

# Validation of Thermodynamic Behavior of Liquid Propellant under Sloshing and Draining

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In recent years, considerable effort has been devoted to studying the future use of liquid methane (LCH<sub>4</sub>) in land, air, and space vehicle applications because of its high density and handling characteristics. This work presents a validation of computational tools for the thermodynamics characterization of a propellant tank undergoing sloshing and draining-induced thermal de-stratification as part of our continuous effort to improve simulation capabilities for support of NASA's current and future flight programs. A multi-phase computational fluid dynamics (CFD) code developed at NASA MSFC, Loci/STREAM-VOF, is applied to predict gaseous pressurant requirements during the ramping, holding, and draining phases of operation with liquid methane. The experimental work conducted at the NASA K-site facility is used for validation. The effort showed that Loci/STREAM-VOF is capable of capturing the important findings from the previous experiments: (1) the pressurant mass required increases with the expulsion time due to longer mass transfer time at the interface; and (2) the pressurant mass required decreases with the increase in inlet temperature. Comparison with experimental data shows consistent good agreement at different expulsion times and different inlet gas temperatures.

## Nomenclature

|       |                                    |
|-------|------------------------------------|
| A     | area                               |
| $c_v$ | heat capacity at constant volume   |
| $c_p$ | heat capacity at constant pressure |
| $C_m$ | mass transfer coefficient          |
| e     | internal energy                    |
| F     | volume of fluid                    |
| g     | gravity vector                     |
| h     | enthalpy                           |
| k     | thermal conductivity               |
| L     | latent heat                        |
| m     | interfacial mass flux              |
| n     | surface normal                     |
| p     | pressure                           |
| R     | gas constant                       |
| Q     | surface heat flux                  |
| S     | surface                            |
| T     | temperature                        |
| t     | time                               |

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u      velocity  
V      volume

#### Greek

$\beta$       thermal expansion coefficient  
 $\kappa$       compressibility  
 $\rho$       density  
 $\tau$       shear stress  
 $\omega$       specific turbulence dissipation rate  
 $\Phi$       dissipation

#### Subscript

face    surface  
g      gas phase  
i      component in x,y, and z direction  
l      liquid phase  
ref    reference  
sat    saturation

## **I. Introduction**

In a cryogenic liquid-fueled propulsion system, the propellant is drained from the tank bottom, and high-temperature helium gas or gaseous propellant is generally injected into the tank to maintain the tank pressure at a sufficiently high level so as to prevent cavitation at the pump inlet. In this process, various thermodynamic phenomena may simultaneously occur, including heat transfer between ullage, liquid and tank wall, liquid-vapor mass transfer, and species transport in the multi-constituent ullage. Sufficient knowledge of these processes and their effects on pressurization performances is essential for the design and optimization of a pressurization system.

Future space exploration missions will require large quantities of cryogenic liquids and the ability to transfer these fluids between earth-to-orbit tankage vehicles, orbiting depots, and space transportation vehicles [1]. Such transfer operations will require supply tank pressurization and pressurized expulsion to achieve the transfer between spacecraft. The technique involves the introduction of a gaseous pressurant into a cryogenic supply tank. When the tank pressure becomes sufficiently high, liquid cryogen is expelled from the tank via a transfer line to the destination point. The principal objective of pressurization analysis is the determination of the required amount of pressurizing gas for transfer operations. An accurate estimate of the amount of pressurant gas necessary for a transfer operation is highly desirable; having excess pressurant carries a substantial weight penalty, while an insufficient amount will result in incomplete cryogen transfer.

This work presents our effort in the validation of computational tools for the thermodynamics characterization of a propellant tank undergoing sloshing and draining-induced thermal de-stratification [2-3]. This paper reports our assessment of a multi-phase CFD code developed at NASA MSFC, Loci/STREAM-VOF, in predicting gaseous pressurant requirements during ramping, holding, and draining phases. In recent years, considerable effort has been devoted to studying the future use of liquid methane (LCH<sub>4</sub>) in land, air, and space vehicle applications because of its high density and handling characteristics. However, it was not known if the results of the previous liquid hydrogen expulsion investigations could be used for the case of gaseous methane (GCH<sub>4</sub>) pressurant requirement predictions. To this end, the experimental data of DeWitt et al. [4] will be used for validation. In the work of DeWitt et al. [4], methane, helium, hydrogen, and nitrogen were used as pressurant gases. The necessary quantities of these gases to expel 90 percent of the LCH<sub>4</sub> propellant were studied as a function of expulsion time at a nominal operating pressure of  $34.47 \times 10^5$  N/m<sup>2</sup> (50 psia), using nominal inlet gas temperatures of 222 and 333 K. Also studied were the effects on methane, helium, and hydrogen pressurant requirements of various slosh excitation frequencies and amplitudes, both with and without slosh suppressing baffles in the tank. This paper concentrates on the validation of pressurant requirements for static and slosh tanks with different inlet temperatures and different expulsion times.

## II. PROCESS

The principal aim of the work documented in this paper is to validate the Loci/STREAM-VOF CFD code and physics models implemented for cryogenic fluid management (CFM) and propellant tank dynamics applications for the purpose of predicting pressurant requirements for the discharge of liquid propellant.

### 2.1 Experimental Description

Figure 1 shows the test facility of Dewitt *et al.* [4], where all tests were conducted inside a 7.61-meter - (25-ft-) diameter spherical vacuum chamber to reduce the external heat leak into the propellant tank to a low value. A heat exchanger and bleed valve subsystem capable of delivering pressurant gas at temperatures of 167 to 405 K (301° to 729° R) was used to control pressurant gas inlet temperature. A ramp generator and control valve were used to manage the initial rate of pressurization of the propellant tank. Tank sloshing was accomplished using a hydraulically operated shaker controlled by a function generator that specified amplitude and frequency. Liquid methane outflow rates were measured using a turbine-type flowmeter located in the transfer line. Pressurant gas inlet flow rates were determined by the use of an orifice located in the pressurant supply line. Tank, line, and differential pressures were measured with bonded strain-gage-type transducers.

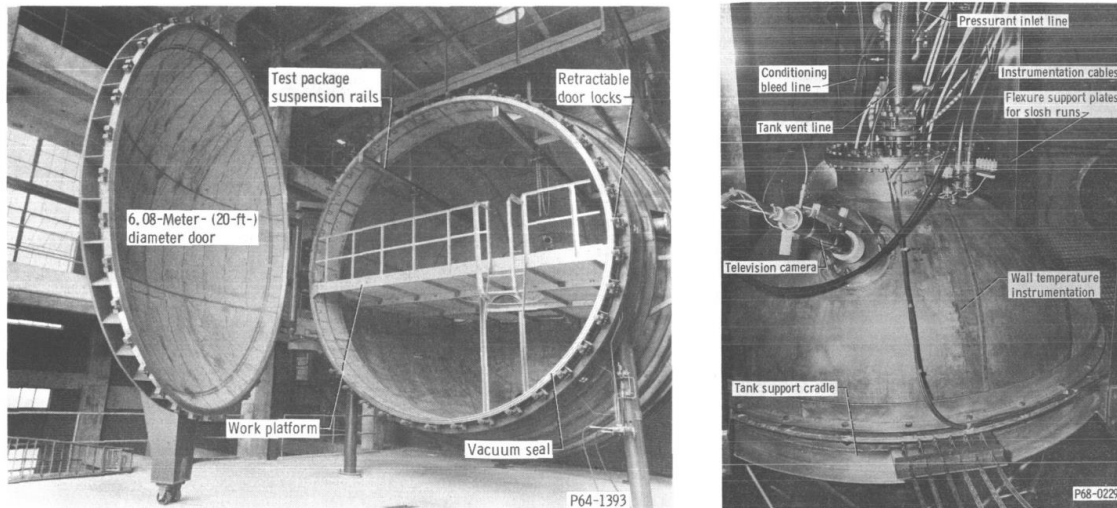


Figure 1. 7.61-meter diameter vacuum chamber and closeup of installed 1.52-meter diameter tank.

The experimental work was conducted using a 1.52-meter - (5-ft -) diameter spherical aluminum tank, as shown in Figure 2. A hemisphere injector (Figure 2 right) was used. This particular geometry was selected because it injects the pressurant uniformly in all directions into the ullage volume.

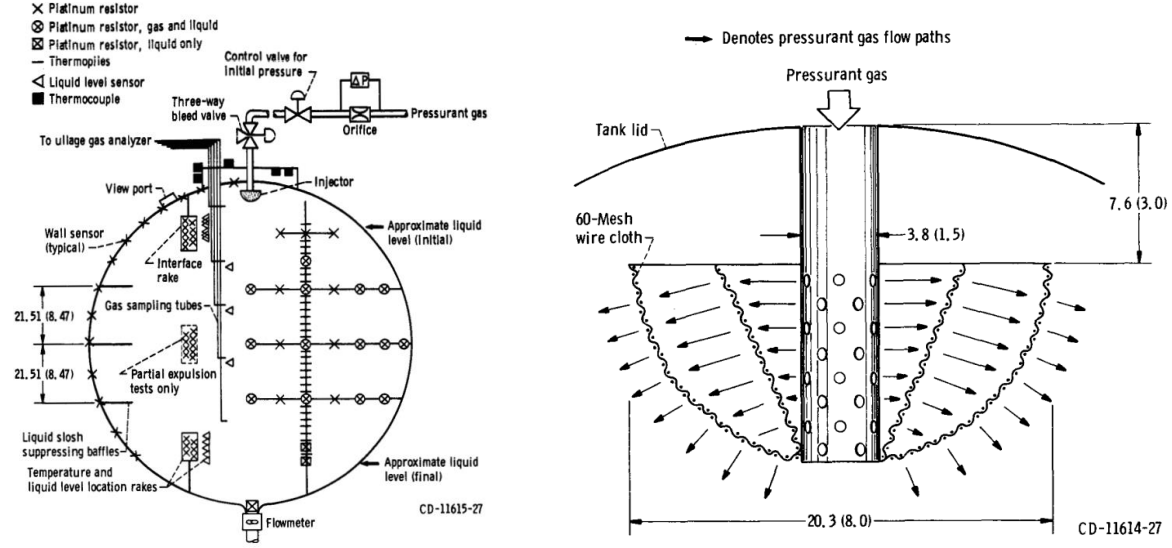


Figure 2. Test tank instrumentation. (in cm (in. )) (left) and injector geometry for hemisphere injector (right).

## 2.2 Computational Tool

The VOF method is a powerful and robust technique for simulating free-surface and gas-liquid interfacial flows such as those encountered in CFM. The geometric algorithms tracking the interface are more accurate than other methods at simulating free-surface flows and allow for simulations with excellent conservation properties when adequately implemented. The Fluid Dynamics Branch (ER42) at Marshall Space Flight Center (MSFC) has developed a VOF module to augment the general-purpose CFD program Loci/STREAM. Loci [5] is a novel software framework that has been applied to the simulation of non-equilibrium flows. The Loci system uses a rule-based approach to automatically assemble the numerical simulation components into a working solver. This technique enhances the flexibility of simulation tools, reducing the complexity of CFD software induced by various boundary conditions, complex geometries, and different physical models. Loci plays a central role in building flexible goal-adaptive algorithms that can quickly match numerical techniques with various physical modeling requirements. Loci/STREAM [6-7] is a pressure-based, all-speed CFD code for generalized grids in the rule-based programming framework Loci. Loci/STREAM uses SIMPLE, SIMPLEC, and PISO algorithms for pressure-momentum coupling and provides various turbulence models which can be executed in Reynolds-Averaged Navier-Stokes (RANS) or Large Eddy Simulation (LES) mode. The coupled simulations between the flow solver and VOF transport are carried out using the Loci/STREAM flow solver and a VOF module developed by CFDRC [8]. The final product, Loci/STREAM-VOF, has been applied to practical rocket propulsion-related VOF applications and has shown significant parallel scalability, up to thousands of CPU cores [9,10]. The VOF solver has been applied to CFM analyses and tank dynamics applications, such as propellant slosh, to extract engineering metrics like slosh frequency and damping that can be used for system-level design and analysis [2,3].

## Governing Equations and Solution Methodology

The governing equations for mass, momentum, and energy implemented in Loci/STREAM-VOF are accompanied by an additional transport equation for the Volume of Fluid (VOF). First, the governing equations for mass, momentum, and energy are:

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_j}{\partial x_j} = 0 \quad (1)$$

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_j u_i}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} + \rho g_i \quad (2)$$

$$\rho c_p \frac{DT}{Dt} - \frac{DP}{Dt} = \frac{\partial}{\partial x_i} \left( k_{eff} \frac{\partial T}{\partial x_i} \right) + \Phi \quad (3)$$

where all the variables are defined in the nomenclature. The above equations are for single-phase fluids. Next, we will discuss the incorporation of two-phase fluids.

### **VOF Module**

To consider the liquid phase, an additional equation for volume fraction,  $F$ , to track the location of the liquid phase is solved in the VOF module. The volume fraction represents the local fraction of the cell volume occupied by the liquid of interest. All cells where the volume fraction is between 0.0 and 1.0 are interface cells in which both fluids and the interface between them exist. The spatial and temporal evolution of the liquid volume fraction is given by the following equation:

$$\frac{\partial F}{\partial t} + u_i \frac{\partial F}{\partial x_i} = 0 \quad (4)$$

where  $u_i$  is the velocity field.

The above equation is nothing but a scalar transport equation; however, the advection of the VOF field using conventional finite-volume discretization techniques is highly diffusive and leads to “smoothing” and destruction of the sharp interface between the gas and liquid. To keep the interface sharp for a very long period of time, the initialization and transport of  $F$  are carried out using purely geometric constructions.

The simulation of two-phase flows with VOF methods consists of three main aspects:

1. VOF initialization, interface construction, and advection of liquid phase;
2. Evaluation of body forces due to gravity and surface tension; and
3. The coupling of body forces and density changes to the solved pressure, momentum, and energy equations.

A detailed description can be found in Reference [8].

### **Coupling between VOF Module and Flow Solver**

For two-phase flow with gas-liquid interfaces, the density is not constant in space, and therefore, the total continuity equation has to be solved. It is given by

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho u) = \frac{\partial \rho}{\partial t} + \sum_s (\rho_f u_f) \cdot n_f = 0. \quad (5)$$

In order to maintain consistency between the VOF module and Loci/STREAM flow solver, appropriate face density values are required. The face densities cannot be modeled with the STREAM implementation, which uses inverse distance weighted values from the cell centers. Instead, a new implementation of the face densities was introduced as

$$\rho_f = \frac{\rho_g V_g + \rho_l V_l}{V_g + V_l} \quad (6)$$

where  $V_g$  and  $V_l$  denote the gas-volume and liquid-volume fluxes across the face at a given time step. This approach is expected to provide a consistent formulation between the explicit VOF advection and the implicit STREAM time-step advances.

STREAM utilizes the cell densities based on the advected VOF and the new face densities. This provides it with the information to calculate mass fluxes into and out of each cell to solve the pressure correction and then the momentum equations.

Based on the previous work by Lowry and Yang [11], the formulation for the pressure correction equation was modified so that it uses  $\ln(\rho)$  for the source term of the  $p'$  equation as recommended by Pericleous *et al.* [12] using a total derivative form of  $\ln(\rho)$  for free surface problems as shown below:

$$\frac{D(\ln \rho)}{Dt} + \nabla \cdot u = 0. \quad (7)$$

### **Energy Conservation Equation Modifications**

Regardless of the liquid or gas phase, the original energy conservation equation is derived based on total energy conservation:

$$\rho \frac{De}{Dt} - \nabla k \nabla T - \Phi + p \nabla \cdot \mathbf{u} = 0. \quad (8)$$

The first term represents the internal energy increase, the second is heat conduction, the third term is dissipation, and the fourth term is the pressure work. The internal energy can be expanded as follows:

$$e = h - \frac{p}{\rho} \quad (9)$$

with the use of equations (8) and (5), we have:

$$\rho \frac{Dh}{Dt} - \frac{Dp}{Dt} - \nabla k \nabla T - \Phi = 0. \quad (10)$$

Using the thermodynamic relation, we have:

$$dh = \left( \frac{\partial h}{\partial T} \right)_p dT + \left( \frac{\partial h}{\partial p} \right)_T dp = c_p dT + \frac{1}{\rho} (1 - \beta T) dp. \quad (11)$$

For an ideal gas,  $\beta T = 1$ , and  $dh = c_p dT$ . Combining equations (10) and (11), one gets:

$$\rho c_p \frac{DT}{Dt} - \beta T \frac{Dp}{Dt} - \nabla k \nabla T - \Phi = 0. \quad (12)$$

In comparison to the gas phase energy equation, the difference is the  $Dp/Dt$  coefficient. Combining the gas phase ( $g$ ) and liquid phase ( $l$ ) equations and weighting by the VOF volume fraction, one gets:

$$(1 - F) \left( \rho c_p \frac{DT}{Dt} - \frac{Dp}{Dt} - \nabla k \nabla T - \Phi \right)_g + F \left( \rho c_p \frac{DT}{Dt} - \beta T \frac{Dp}{Dt} - \nabla k \nabla T - \Phi \right)_l = 0. \quad (13)$$

After rearranging, the final equation becomes:

$$\left[ (1 - F)(\rho c_p)_g + F(\rho c_p)_l \right] \frac{DT}{Dt} - [1 - F + F(\beta T)_l] \frac{Dp}{Dt} - \nabla k \nabla T - \Phi = 0. \quad (14)$$

### **Mass Transfer Rate**

The mass transfer rate between the gas and liquid phase,  $\dot{m}$ , is based on the kinetic theory of the Hertz-Knudsen equation,

$$\dot{m} = C_m \left( \frac{1}{2\pi R_g T_{in}} \right)^{1/2} (p_{sat} - p_g) A_{in}. \quad (15)$$

where  $\dot{m}$  is mass evaporation rate in kg/s,  $C_m$  is the mass transfer coefficient that lies between 0 and 1,  $R_g$  is the gas constant,  $T_{in}$  is the interfacial temperature,  $p_{sat}$  is the saturation pressure based on the interfacial temperature, and  $p_g$  is the gas phase pressure. The Clausius-Clapeyron or Antoine equation can be used to compute the saturation pressure based on the local temperature. The Antoine equation is given by:

$$\log_{10}(P) = A - \frac{B}{T+C}. \quad (16)$$

where  $P$  is vapor pressure (bar), and  $T$  temperature (K). For methane the constants in Equation (16) are:  $A=3.9895$ ,  $B=443.028$ , and  $C=-0.49$ . The mass flux in Equation (15) is subtracted from the liquid phase equation (VOF equation) and is added to the condensable gas species equation. The associated latent heat ( $\dot{m}L$ ) is added to the gas phase energy and subtracted from liquid energy.

### 2.3 Simulation Model

Our simulation model and mesh are given in Figure 3, with an isometric view of the volume and a cross-section of the mesh. There are a total of 3.27 million hexahedral cells covering the half-sphere (Figure 3(b)). In order to include the heat conduction within the solid wall a separate, coincident mesh representing the thin aluminum tank wall is also included. A butterfly mesh is used to keep uniform cell size and orthogonality (Figure 3(c)). In the interface and ullage region, the mesh size is between 2 mm and 3 mm. For the case of a static tank (without slosh), the flow is axisymmetric, and to save computing time, a one-degree wedge with one cell in the azimuthal direction, shown in Figure 3(d), is used.

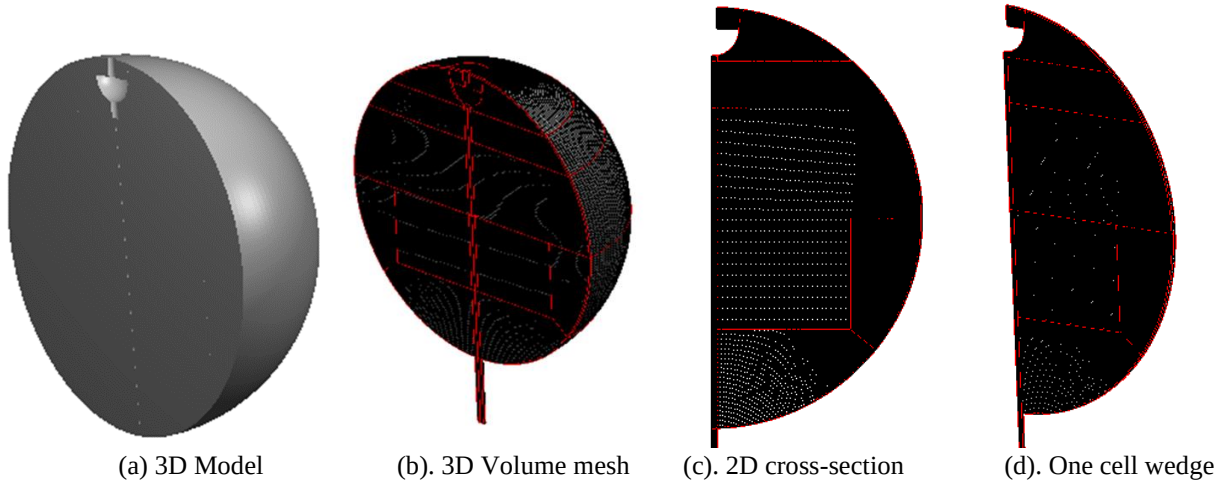


Figure 3. CFD simulation model and mesh. (a). 3D model; (b). 3D mesh for the case with slosh; (c). 2D cross-sectional view; (d). One-degree wedge mesh for the case without slosh.

### 2.4 Boundary Conditions

The applied boundary conditions are such that all the walls are non-slip and adiabatic. The diffuser inlet is specified either as a fixed pressure boundary condition or a fixed mass flow rate based on the experimental condition. During the draining, the outlet boundary is specified as the fixed mass flow rate.

### 2.5 Initial Conditions

During the experiment [4], The spherical tank was filled from the bottom to approximately a 2 percent ullage condition. The temperature control circuit was used to get the desired pressurant gas temperature level during the flow period. The liquid level in the tank was adjusted to a desired value (~ 5 percent ullage) by either topping or slow draining. Then the tank was pressurized over a predetermined time period to the nominal operating pressure of  $3.447 \times 10^5$  newtons per square meter (50 psia). Tank pressure was held constant for almost 24 seconds to stabilize internal temperatures. The tank expulsion period was then started. As such, our initial condition starts with cold liquid and gas temperature with a liquid fill level of 95%, as shown on the left in Figure 4 (a).

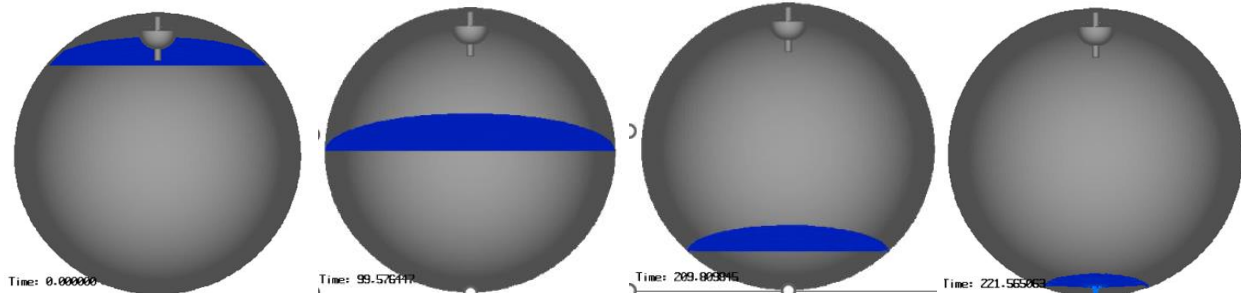


Figure 4. CFD simulation model for tank draining. Left: the initial liquid level. Right: the final stage with gas ingestion.

## 2.6 Fluid/Material Properties

Fluid and material properties were extracted from the National Institute of Standards and Technology (NIST) databases [16]. The liquid-related properties and solid conduction properties are listed in Table 1. The gas properties are taken from the existing thermodynamic table in Loci/STREAM.

Table 1. Thermodynamic Properties of Methane Used in the Simulation.

| Parameters | Description                               | Value                          |
|------------|-------------------------------------------|--------------------------------|
| $\rho_l$   | Liquid density                            | 421.14 kg/m <sup>3</sup>       |
| $(c_p)_l$  | Liquid-specific heat at constant pressure | 3487.2 J/Kg-K                  |
| $k_l$      | Liquid thermal conductivity               | 0.18254 W/m-K                  |
| $\mu_l$    | Liquid dynamic viscosity                  | 1.1478x10 <sup>-4</sup> Kg/m-s |
| $\beta$    | Liquid volume expansion coefficient       | 0.0168 /K                      |
| L          | Latent heat                               | 5.0933x10 <sup>5</sup> J/kg    |
| $\sigma$   | Surface tension                           | 0.001270 N/m                   |
| $\rho_s$   | Solid density                             | 1200 kg/m <sup>3</sup>         |
| $(c_p)_s$  | Solid-specific heat at constant pressure  | 400.0 J/Kg-K                   |
| $k_s$      | Solid thermal conductivity                | 0.14 W/m-K                     |

## 2.7 Physics Models and Simulation Options

As the liquid density is assumed to be constant, the buoyancy force in the liquid phase is taken into account by the Boussinesq approximation. The liquid density is considered as a linear function of temperature in the gravity term:

$$F_g = \rho_l g - \rho_{ref} g = [\rho_{ref} - \beta_l \rho_{ref} T - \rho_{ref}] g = -\beta_l \rho_{ref} T. \quad (17)$$

Both laminar flow and turbulence models are evaluated. Two turbulence models are applied: the k- $\omega$  shear stress transport model (k- $\omega$ -SST) and the k- $\omega$ -SST Delayed Detached Eddy Simulation (DDES).

The initial time step size for the simulation was set to dt=1e-2 sec. for all cases. For the calculation of a stable time step for the VOF module, a CFL number of 0.1 was chosen.

## III. RESULTS

In the following, the simulation efforts for the validation of Loci/STREAM-VOF with the K-site slosh and drain experiment [4] are discussed. A baseline model case for the test denoted as Run 10 is presented first for the ramp and hold phases. After that, analysis of draining of a static tank without sloshing is presented for different expulsion rates and pressurant inlet temperatures. Finally, an assessment of the effect of sloshing is presented for a non-baffled tank configuration.

### 3.1 Validation of Ramp and Hold Phases of Run 10

The simulation details and model parameters based on experimental conditions for Run 10 of the experiment [4] are:

- The pressure ramp at the inlet was from 1.035x10<sup>5</sup> to 3.37x10<sup>5</sup> (N/m<sup>2</sup>) within the first 34 seconds;
- Constant pressure of 3.37x10<sup>5</sup> N/m<sup>2</sup> during hold (from 34s to 58s) and liquid expulsion;
- Constant temperature at the inlet (344K);
- Antoine Equation for the calculation of saturation conditions;
- Mass transfer coefficient  $c_m=1.0e-3$  for the Hertz-Knudsen model;
- k- $\omega$  SST DDES turbulence model; and
- Conjugate heat transfer activated only for sensitivity study.

The use of mass transfer coefficient  $c_m=1.0e-3$  and  $k-\omega$  SST DDES model is based on our previous experience with the propellant tank self-pressurization study [3-4]. The sensitivity to the simulation parameters and models is investigated during the study.

#### *Inlet as Time Dependent Pressure Condition*

First, we can consider the inlet as a prescribed linearly ramping pressure condition. The ramp rate is from  $1.035 \times 10^5$  N/m<sup>2</sup> to  $3.37 \times 10^5$  N/m<sup>2</sup> within 34 seconds. Figure 5 shows the VOF during the ramp (left) and temperature distributions at the end of the ramp and hold phases. One can see that after the ramp period, the ullage is very much filled with the hot gas from the diffuser, and it appears that there is negligible change in the temperature distribution during the hold phase. At the end of the hold phase, the liquid temperature at the interface reaches the thermodynamic equilibrium temperature of 130K, corresponding to an ullage pressure of  $3.37 \times 10^5$  N/m<sup>2</sup>. On the right of Figure 5 is the temperature distribution limited to the maximum saturation temperature at the hold pressure. Clearly, there is a thermal stratification layer inside the liquid at the interface.

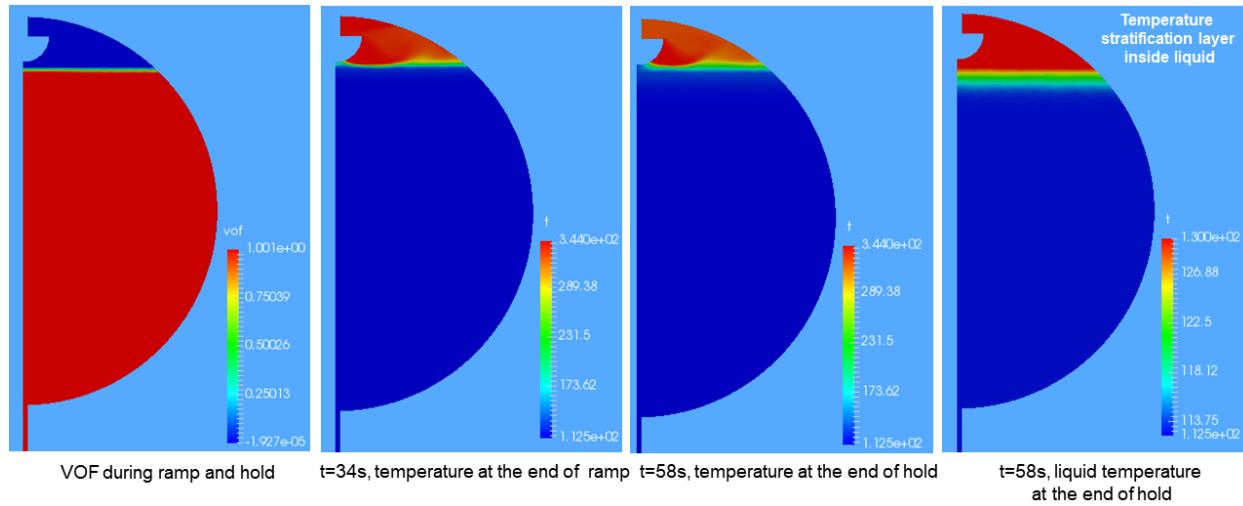


Figure 5. Temperature distribution of the ullage and in the top portion of the liquid during the initial ramp, at the end of pressure ramp, and at the end of pressure hold from the inlet diffuser.

Figure 6 shows the pressure variation during the ramp phase and hold phase from this CFD simulation. Here, a linear increase in pressure is assumed. The corresponding mass flow rate at the inlet due to the pressurization is also given. Except at the beginning, the mass flow rate increases linearly with time. After the hold, the mass flow rate reduces and approaches a small value, implying a near-equilibrium state at the gas-liquid interface.

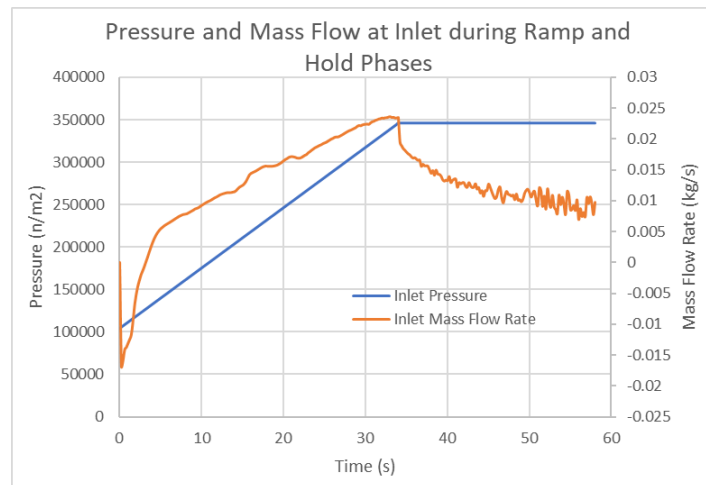


Figure 6. Pressure and mass flow rate at the diffuser inlet during ramp and hold phases.

Table 2 compares the experimental measurement and CFD simulation in terms of the initial mass, mass added from the inlet, and the mass transferred from the gas-liquid interface. The table shows that CFD predicts the mass added and mass transferred reasonably well in comparison with the experimental measurement.

Table 2. Comparison of CFD and experiment [4] on various masses.

|                   | Ramp Phase (34 seconds) |                 |                       |
|-------------------|-------------------------|-----------------|-----------------------|
|                   | Initial Mass (kg)       | Mass Added (kg) | Mass Transferred (kg) |
| <b>Experiment</b> | <b>0.153</b>            | <b>0.503</b>    | <b>0.361</b>          |
| <b>CFD</b>        | <b>0.151</b>            | <b>0.472</b>    | <b>0.417</b>          |

#### Inlet as Prescribed Mass Flow Rate Condition

As the total mass added from the inlet is given from the experiment during the ramp, another way of specifying the inlet boundary condition is to use a prescribed mass flow rate. Here, we can assume the mass flow rate is constant during the ramp. This inlet condition is simulated for two different mass transfer coefficients ( $c_m=1.0e-3$  and  $c_m=1.0e-4$ ) and for two different mesh resolutions. The results are given in Figure 7. A good match from the CFD against the experiment value at the end of the ramp phase is observed. Mass transfer coefficient sensitivity was also studied for a lower value of  $c_m=1.0e-4$ . Even with a drop in mass transfer coefficient by one order of magnitude, the pressure trace is consistent, showing the insensitivity to the use of  $c_m=1.0e-3$  in this study. When the mesh resolution is reduced by 25%, some variations of pressure during the transient process are observed, but at the end of the ramp phase, the predicted pressure agrees well with the experiment.

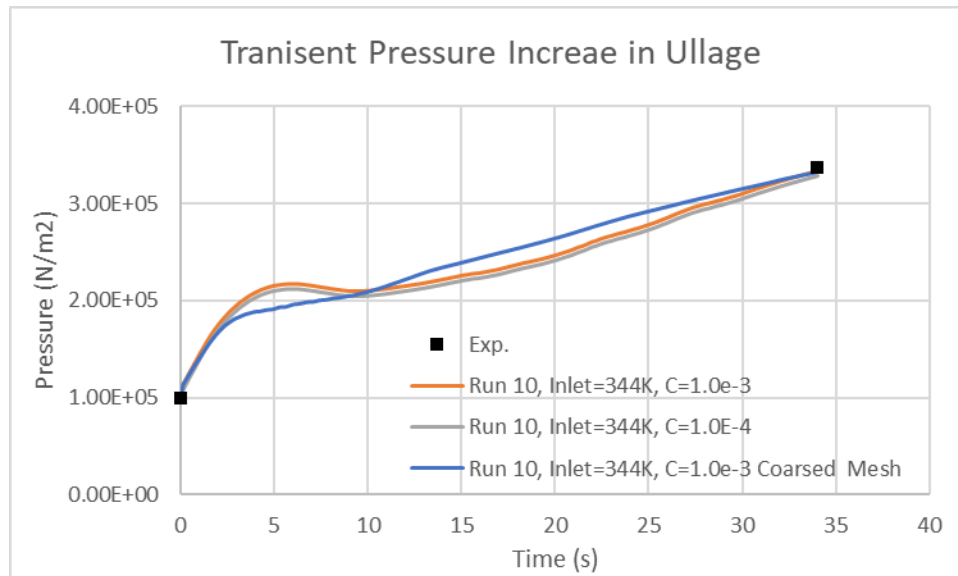


Figure 7. The sensitivity of mesh density and mass transfer coefficient on the pressure increases in ullage due to the prescribed mass flow rate at the diffuser inlet.

### 3.2 Validation of Pressurant Mass Requirement during Static Expulsion of Run 10

The simulation for the above ramp and hold continued with the outlet at the bottom of the tank specified as a prescribed mass flow rate boundary condition. For Run 10, there was no slosh, and the expulsion time was 410 seconds (468 seconds from the start of the ramp). When the desired final propellant level in the tank, which was specified as 5% liquid in the experiment, was reached, the expulsion was terminated. Figure 8 shows the computed and measured mass flow rate during the expulsion. In general, good agreement between the prediction and measurement is observed. The fluid dynamics of liquid during the expulsion are shown in Figure 9. The interface velocity during draining can be seen.

The pressurant mass requirement during the expulsion can be obtained by integrating the inlet mass flow rate of Figure 8. The integration result is listed in Table 3, along with the experimental data. The agreement between CFD and the experiment is considered good. The deviation for the total pressurant mass during the expulsion is 2.88 percent.

The CFD simulation sensitivities to the mass transfer coefficient and the use of a laminar or turbulence model have also been investigated. Figure 10 shows the inlet mass during the expulsion. From the experiment, since only the final total mass is given, the linear increase in the mass is assumed for reference purposes. At the end of the expulsion, the total added masses for different mass transfer coefficients are listed on the right of Figure 10. One can see that for a variation of two orders-of-magnitude in mass transfer coefficient (from  $1.0\text{e-}4$  to  $1.0\text{e-}2$ ), the predicted total mass requirements are within 10% of the experimental value.

The same simulations of varied mass transfer coefficients using a laminar model are shown in Figure 11. Again, agreements between CFD and simulation are reasonably good, considering that the mass transfer coefficient varied for two orders of magnitude. In general,  $c_m=1.0\text{e-}3$  gives consistently good results, while the  $k-\omega$  SST DDES model predicts slightly more mass (2.8%), and the laminar model gives slightly less mass (- 7.3%). Based on the above study, we will use the  $k-\omega$  SST DDES model and  $c_m=1.0\text{e-}3$  for the rest of the simulations.

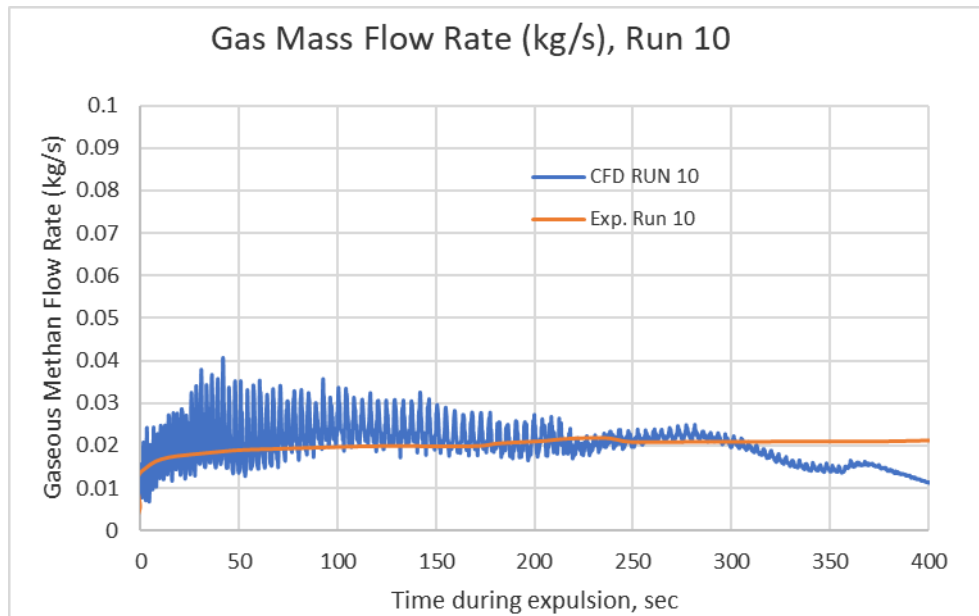


Figure 8. Computed and measured mass flow rate at diffuser inlet during expulsion for Run 10.

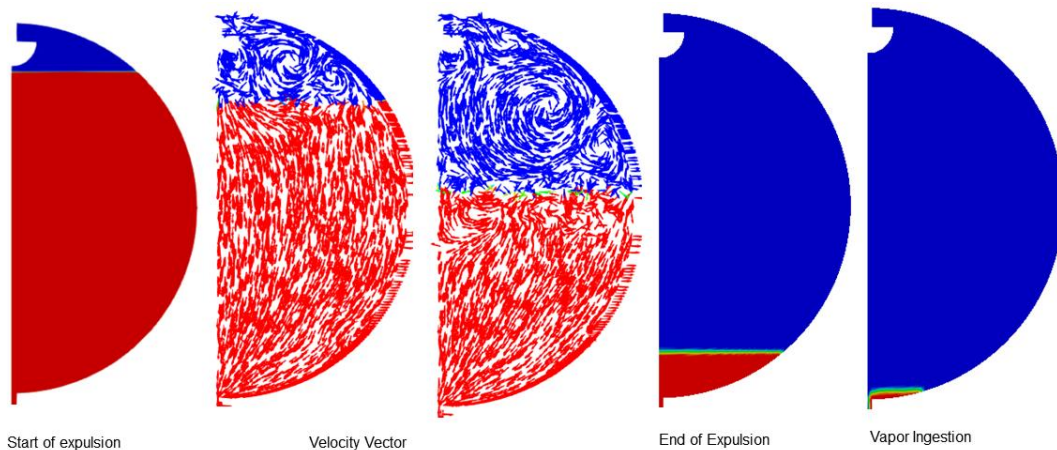
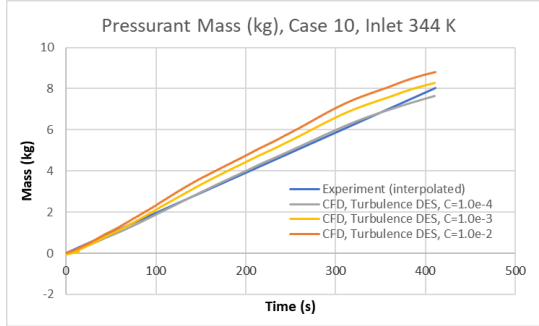


Figure 9. Flow field during the expulsion for Run 10.

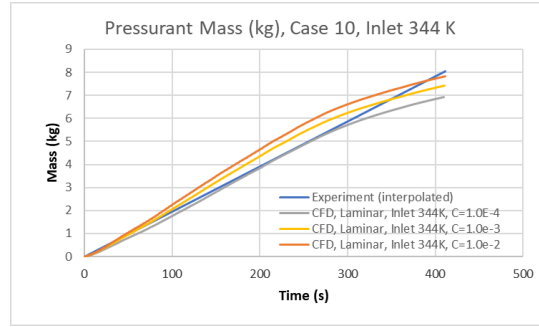
Table 3. Comparison of mass added during the expulsion.

| DDES Model<br>( $C=1.0e-3$ ), Inlet<br>344K | Expulsion Time<br>(s) | Mass<br>Added (kg) | % Error in<br>Mass |
|---------------------------------------------|-----------------------|--------------------|--------------------|
| Exp. Run 10                                 | 410                   | 8.03               |                    |
| CFD Run 10                                  | 410                   | 8.26               | 2.88%              |



| K- $\omega$ SST DDES Model | Final<br>Pressure | Mass Added<br>(kg) | % Error in<br>pressure |
|----------------------------|-------------------|--------------------|------------------------|
| Exp. #10 (Inlet 334 K)     | 3.44E5            | 8.028              |                        |
| CFD 344K, $C_m=1.0e-4$     | 3.44E5            | 7.628              | -4.9%                  |
| CFD 344K, $C_m=1.0e-3$     | 3.44E5            | 8.254              | 2.8%                   |
| CFD 344K, $C_m=1.0e-2$     | 3.44E5            | 8.787              | 9.45%                  |

Figure 10. Pressurant requirement sensitivity to the mass transfer coefficient with  $k-\omega$  SST DDES model.



| Laminar Model          | Final<br>Pressure | Mass Added<br>(kg) | % Error in<br>pressure |
|------------------------|-------------------|--------------------|------------------------|
| Exp. #10 (Inlet 334 K) | 3.44E5            | 8.028              |                        |
| CFD 344K, $C=1.0e-4$   | 3.44E5            | 6.930              | -13.6%                 |
| CFD 344K, $C=1.0e-3$   | 3.44E5            | 7.408              | -7.72%                 |
| CFD 344K, $C=1.0e-2$   | 3.44E5            | 7.836              | -2.39%                 |

Figure 11. Pressurant requirement sensitivity to the mass transfer coefficient with laminar flow model.

### 3.3 Validation of Pressurant Mass Requirement during Static Expulsion of Runs 9 and 11

The expulsion runs 9 and 11 in the experiment [4] have the same inlet temperature and similar ramp and hold timing. The difference is the expulsion time. For Run 9, the expulsion time is 637 seconds, and for Run 11, it is 233 seconds. The simulated inlet mass for each case and comparisons to experimental values, assuming a linear variation, are shown in Figure 12. Experimental measurements indicated that the pressurant mass required increases with the expulsion time because it allows more time for mass transfer at the interface. This physics is well captured by the present simulation. By the end of expulsion, the predicted masses for different runs are in good agreement with measurement. The errors, as listed in Table 4, are within 7% for all three expulsion times.

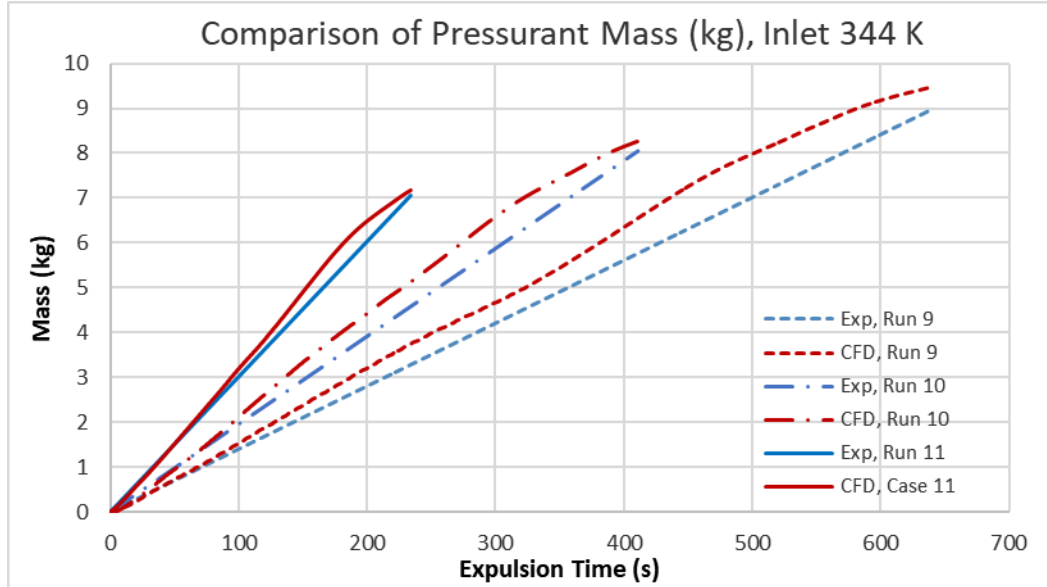


Figure 12. Total from mass at different times during expulsion for Runs 9, 10, and 11.

Table 4. Comparison of mass added for different expulsion time runs.

| DDES Model<br>( $C=1.0e-3$ ), Inlet 344K | Expulsion Time<br>(s) | Mass Added<br>(kg) | % Error in<br>Mass |
|------------------------------------------|-----------------------|--------------------|--------------------|
| Exp. Run 11                              | 233                   | 7.03               |                    |
| CFD Run 11                               | 233                   | 7.17               | 1.99%              |
| Exp. Run 10                              | 410                   | 8.03               |                    |
| CFD Run 10                               | 410                   | 8.26               | 2.88%              |
| Exp. Run 9                               | 637                   | 8.95               |                    |
| CFD Run 9                                | 637                   | 9.49               | 6.03%              |

### 3.4 Validation of Pressurant Mass Requirement during Static Expulsion at Different Inlet Temperature

In the experimental work of Reference [4], the complete tank expulsions were made using GCH<sub>4</sub>, GHe, GH<sub>2</sub>, and GN<sub>2</sub> pressurants. The test parameters were inlet gas temperature and expulsion time. To explore the effect of inlet temperature, the test Runs of 6, 7, and 8 are also simulated where the inlet temperature was lower, at 222K. The results and comparison to the experiment are given in Figure 13. In general, for a given inlet temperature, there is an increasing pressurant requirement for increasing expulsion time. On the other hand, the lower inlet temperature leads to higher pressurant mass requirements as the ullage is occupied by the inlet gas at its own temperature. For fixed ullage pressure, lower gaseous temperature means higher gas density and a higher amount of gaseous mass to occupy the ullage. For the lower inlet temperature case of 222K, the simulation slightly underpredicts the gas requirement, while for the higher temperature case of 344K, the simulation slightly overpredicts, but all agree with the experiment well.

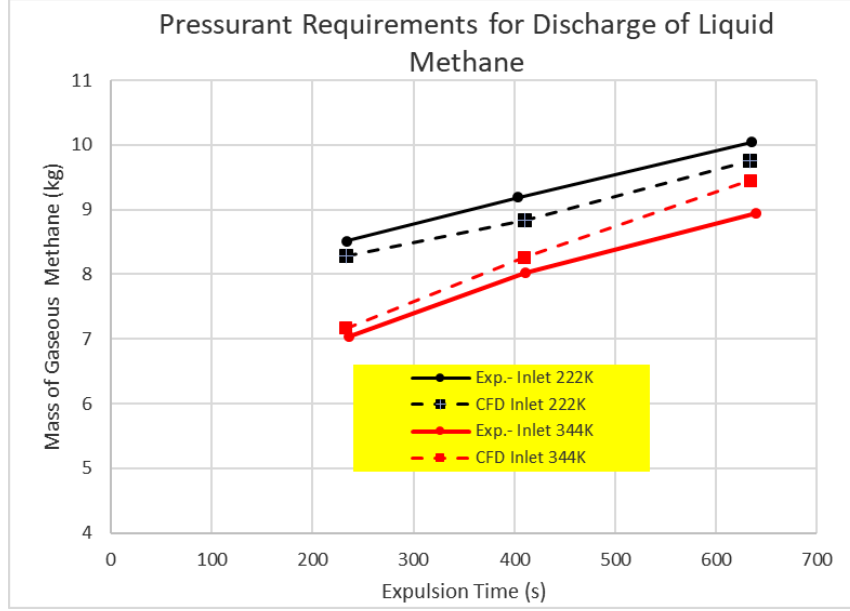


Figure 13. Total gaseous methane requirement for different expulsion times and different inlet temperatures.

### 3.5 Validation of Pressurant Mass Requirement For Slosh Expulsion of Run 29 in Unbaffled Tank

Expulsion tests including slosh in an unbaffled tank were conducted by DeWitt and McIntire [4] while the tank was being oscillated at an amplitude of 0.0223m and at a frequency corresponding to the natural frequency of the liquid remaining in the tank. Starting at the beginning of expulsion, the slosh amplitude was increased linearly from 0.0 to 0.0223m over approximately a 60-second time period. The purpose of the ramped amplitude was to allow the development of the slosh motion without a sudden loss of tank pressure at the beginning of expulsion. Excessive liquid propellant splashing resulted if the full slosh amplitude was imposed on the tank immediately at the start of expulsion. This splashing resulted in excessive cooling of the ullage gas and a drop-off in the tank pressure.

To simulate this slosh expulsion, we first validated the slosh frequency from our VOF model. At the selected liquid fill heights of 83%, 50%, and 33%, the equilibrium flat liquid surface is given a small perturbation in the slope, as shown in Figure 14. With this state as the initial condition, the simulation starts without any expulsion. The mass center displacement, which shows sinusoidal oscillation, is then monitored. The oscillation frequency is the sloshing frequency for that particular liquid fill height. To compare to experimental data, a slosh frequency parameter is defined as:

$$\sqrt{\lambda} = 2\pi f \sqrt{\frac{R}{g}} \quad (18)$$

This parameter is plotted in Figure 15, which shows excellent agreement with the experimental values of Reference [13]. The above curve is then fitted as an analytical function to enable the driving frequency to correspond to the natural frequency of the liquid remaining in the tank. The tank motion acceleration is imposed by a body force in the non-inertial frame added to the VOF momentum equation.

Figure 16 shows the VOF iso-surface of 0.5 and the temperature distribution in the center plane of the tank during the propellant expulsion. In comparison to the case without the slosh of Run 10 (see Figure 9), the interface is no longer flat but rather shows the waveforms. Figure 17 is the lateral displacement of the liquid mass center, which corresponds to the amplitude of the slosh during the expulsion from this CFD simulation. One can see that the oscillation amplitude of the mass center (the slosh amplitude) increases with time after the expulsion starts, which is also the time the tank is driven at its own natural slosh frequency. However, the resonance does not occur until at a later time of about 50 seconds. The oscillation amplitude then decays and then starts to increase again, leading to another resonance at about 80 seconds. It is interesting to see that rather than at continuous frequencies, slosh resonates at discrete frequencies. Figure 16 also shows the temperature distribution during the slosh. In addition to the increased surface area, the slosh causes the distortion of the temperature gradient in both gas and liquid phases. As a result, the mass transfer between the gas-liquid interface is expected to increase.

The experimental mass flow rate from the diffuser and the simulated one are given in Figure 18. Again, from the mass flow rate, one notices that while the tank is driven at the natural frequency of the remaining liquid in the tank, the slosh resonance does not occur all the time but rather in several instances. For example, one can count six peaks on the mass flow rate for the first 170 seconds of the experiment. Our simulation shows a similar number of peaks. Our first peak does not have as high of a value as observed in the experiment, but the second, third, and fourth peaks all match with the experiment well in the timing and the peak value. Even though some discrepancies in the flow rate value are observed at a later time, the time-dependent trends between CFD and the experiment are very similar.

The comparison of time-integrated masses at the inlet during expulsion from the experiment and from this simulation is given in Figure 19. In general, the simulation follows the correct trend observed from the experiment: much higher mass requirement when slosh is present. Quantitatively, the predicted pressurant mass requirement is within 20% of the experimental value.

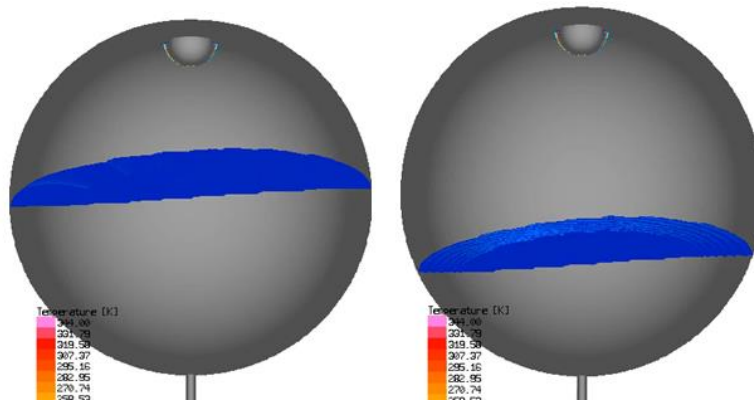


Figure 14. Initial liquid position at two fill levels to determine the sloshing frequency.

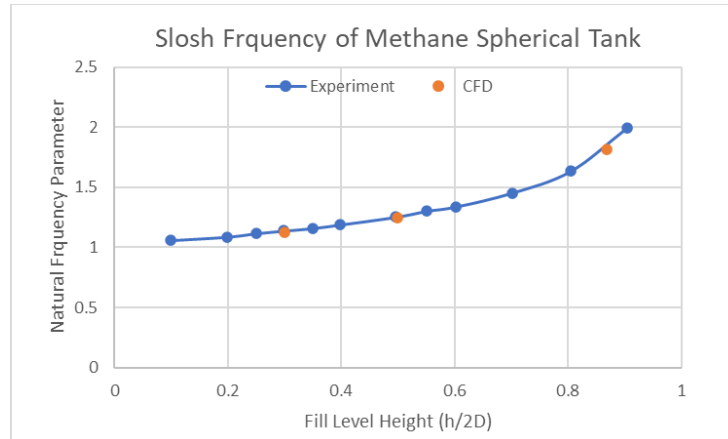


Figure 15. Comparison of slosh frequency from the simulation at selected fill heights with experiment [13]

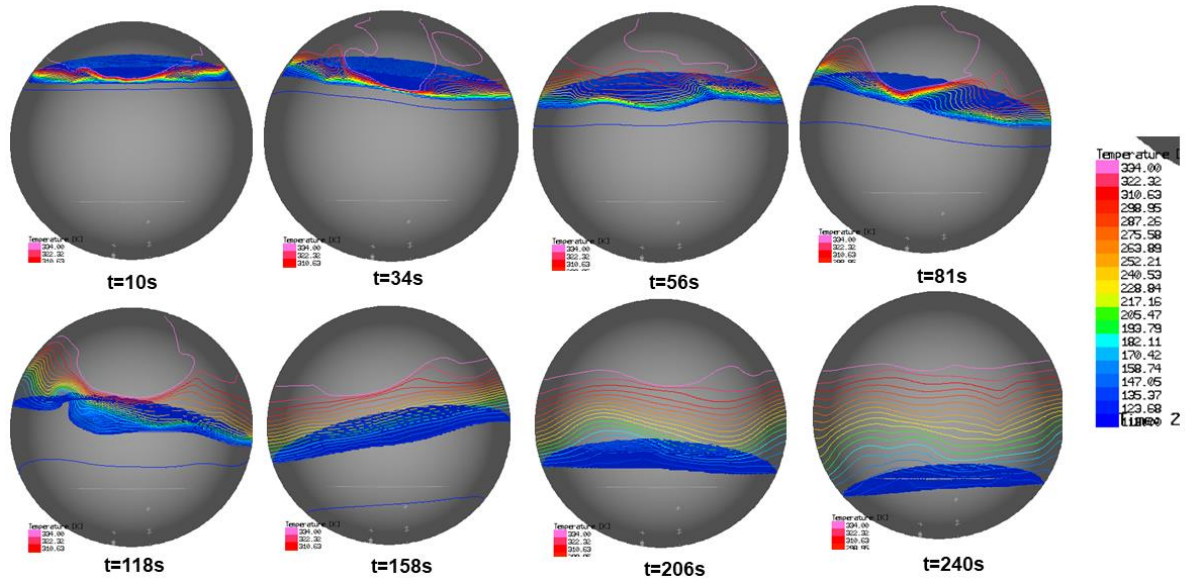


Figure 16. VOF and temperature field inside the tank during slosh expulsion for Run 29.

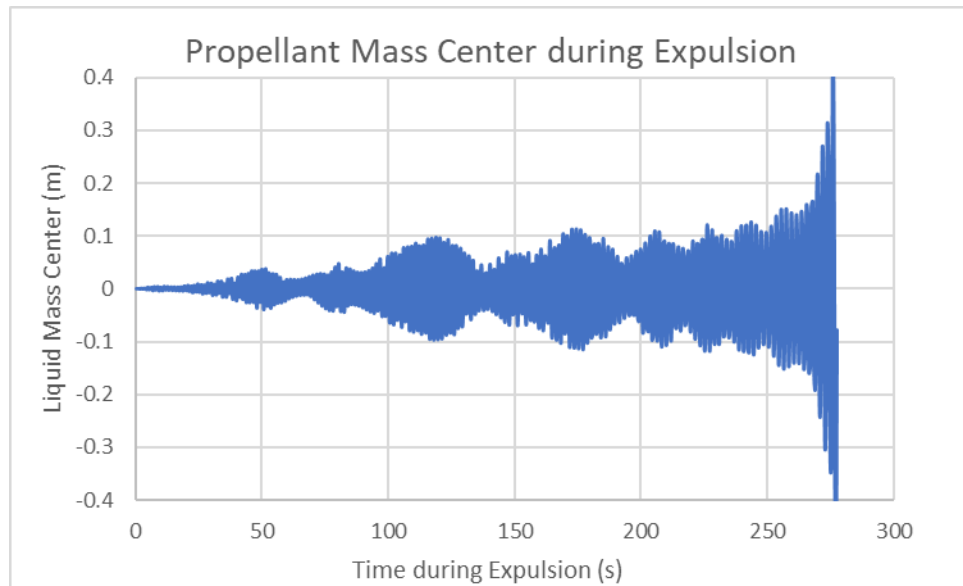


Figure 17. Propellant mass center lateral displacement during expulsion due to tank slosh.

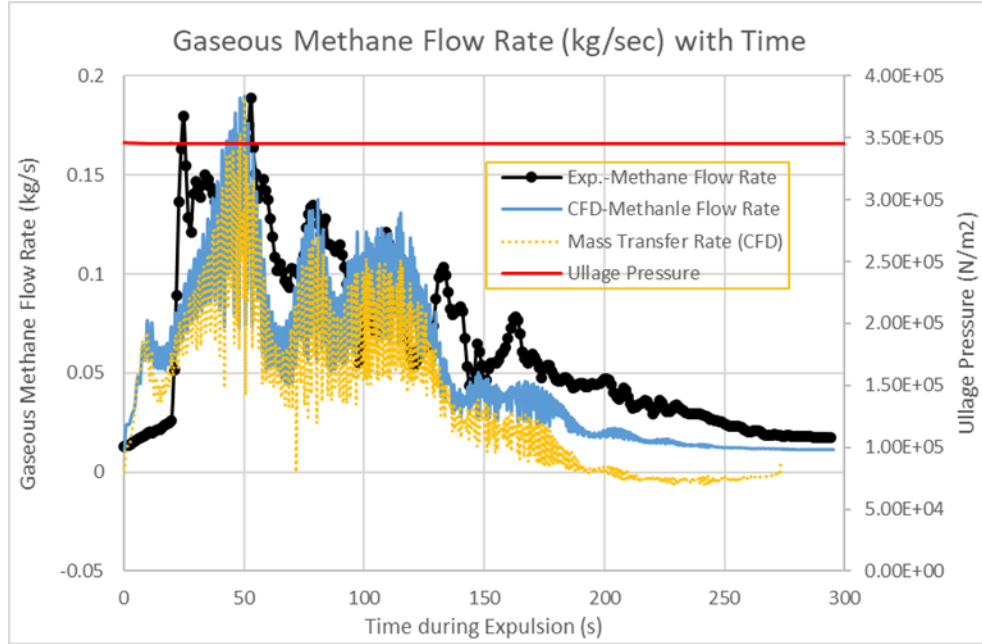


Figure 18. Gaseous methane flow rate with time for slosh expulsion Run 29.

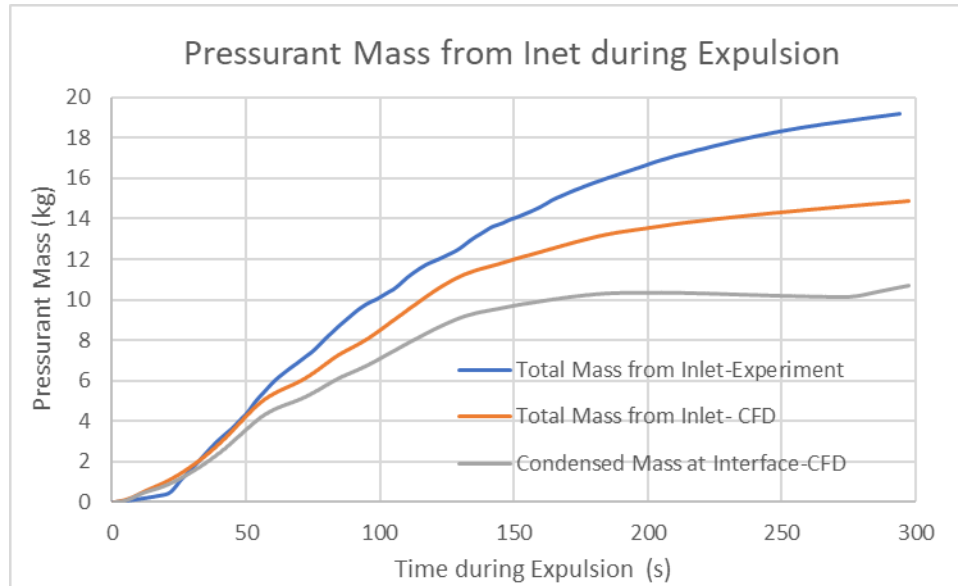


Figure 19. Comparison of pressurant mass requirement during expulsion with slosh.

#### IV. Conclusion

This paper documents a model validation effort for the prediction of cryogenic propellant tanks under static and slosh expulsions using the Loci/STREAM-VOF two-phase CFD code developed at NASA MSFC. In the past, the MSFC Propulsion Fluid Dynamics Branch has validated and used the Loci/STREAM-VOF code extensively for propellant slosh applications, which are dominated by fluid motion. CFM applications require accurate modeling of heat transfer and thermodynamics. Therefore, detailed validation of those physics is essential to ensure simulation accuracy and success. For the present study, Loci/STREAM-VOF simulations were compared with data from NASA K-site experiments on pressurant requirements for the discharge of liquid methane from a 1.52-meter diameter spherical tank under both static and slosh conditions. This study investigated several parametric sensitivities and made several comparisons with experimental measurements.

- The sensitivity of the mass transfer coefficient on the pressurant requirement in the Hertz-Knudsen model has been investigated for the initial pressure ramp phase and the static tank expulsion. A previous baseline value of  $c_m=1.0e-3$  for CFM tank self-pressurization [3] and for ullage collapse [4] is found to be adequate for tank expulsion. Even with the change of two orders of magnitude from  $c_m=1.0e-4$  to  $c_m=1.0e-2$ , the resulting change in inlet mass is within 10% of the experimental data for the ramp phase and for the static tank expulsion phase.
- CFD predictions for the pressurant mass requirements compare well with the experiment measurement under the ramp phase. CFD simulation also shows a consistent trend of increased inlet mass with increased expulsion time during the expulsion phase. For a lower inlet temperature, the mass requirement increases, as seen from the experiment. The quality comparisons are all very good, typically within 10% of the experimental value.
- The hybrid RANS-LES  $k-\omega$  SST DDES model has been used and gives a consistent trend with the experiment.
- For the tank expulsion simulation with slosh, our preliminary results show a significant increase in the pressurant mass requirement, as found in the experiment. When driven at the resonant frequency corresponding to the remaining liquid in the tank, the slosh responds at discrete rather than continuous frequencies, which is consistent with the experiment. The comparison between this simulation and the experiment for the pressurant mass requirement is within 20%.

Based on these results, the Loci/STREM-VOF model is expected to provide accurate predictions for tank expulsion under static and slosh conditions when following the recommended simulation methodology from the above observations. More validation efforts are underway for other pressurant fluids and other tank-driving conditions.

### Acknowledgments

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