Effect of Interfacial Turbulence and Accommodation Coefficient on CFD Predictions of Pressurization and Pressure Control in Cryogenic Storage Tank

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Background

- NASA has identified cryogenic storage & transfer as an area with greatest potential for cost saving.
- Zero-Boil-Off (ZBO) or Reduced Boil-Off (RBO) dynamic storage tank pressure control that involves some mode of mixing of the bulk liquid with or without active or passive cooling is needed to realize cost savings.
- Optimization of ZBO or RBO tank design for microgravity applications will most probably be accomplished with only ground-testing due to budgetary constraint.
- State-of-the-Art validated storage tank CFD models will play an crucial role in extrapolation of the 1g tested storage tank design to microgravity and partial gravity applications.
- Correct implementation of Interfacial & bulk turbulence and evaporative condensing mass transfer is crucial for the fidelity and validity of the CFD models.
Fundamental Multiphase Science Issues

- Natural Convect (turbulence)
- Forced Mixing (turbulence)
- Evaporation Condensation
- Microgravity Superheats
- Non-Condensable Gases
- Transport Barrier
- Marangoni Convection
- Interfacial Kinetics
- Free Surface Dynamics
- Contact Angle Dynamics
- Sloshing/Droplet Transport
- Phase Control/Positioning
Two-Phase Sharp Interface Storage Tank CFD Model

<table>
<thead>
<tr>
<th>Equation</th>
<th>Liquid</th>
<th>Ullage</th>
</tr>
</thead>
<tbody>
<tr>
<td>Continuity</td>
<td>√</td>
<td>√</td>
</tr>
<tr>
<td>Navier Stokes</td>
<td>√</td>
<td>√</td>
</tr>
<tr>
<td>Energy</td>
<td>√</td>
<td>√</td>
</tr>
<tr>
<td>Turbulence (k-ω SST)</td>
<td>√</td>
<td>√</td>
</tr>
</tbody>
</table>

Interfacial Energy Balance:

\[ LJ_v = -k_l \nabla T_l \cdot \hat{n} + k \cdot \nabla T \cdot \hat{n} \]

Schrage Interfacial Mass Transfer:

\[ J_v = \frac{2\sigma}{2 - \sigma} \frac{1}{\sqrt{2\pi R T_l}} \left[ P_{sat}(T_l) - P_v \right] \]

\[ P_{sat}(T_l) \frac{P_v}{P_r} = e^{\left[ \frac{L}{R} \left( \frac{1}{T_r} - \frac{1}{T_l} \right) \right]} \]

Continuity:

\[ \frac{\partial \rho}{\partial t} + \nabla (\rho \vec{v}) = 0 \]

Momentum:

\[ \frac{\partial}{\partial t} (\rho \vec{v}) + \nabla (\rho \vec{v} \cdot \vec{v}) = -\nabla p + \nabla \left[ \mu_{eff} \left( \nabla \vec{v} + \nabla \vec{v}^T \right) \right] + \rho \vec{g} + F_{vol} \]

Energy:

\[ \frac{\partial}{\partial t} (\rho E) + \nabla (\rho E + p) = \nabla (k_{eff} \nabla T) + S_h \]
Two-Phase VOF Storage Tank CFD Model

**Continuity:**
\[
\frac{\partial \rho}{\partial t} + \nabla (\rho \vec{v}) = 0
\]

**Momentum:**
\[
\frac{\partial}{\partial t} (\rho \vec{v}) + \nabla (\rho \vec{v} \cdot \vec{v}) = -\nabla p + \nabla \left[ \mu_{eff} \left( \nabla \vec{v} + \nabla \vec{v}^T \right) \right] + \rho \vec{g} + \vec{F}_{vol}
\]

**Energy:**
\[
\frac{\partial}{\partial t} (\rho E) + \nabla (\rho E + p) = \nabla \left( k_{eff} \nabla T \right) + S_h
\]

**Volume of Fluid (VOF) model:**
Energy and Temperature are defined as mass average scalars:
\[
E = \sum_{q=1}^{2} \alpha_q \rho_q E_q
\]

**Properties:**
\[
\rho = \sum_{q=1}^{2} \alpha_q \rho_q, \quad \mu_{eff} = \sum_{q=1}^{2} \alpha_q \mu_{eff} q, \quad k_{eff} = \sum_{q=1}^{2} \alpha_q k_{eff} q
\]

**Continuity of Volume Fraction of the \( q \)-th phase:**
\[
\frac{1}{\rho_q} \left[ \frac{\partial}{\partial t} (\alpha_q \rho_q) + \nabla \cdot (\alpha_q \rho_q \vec{v}) \right] = S_{\alpha_q}
\]

**Interfacial mass transfer per unit volume:**
\[
S_{\alpha_q} = \mathbf{m}_i \cdot \mathbf{A}_i \left[ \frac{kg}{m^3 \cdot \text{sec}} \right]
\]
\[
\mathbf{A}_i = |\nabla \alpha|, \text{ is an interfacial area density in } 1/m, \quad \mathbf{m}_i \text{ is a mass flux vector in } kg/(m^2 \cdot \text{sec}).
\]

where \( \alpha \) is a volume fraction of the primary phase

**Schrage’s Relation:**
\[
|\mathbf{m}| = \left( \frac{2\sigma}{2-\sigma} \right) \left( \frac{M}{2\pi R} \right)^{1/2} \left( \frac{P_i}{T_{i}^{1/2}} - \frac{P_v}{T_v^{1/2}} \right) \left[ \frac{kg}{m^2 \cdot \text{sec}} \right]
\]

\( \sigma \) is a surface tension coefficient in N/m, \( M \) is the molecular weight of the phase, \( R \) is the gas constant, \( P_i \) and \( P_v \) are the internal and external pressures, and \( T_{i} \) and \( T_v \) are the internal and external temperatures.
Self-pressurization tests were run with LH₂.

Cylindrical midsection with:
- height = 3.05 m
- diameter = 3.05 m

Ullage pressure, 2 Fluid temperature rakes,
Large number of Wall Temperature measurements

Boil-off test was performed prior to tank lockup and self-pressurization

Most tests include 20, 50, 90% fill levels

Heat Flux = 2.05 W/m²

Tank Internal volume 37.5 m³

2:1 elliptical top and bottom domes

Tank is enclosed in a vacuum shroud.

MHTB Facility (1996-2005)

Multi-purpose Hydrogen Test Bed (MHTB) at NASA Marshall Space Flight Center
Effect of Accomodation Coefficient
MHTB Pressurization – MHTB 90%

Sharp Interface Model

Heat Flux = 2.05 W/m²
Effect of Accommodation Coefficient – MHTB 90%
Sharp Interface Model

MHTB 90% Self-Press with Sharp Interface - Schrage model

Heat Flux = 2.05 W/m²

\[
|\dot{m}| = \left( \frac{2\sigma}{2 - \sigma} \right) \left( \frac{M}{2\pi R} \right)^{1/2} \left( \frac{P_i}{T_i^{1/2}} - \frac{P_v}{T_v^{1/2}} \right)
\]

(7)
Effect of Accommodation Coefficient- (MHTB 90%)

**Sharp Interface Model**

Heat Flux = 2.05 W/m²

\[ |\dot{m}| = \left( \frac{2\sigma}{2 - \sigma} \right) \left( \frac{M}{2\pi R} \right)^{1/2} \left( \frac{P_{sat}(T_i) - P_v}{T_i^{1/2}} \right) \]
Effect of Accommodation Coefficient - MHTB (50%)

VOF Model

Liquid Heat Flux = 2.05 W/m²
Vapor Heat Flux = 0.90 W/m²
1G MHTB Pressure Control Results: LH2, Large Tank Droplet Spray Bar - VOF
Computation of mass transfer using Schrage in the sharp Interface model is insensitive to the magnitude of accommodation coefficient. \( \alpha \) close to 1 seems to work fine.

Computations of mass transfer using Schrage in the VOF method also show a certain degree of insensitivity to the magnitude of accommodation coefficient but small values around \( \alpha = 0.01 \) seem to be necessary for numerical practicality and stability.

This is only true for a stable flat interface between bulk phases. Mass transfer computations based on Schrage equation for droplets and during slosh dynamics or boiling situations are quite sensitive to magnitude of accommodation coefficient.

Schrage might not represent the right mass transfer kinetics under these conditions.
Effect of Turbulence
Effect of Turbulence: MHTB (50%)

Liquid Heat Flux = 2.05 W/m²
Vapor Heat Flux = 0.90 W/m²
MHTB Self Pressurization: Effect of Turbulence

Pressure Time History

Laminar vs. Turbulent

Temp Profile at end of Self-Press

Liquid Heat Flux = 2.05 W/m²
Vapor Heat Flux = 0.90 W/m²
1. Test fluid is liquid **hydrogen**

2. Flightweight insulated 2219-T62 aluminum ellipsoidal tank
   - Internal volume: $4.95 \text{ m}^3 = 175 \text{ ft}^3$
   - Tests conducted in vacuum chamber.
   - Test article is enclosed by a cryoshroud whose temperatures are maintained with electrical heaters.
   - Tank is insulated with 2 blankets of MLI.

3. Steady boil-off test and measurement performed at 95% liquid fill fraction and 117 kPa (or 1.17 bar) tank pressure.

4. Tank fill level was reduced to desired fill level (29%, 49%, 83%)

5. Several hours of additional venting at 103 kPa were performed to achieve stationary state.

6. Self-pressurization tests were initiated from a stationary stratified state.

7. Two Cryoshroud Temps $\rightarrow$ Two heat loads (2 & 3.5 W/m²)

8. Grashof Number (Gr) based on 3.5 W/m² average heat flux into tank $\rightarrow$ vapor: $Gr = 2.21e+13$; liquid: $Gr = 1.33e+14$
   (which corresponds to turbulent natural convection for a steady-state natural convection flow)
Effect of Turbulence: K-Site (50%)

Tank Pressure & Interfacial Mass Transfer

- black - Exp
- red - VOF Implicit Laminar-Conjugate
- blue - VOF Implicit Turbulent-Conjugate
- red dashed - m_dot - VOF - Laminar
- blue dashed - m_dot - VOF - Turbulent

K-Site VOF, Conjugate HT, Laminar, 3.5 W/m^2

K-Site VOF, Conjugate HT, Turbulent, 3.5 W/m^2

60,000 seconds of self-pressurization
K-Site Self-Pressurization: Effect of Turbulence

Results: 3.5 W/m$^2$ heat flux

Temperature in the vapor at SD8
K-Site Self-Pressurization: Effect of Turbulence

Results: 3.5 W/m² heat flux

Temperature in the liquid at SD16
K-Site Self-Pressurization: Effect of Turbulence

Results: 2.0 W/m² heat flux

Tank Pressure

- Experiment
- CFD Turbulent k-w-SST Conjugate
- CFD Laminar Conjugate

Stream Function, kg/s

- 3.8e-03
- 3.4e-03
- 3.0e-03
- 2.7e-03
- 2.3e-03
- 1.9e-03
- 1.5e-03
- 1.1e-03
- 7.6e-04
- 3.8e-04
- 6.8e-05
K-Site Self-Pressurization: Effect of Turbulence

Velocity Magnitude

10000 seconds

30000 seconds

60000 seconds

19
Laminar models agree closely with the pressure evolution and vapor phase temperature stratification but under-predict liquid temperatures.

Turbulent SST k-w and k-e models under-predict the pressurization rate and extent of stratification in the vapor but represent liquid temperature distributions fairly well.

These conclusions seem to equally apply to large cryogenic tank simulations as well as small scale simulant fluid pressurization cases.

Appropriate turbulent models that represent both interfacial and bulk vapor phase turbulence with greater fidelity are needed.

Application of LES models to the tank pressurization problem can serve as a starting point.
K-Site Self-Pressurization: Effect of Turbulence Sharp Interface Model

Results: 3.5 W/m² heat flux