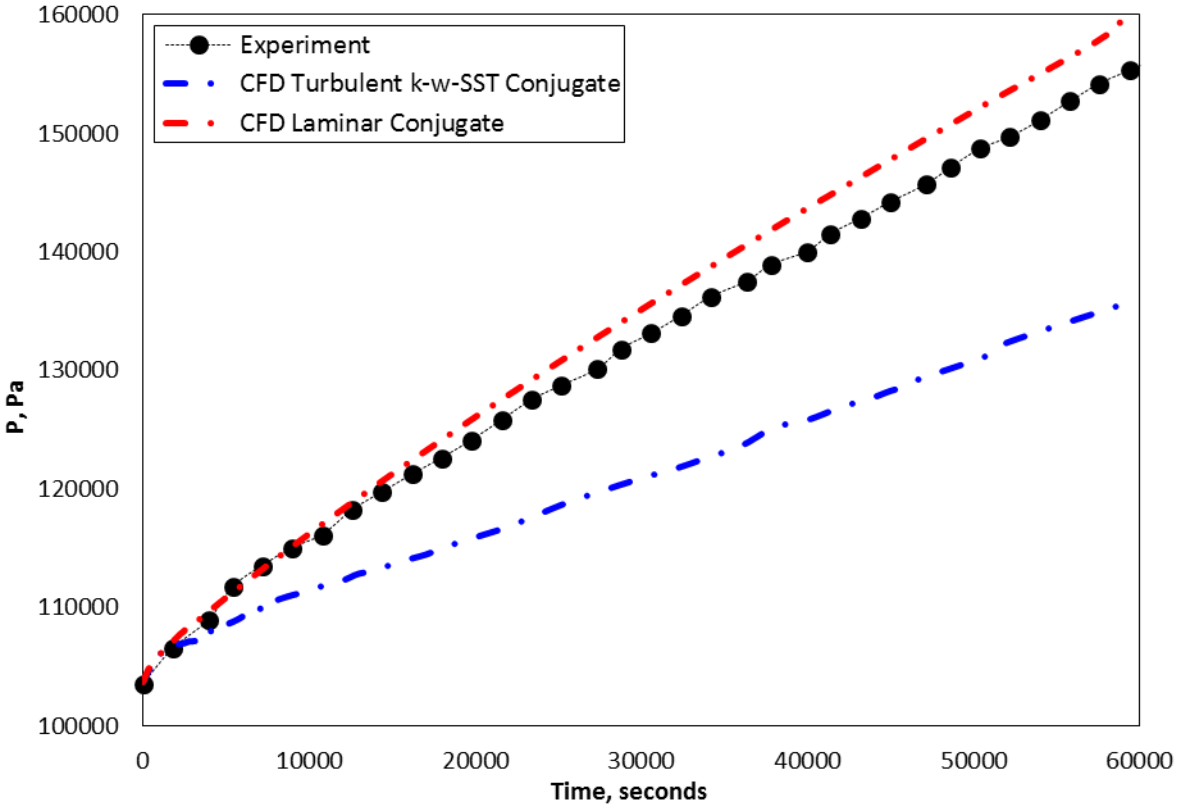

Figure 4: Tank pressure during tank pressurization with 2 W/m^2: CFD vs. Experiment

VI. Conclusion

Preliminary CFD results for cryogenic tank self-pressurization are presented and compared with the experimental data provided by Hasan et al.[1]. Simulations were performed for 2 and 3.5 W/m^2 wall heat fluxes. Results of the laminar and turbulent VOF models are compared. The effect of including tank wall into calculations is evaluated.

The laminar VOF model with heat transfer through the tank wall compares well with the measured tank pressure values. Predicted tank pressures are within 7% of the measured ones for the 3.5 W/m^2 heat flux case and within 3% for the 2 W/m^2 heat flux case. Including tank wall into calculations results in a better agreement with the experimental data for the laminar VOF model. The turbulent VOF model with and without heat transfer through the tank wall significantly underpredicts experimental tank pressure rise.

There is a need to further investigate the reason why laminar VOF model is in a better agreement with experimental data, despite the fact that the natural convection flow inside the tank is turbulent (vapor: Gr = 2.21e+13; liquid: Gr = 1.33e+14).

Acknowledgments

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