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

Mohammad Kassemi*, Olga Kartuzova, Sonya Hylton
National Center for Space Exploration (NCSER)
NASA Glenn Research Center
Cleveland, OH 44135

*Mohammad.Kassemi@nasa.gov

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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 RBF 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>
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<tbody>
<tr>
<td>Continuity</td>
<td>✓</td>
<td>✓</td>
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<td>Navier Stokes</td>
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</tr>
<tr>
<td>Energy</td>
<td>✓</td>
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<tr>
<td>Turbulence (k-ω SST)</td>
<td>✓</td>
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</tbody>
</table>

### Interfacial Energy Balance:

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

\[T_l = T_{sat}(P_v)\]

### Schrage Interfacial Mass Transfer:

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

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

Continuity:

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

Momentum:

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

Energy:

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

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

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

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

### Volume of Fluid (VOF) model:

### Energy and Temperature are defined as mass average scalars:

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

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

### Interfacial mass transfer per unit volume:
\[
S_{\alpha_q} = \dot{m}_i \cdot \vec{A}_i \left[ \frac{\text{kg}}{m^3 \cdot \text{sec}} \right]
\]

Where \( \vec{A}_i = |\nabla \alpha| \), is an interfacial area density in \( 1/m \), \( \dot{m}_i \) is a mass flux vector in \( \text{kg}/(m^2 \cdot \text{sec}) \).

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

\( \alpha = 0 \)

\( \alpha = 1 \)
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.

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Effect of Accommodation Coefficient
MHTB Pressurization – MHTB 90%

Sharp Interface Model

Heat Flux = 2.05 W/m²

MHTB Sharp Interface 90% fill ratio, Turbulent, AC=1

Time [s] = 2000

MHTB Sharp Interface 90% fill ratio, Turbulent, AC=1

Time [s] = 25000
Effect of Accommodation Coefficient – MHTB 90%

Sharp Interface Model

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

Heat Flux = 2.05 W/m²

\[ |\dot{m}| = \left( \frac{2\sigma}{2 - \sigma} \right) \left( \frac{M}{2\pi R} \right)^{1/2} \left( \frac{P_i}{T_i^{1/2}} - \frac{P_v}{T_v^{1/2}} \right) \]
Effect of Accommodation Coefficient - (MHTB 90%)
Sharp Interface Model

Heat Flux = 2.05 W/m²

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

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 $\alpha = .01$ 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
MHTB Self-Pressurization: Effect of Turbulence

![VOF Laminar and VOF Turbulent scenes with temperature maps and graph showing effective thermal conductivity vs distance from tank centerline.](image-url)
Tank Self-Pressurization Experiments at K-site Facility (1990-91)

1. Test fluid is liquid *hydrogen*

2. Flightweight insulated 2219-T62 aluminum ellipsoidal tank
   - Internal volume: 4.95 m$^3$ = 175 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/m$^2$)

8. Grashof Number (Gr) based on 3.5 W/m$^2$ 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

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/m² heat flux

Temperature in the vapor at SD8

- Experiment
- VOF Laminar - Conjugate
- VOF Turbulent - Conjugate

Laminar

T, K

Turbulent

T, K

(16)
K-Site Self-Pressurization: Effect of Turbulence

Results: 3.5 W/m² heat flux

Temperature in the liquid at SD16

- Experiment
- VOF Laminar - Conjugate
- VOF Turbulent - Conjugate

T, K

0 10000 20000 30000 40000 50000 60000 70000

T, K

Laminar

Turbulent

(17)
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

T, K

36.0
33.6
32.2
30.8
29.4
28.0
26.6
25.2
23.6
22.2
20.8
20.0

0.8e-03
3.0e-03
3.6e-03
4.0e-03
4.4e-03
4.8e-03
5.6e-04
7.6e-04
3.8e-04
0.0e+00
K-Site Self-Pressurization: Effect of Turbulence

Velocity Magnitude

Laminar

Turbulent

10000 seconds

30000 seconds

60000 seconds
Effect of Turbulence - Summary

- 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