

Computational Analyses of Pressurization in Cryogenic Tanks

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and

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**44rd AIAA/ASME/SAE/ASEE
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Motivation

Analyses of Tank Pressurization Systems



Exploration Missions

- Heat Transfer from different sources such as solar radiation contributing to solar radiation
- Large amplitude Sloshing during vehicle maneuvers, engine burn, orbital insertion
- Thermal stratification in variable gravity environments
- Control systems condition the tank during orbital engine start-up

Ground Test Operations

- Ultra-high pressure source of gas at ambient temperature used to pressurize tanks
- Turbulent Mixing in Tank
- Tank comprises of entire fluid dynamic spectrum from compressed cryogenic liquid, supercritical, superheated compressible
- Scenarios include cryo-collapse in the tank

REGIMES OF TANK PROBLEMS AND APPROPRIATE MODELS(Exploration)

Lumped Parameter
Thermodynamic Models
Simplified CFD Models

Simplified CFD Models
with more elaborate heat
transfer

Multi-Phase CFD models
Interface tracking /
capturing techniques
Surface Tension

Multi-Phase CFD models
Mesh motion/grid
adaption
Elaborate Multi-Phase
CFD models with
Dispersed Phase etc.

Pre-Pressurization



Re-Pressurization /
Pressurization in
variable g environ



Re-pressurization
at Stage Separation



Upper Stage Burn

Self-Pressurization
Thermal/Pressure
Control Systems

Free/Forced Convection
Heat Transfer

+

Low Amplitude Slosh

+

High Amplitude Slosh

+

Flow dynamics
associated with drain

REGIMES OF TANK PROBLEMS AND APPROPRIATE MODELS(Ground)

Thermodynamic Heat
Transfer Models

System Level Codes
such as RPTA
Multi-Phase CFD Models
with Real Fluid Effects

Multi-Phase CFD Models
with Interface Tracking

Tank Chill Down



Tank Pressurization



Runtime Propellant
Draw Down & Purge

Heat Transfer

+

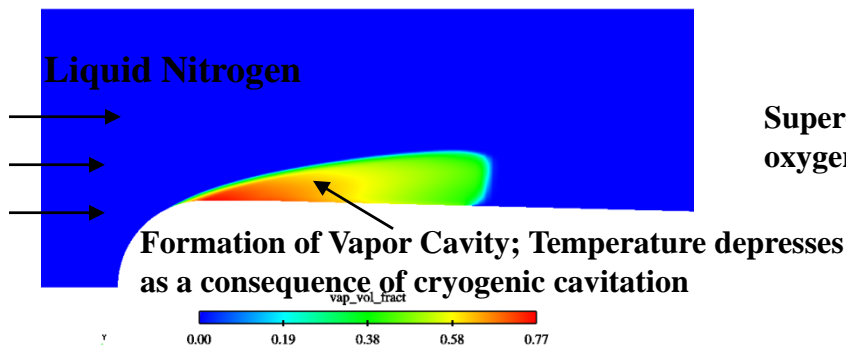
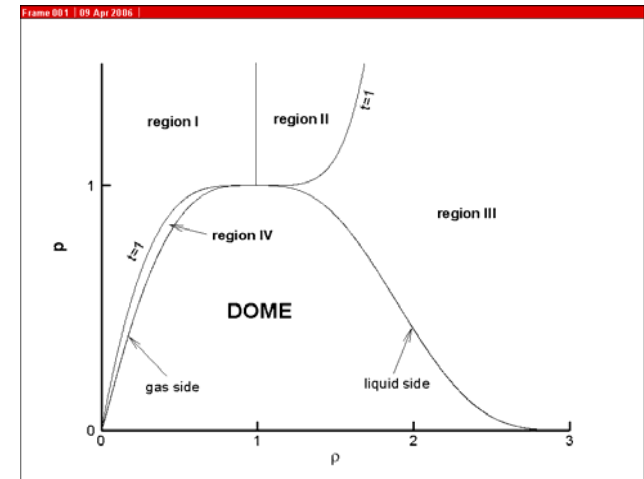
Mixing, Phase Change,
Existence of Sub-
critical/Supercritical
States

+

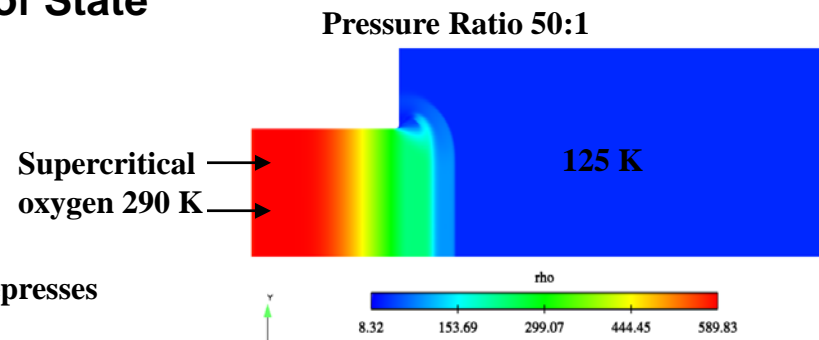
Drain related flow
dynamics

Generalized Multi-Phase Computational Framework

- **Computational Framework For Mixture Set of Equations**
 - Gas-Liquid Interface Captured as part of Solution Procedure
 - Acoustics of Two-Phase Regime Accurately Captured
 - Phase Change Problems such as cryogenic cavitation modeled by Finite Rate Kinetics
 - Tank Pressurization Problems require a broader operating envelope (P,T) from classical cryogenic cavitation problems
 - Properties related to Sub-critical and Supercritical States are obtained directly from Specialized Equations of State



Cryogenic Cavitation



Supercritical Flow in Chamber with Sub-critical conditions

GENERALIZED PRECONDITIONING FORMULATION

- **Generalized Real Fluid, Multi-Component Formulation**

- Allows for user specified mixture of gases and liquid
- Phase change driven by vapor pressure of liquid phase

$$\Gamma \frac{\partial Q_v}{\partial t} + \frac{\partial E}{\partial x} = S + D_v;$$

$$\Gamma = \frac{\partial Q}{\partial Q_v}; \quad A = \Gamma^{-1} \frac{\partial E}{\partial Q_v}$$

- **Versatile Formulation**

- Pressure and Temperature are solved for directly allowing “stiff” components to be modeled
- Flux formulation retained in generalized thermodynamic form
(ρ_P, ρ_T, H_p, H_t)
- Thermodynamic properties can be specified as user input either in analytical form or tabular look-up

- **Framework has been used to model wide range of problems ranging from transcritical injectors, low-speed tank problems, to cavitating turbopumps**

$$Q = \begin{bmatrix} \rho \\ \rho u \\ \rho e \\ \rho Y_i \end{bmatrix}; \quad Q_v = \begin{bmatrix} p \\ u \\ T \\ Y_i \end{bmatrix};$$

$$\Gamma = \begin{bmatrix} \rho_p & 0 & \rho_T & \rho_{y_i} \\ u \rho_p & \rho & u \rho_T & u \rho_{y_i} \\ H \rho_p - (1 - \rho h_p) & \rho u & H \rho_T - (1 - \rho h_T) & H \rho_{y_i} + \rho h_{y_i} \\ Y_i \rho_p & 0 & Y_i \rho_T & Y_i \rho_{y_i} + \rho \delta_{ij} \end{bmatrix}$$

$$d\rho = \frac{\rho}{P} dP - \frac{\rho}{T} dT - \rho \sum_1^{NS-1} \left(\frac{\bar{M}}{M_i} - \frac{\bar{M}}{M_s} \right) dy_i$$

Compressible Multi-Component Systems



SOLUTION PROCEDURE

- System cast in “Compressible” Framework
 - Eigensystem Characteristics Similar for All Systems
 - “Effective” Speed of Sound is defined for multi-fluid mixtures
 - Exploit Compressible System Techniques to Efficiently Solve equations
 - Use Approximate Riemann Solver of Roe
 - Can Use Any Characteristics Based Flux /Flux-difference Splitting Method
- Preconditioning Technique to Over Come Numerical Stiffness
 - Γ Matrix Is Modified Using Scaling Parameter β
 - Reduces Eigen-values to More Matched Form

$$\Gamma_P = \begin{bmatrix} \beta\rho_p & 0 & \rho_T & \rho_{y_i} \\ u\beta\rho_p & \rho & u\rho_T & u\rho_{y_i} \\ H\beta\rho_p - (1-\rho h_p) & \rho u & H\rho_T - (1-\rho h_T) & H\rho_{y_i} + \rho h_{y_i} \\ Y_i\beta\rho_p & 0 & Y_i\rho_T & Y_i\rho_{y_i} + \rho\delta_{ij} \end{bmatrix}$$

Modified Γ Matrix

$$F_m = \frac{1}{2} \left[F(Q_{v,m}) + F(Q_{v,m}^+) \right] - \frac{1}{2} \left[\Gamma_P (\Gamma_P^{-1} A) (Q_{v,m}^+ - Q_{v,m}) \right]$$

$$F_m = \frac{1}{2} \left[F(Q_{v,m}) + F(Q_{v,m}^+) \right] - \frac{1}{2} \left[\Gamma_P (\tilde{R}_P \tilde{\Lambda}_P \tilde{L}_P) (Q_{v,m}^+ - Q_{v,m}) \right]$$

Modified Flux

$$\Lambda_P = \left(\frac{u}{2} \left(1 + \frac{1}{\beta} \right) + c'_m, \frac{u}{2} \left(1 + \frac{1}{\beta} \right) - c'_m, u, u, u, u, u \right)$$

$$c'_m = \frac{1}{2} \sqrt{u^2 \left(1 - \frac{1}{\beta} \right)^2 + 4 \frac{c_m^2}{\beta}}; \quad \beta = \left(\frac{c_m^2}{u^2} \right)$$

Eigen Values of $[A]$

EOS OPTIONS FOR GAS/LIQUID MIXTURES

Mixture Density is defined as

$$\rho_m = \sum_{i=1}^{ns} \rho_i \phi_i \quad \text{where} \quad \phi_i = \frac{y_i \rho_m}{\rho_i}$$
$$\therefore \rho_m = \frac{1}{\sum_{i=1}^{ns} \left(\frac{y_i}{\rho_i} \right)}$$

ρ_i obtained from EOS for each fluid independently

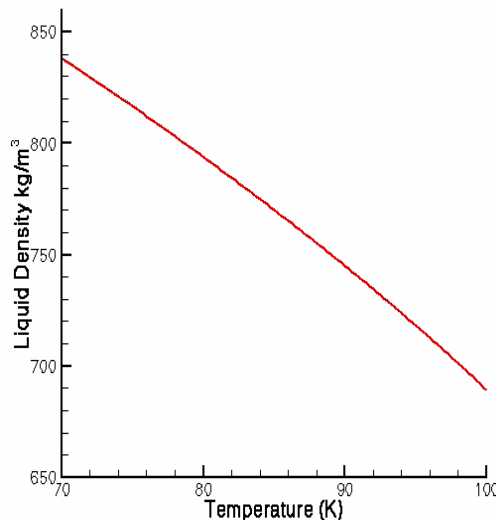
$$h_m = \sum_{i=1}^{NS} \rho_i \phi_i h_i = \sum_{i=1}^{NS} y_i h_i$$

h_i obtained from EOS for each fluid independently

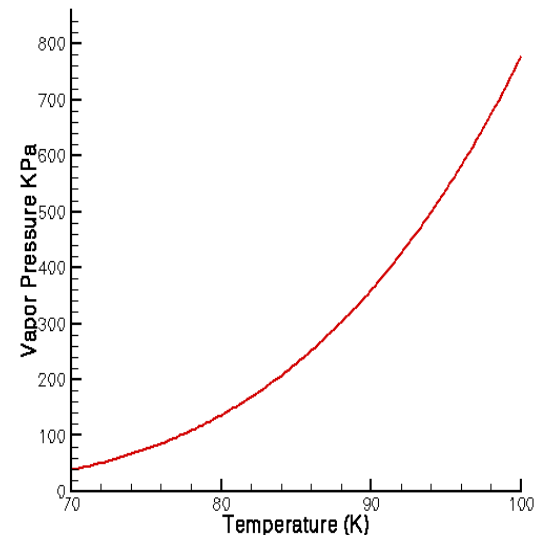
Note that the EOS can be (a) ideal gas equation (b) curve fits (c) cubic or higher order polynomial equations of state (SRK/BWR) (d) any specified equation of state (HBMS)

GAS-LIQUID EOS ROUTINES

- Mixtures of Simple Gases and Liquids
 - Utilized for operating temperatures far from Critical Point
 - Gases Modeled with Ideal Gas Equation
 - Liquids Modeled with Linearly Varying Properties
 - Properties of Cryogenic Liquids show Strong Dependence on Temperature



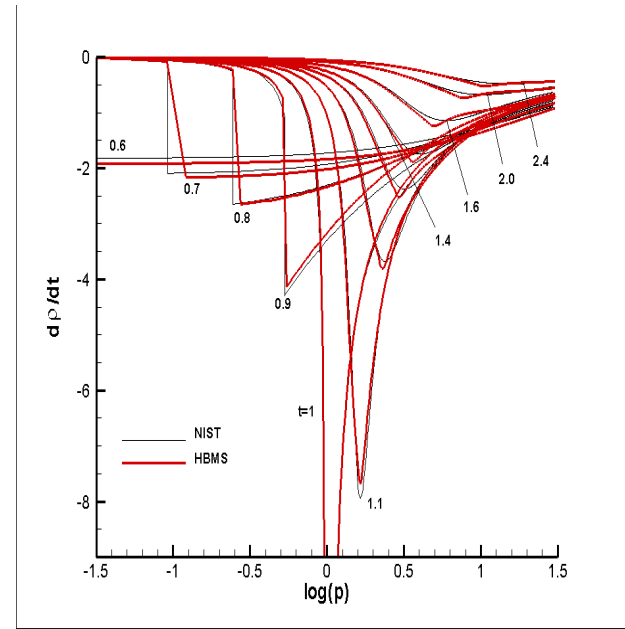
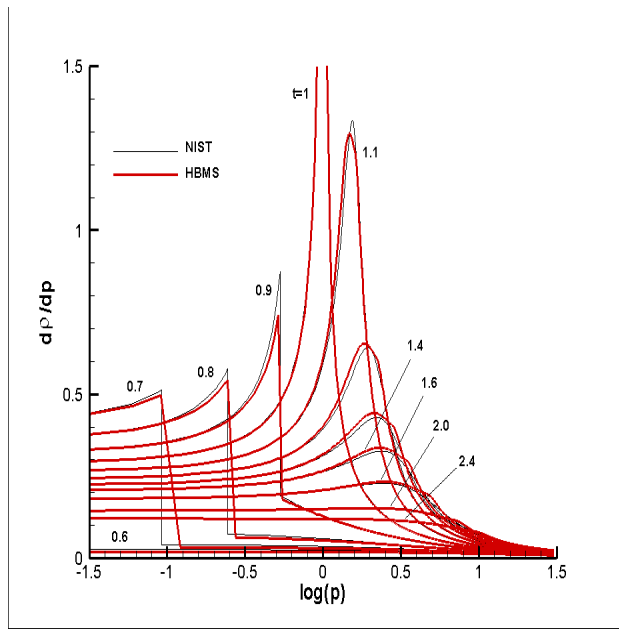
Liquid Nitrogen Density



Vapor Pressure

Gas-Liquid EOS Routines

- For Regimes that include Supercritical Flow along with Sub-critical States Specialized EOS Routines need to be used
 - Close to Critical Point Vapor Phase Exhibits Non-Ideal behavior
 - Property Derivatives Exhibit non-linearities and discontinuous slopes near critical Point
 - Several Generalized EOS Routines that Span Supercritical/Sub-critical Regimes Implemented

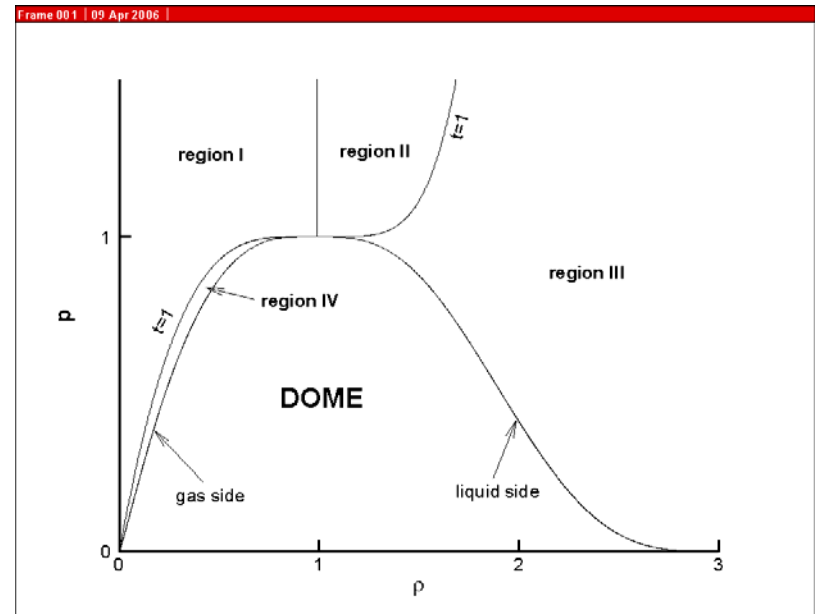


HBMS Model For Real Fluids

- HBMS Model Developed by Hirschfelder, Beuler, McGee and Sutton

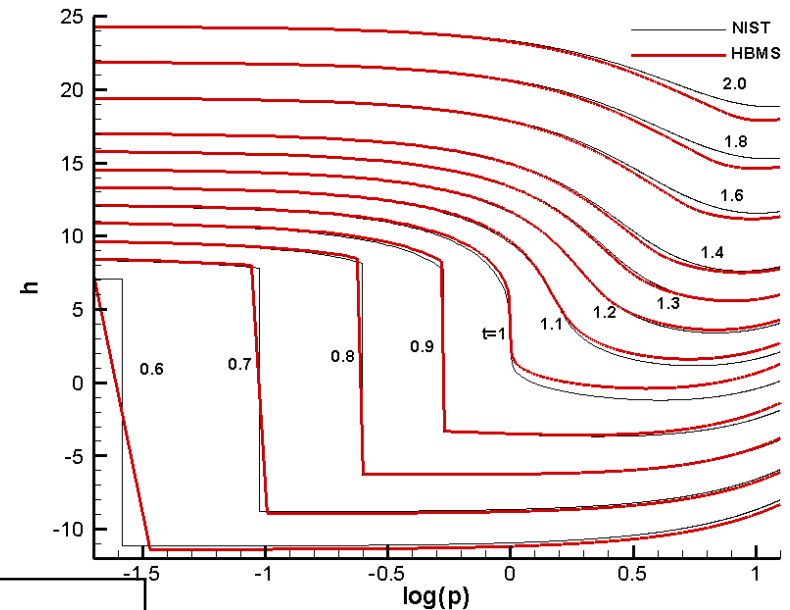
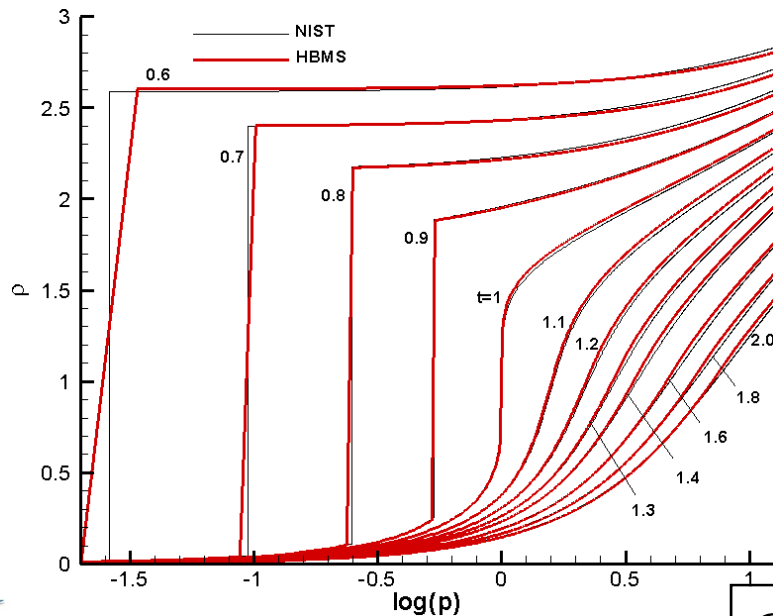
- Hirschfelder, J. O., Buehler, R. J., McGee, H. A., and Sutton, J. R., "Generalized Equation of State for Gases and Liquids", Industrial and Engineering Chemistry, **50**, #3, p375, 1958.
- Hirschfelder, J. O., Buehler, R. J., McGee, H. A., and Sutton, J. R., "Generalized Thermodynamic Excess Functions for Gases and Liquids", Industrial and Engineering Chemistry, **50**, #3, p386, 1958.
- Hirschfelder, J. O., Buehler, R. J., McGee, H. A., and Sutton, J. R., "Correction and Correspondence", Industrial and Engineering Chemistry: Fundamentals, **1** p 224, 1962.

- Three Region Correlation of Real Fluid Properties based on Principle of Corresponding States
- Region I
 - Density < 1
- Region II
 - Temp > 1 Density > 1
- Region III
 - Temp < 1 Density > 1
- All thermodynamic properties and derivatives expressed as functions of density and temperature
- Implementation in CRUNCH requires a density decode at local pressure and temperature
- Evaluate density based on pressure and temperature using a Newton Iteration
- Function has multiple zeroes, iteration sensitive to initial guess
- Regions I and II density initialized by ideal gas law, Region III by liquid density, and Region IV by 0.



HBMS Model for Real Fluids (cont.)

- HBMS shows good comparisons with NIST for oxygen and nitrogen
- Derivatives show discontinuous slopes near the critical pt
 - Questions arise about numerical stability in a CFD Framework
- In the sub-critical regime comparisons are particularly good. However, comparisons deteriorate in the supercritical region



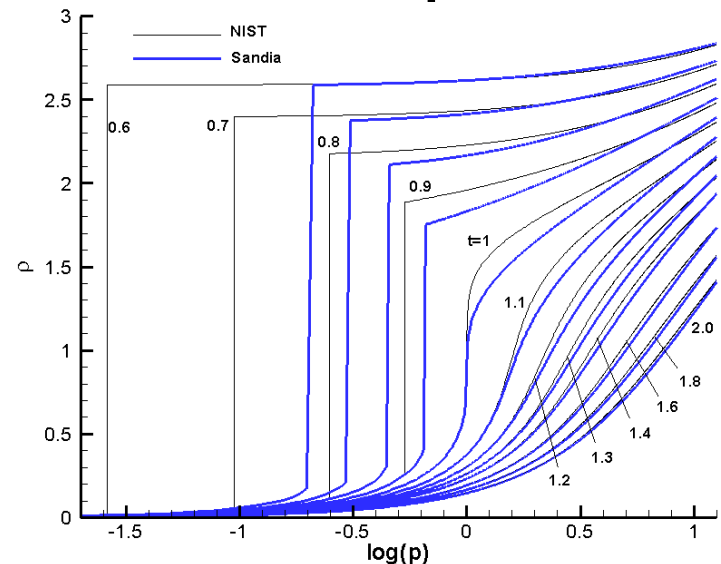
Oxygen

Cubic EOS for Real Fluids

- Routines based on SRK (**S**oave, **R**edlich and **K**wong) and PR (**P**eng, **R**obinson) equations of state
- Routines developed by Joe Oefelein at Sandia
- Belong to a general class of “cubic equations of state”
- Unlike HBMS, Sandia EOS routines are prescribed as functions of pressure and temperature and can be directly used in a density based CFD code such as CRUNCH CFD
- Comparisons with NIST indicate correct Trends but Saturation Line Shifted – Properties on either side of dome well predicted

$$P = \frac{RT}{V - b} - \frac{a}{V^2 + ubV + wb^2}$$

where R is the universal gas constant, V is molar volume
u and w are model constants depending on PR or SRK
and a and b are constants for a given substance which
maybe a mixture in which case they are dependent on
mixture composition

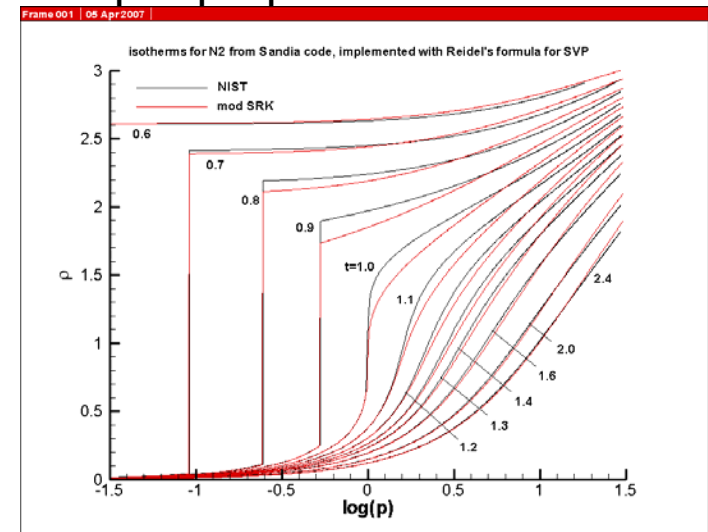
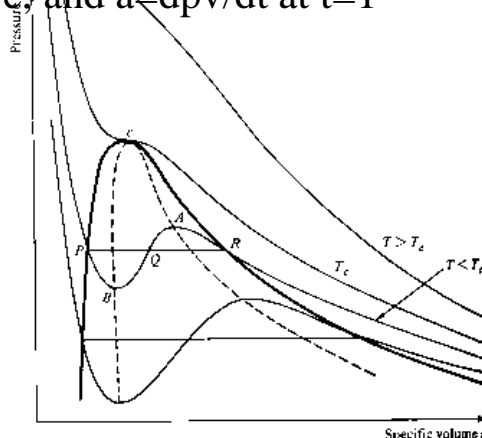


Correction to Cubic EOS (SRK)

- Since SRK/PR EOS use a cubic EOS choice of vapor pressure in these models is an approximation
 - Consequently the saturation line is shifted giving rise to erroneous properties near the saturation line
- Vapor Pressure can be directly computed using Reidel's formula
 - Part of the cubic replaced by the saturation line
 - Determination can be made based on the local pressure and the vapor pressure whether to extract liquid or vapor properties

$$p_v = \exp \left\{ \alpha \ln(t) - 0.0838(\alpha - 3.75) \left[\frac{36}{t} - 35 - t^6 + 42 \ln(t) \right] \right\}$$

where $p_v = P_v/P_c$ and $t = T/T_c$, in which P_c is the critical pressure, and $a = dp_v/dt$ at $t=1$



Isotherms after Correction

Thermophysical Properties

- Thermophysical property models implemented in CRUNCH CFD for properties such as viscosity and thermal conductivity spanning different sub-critical/supercritical regimes
 - Sandia model has its own routines for viscosity and thermal conductivity
 - Lemmon Jacobsen model implemented for nitrogen and oxygen
 - E.W. Lemmon and R.T. Jacobsen, International Journal of Thermophysics, Vol. 25, No.1, Jan. 2004, p.21-69

Viscosity

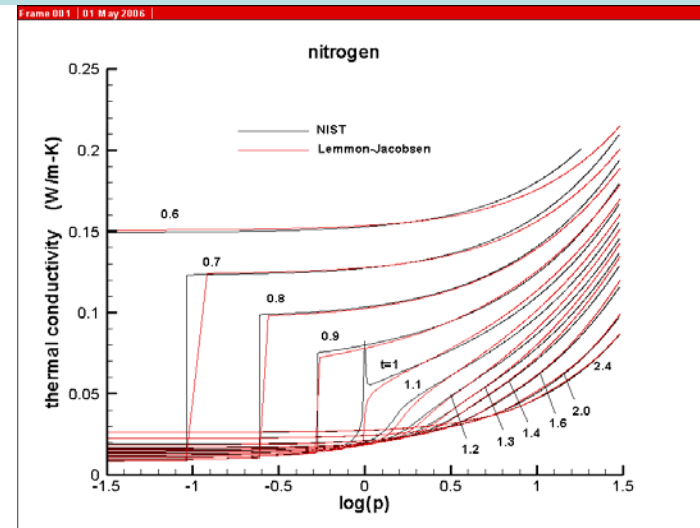
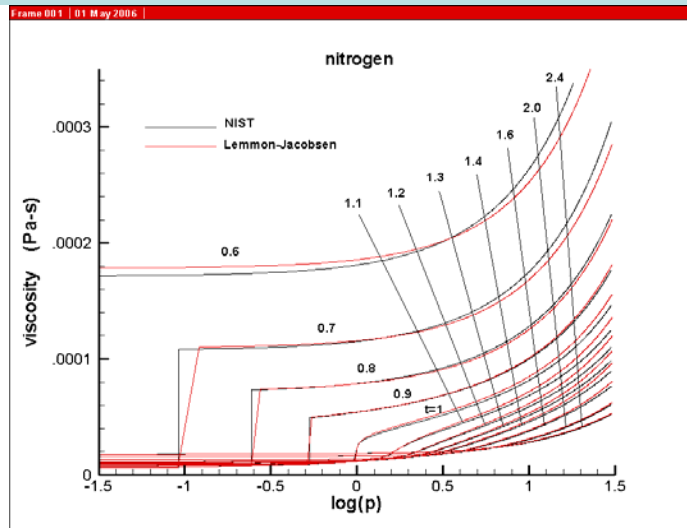
$$\eta = \eta^0(T) + \eta^r(\tau, \delta)$$

$\eta^0(T) = \frac{0.0266958\sqrt{MT}}{\sigma^2\Omega(T^*)}$

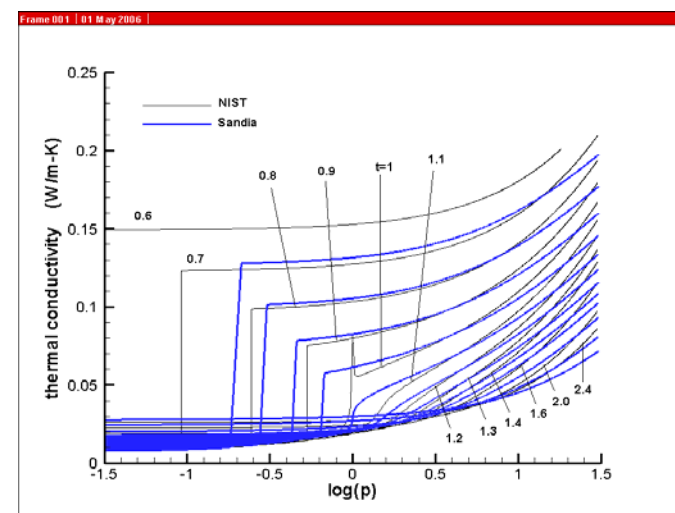
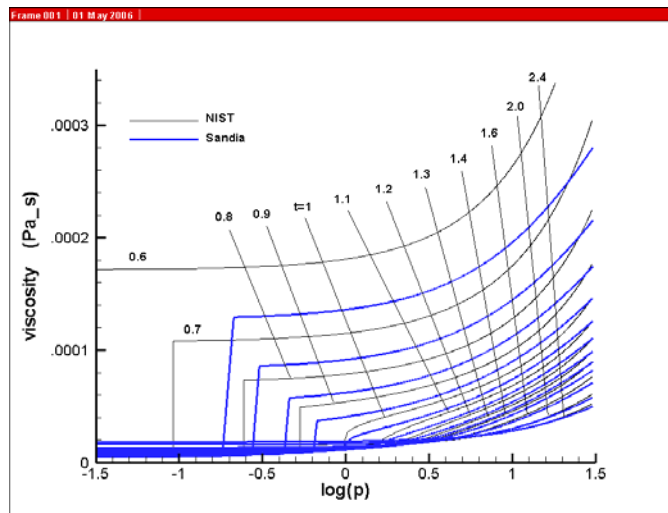
$\Omega(T^*) = \exp\left(\sum_{i=0}^4 b_i [\ln(T^*)]^i\right)$

Dilute gas viscosity $\rightarrow \eta^0(T)$
 Leonard Jones Parameter $\rightarrow \sigma$
 Ratio of density to critical density $\rightarrow \delta$
 Ratio of critical temp to temp $\rightarrow \tau$
 Collision Integral $\rightarrow \Omega(T^*)$

Thermophysical Properties (Cont.)



Lemmon Jacobsen Model for nitrogen



Sandia Model for nitrogen

EOS Framework for Mixture Routines

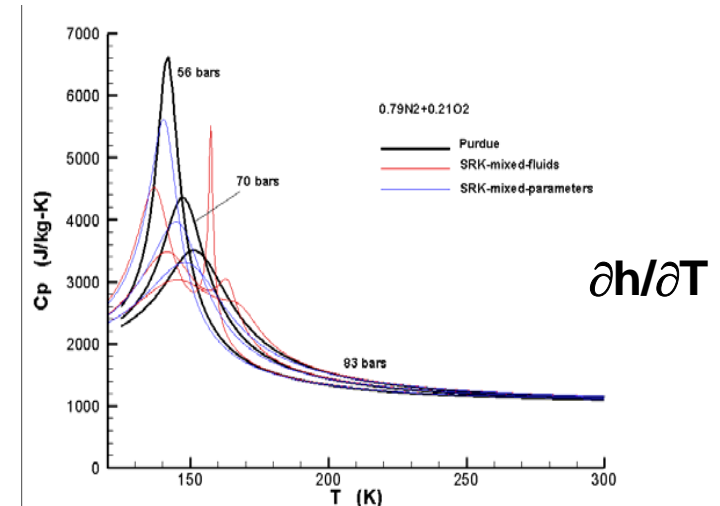
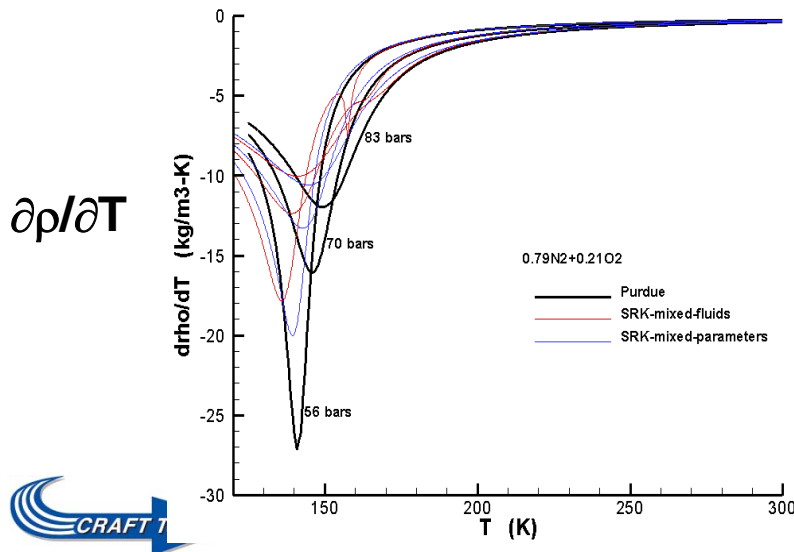
- **A mixture model for property routines where multiple fluids could exist in different states**
 - Eg. Gas, liquid, supercritical
 - Two issues make this complicated
 - Ambiguity of definition of critical point or critical surface
 - In supercritical regimes mixing rules cannot be represented by simple linear combinations of mass fractions of constituents
 - Tank problems such as the pressurization problem is unique because of the existence of multiple states i.e. subcritical gas, liquid, supercritical of the ullage and the propellant
- **Two approaches taken to development of a mixture model**
 - Defining a mixture based on combination of properties of constituent components (Amagat's Law)
 - Defining a cubic equation such as PR/SRK based on a composite fluid

$$P = \frac{R_u T}{V - b} - \frac{a}{V^2 + ubV + wb^2} \quad a = \sum_{i=1}^n \sum_{j=1}^n x_i x_j a_i^{1/2} a_j^{1/2} \quad b = \sum_{i=1}^n x_i b_i$$

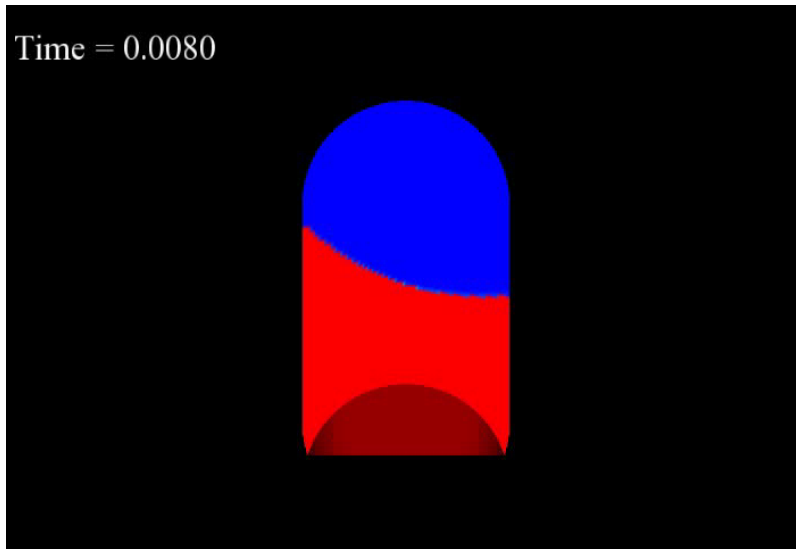
EOS Framework for Mixture Routines(cont.)

Comparisons of mixture formulation and composite fluid formulation in determining properties for mixture oxygen and nitrogen for which NIST data is available

- Comparisons are made for temperatures ranging from 120 K to 300 K through critical point of Oxygen (155 K)
- Both approaches similar in supercritical regime
- Near Critical Point of Oxygen both approaches show significant deviation
 - Composite Fluids Approach Closer to NIST Data
 - Composite Fluids Approach shows Smooth Variation near Critical Point



VALIDATION FOR TANK SLOSHING – MSFC DROP TANK EXPERIMENT



CRUNCH CFD[®] Simulation

- Sloshing in a drop tank experiment at NASA MSFC simulated; liquid simulant; petroleum ether, vapor simulant: air
- Multi-Phase Simulation Performed with gas-liquid interface being resolved as part of the solution
- No Additional Interface tracking or interface fitting technique or grid adaptation used in this case
- Initial liquid surface displaced to provide source for sloshing

Physical Properties: Petroleum Ether

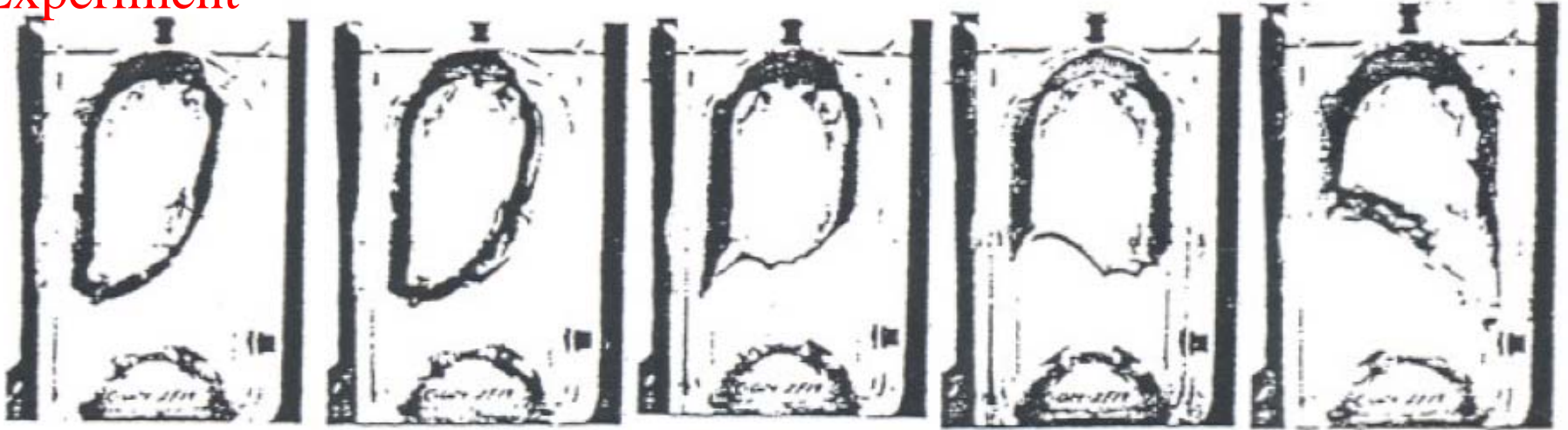
- Density = 618 kg/m³
- Surface Tension=0.0149 N/m (neglected)
- Viscosity =0.0002488 kg/m-s

Gravity Acceleration Profile:

-9.8 m/s ²	0.0 < t < 0.08 s
-1.75 m/s ²	0.08s < t < 0.09 s
-1.06 m/s ²	0.09s < t < 0.10 s
-0.89 m/s ²	0.10s < t < 0.20 s
-0.51 m/s ²	0.20s < t < 0.30 s
-0.21 m/s ²	0.30s < t < 0.356 s
-0.10 m/s ²	0.356s < t < 4.0 s

Comparison of Experiment and Computational Flowfield with Gas-Liquid Iso-Surface

Experiment



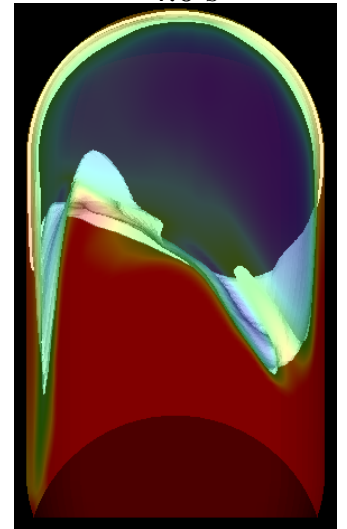
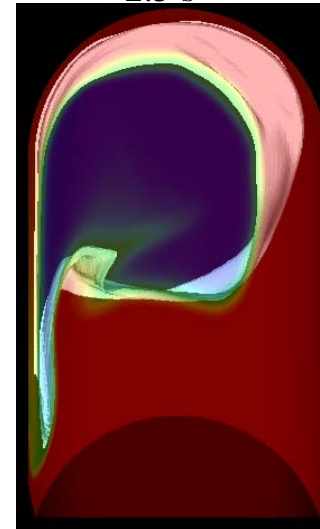
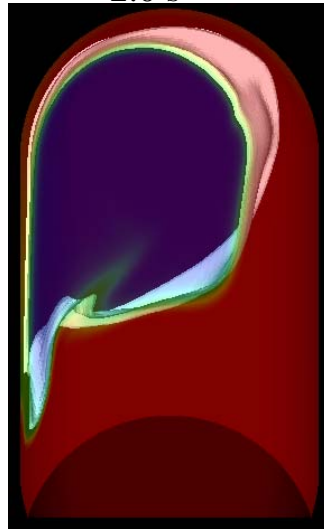
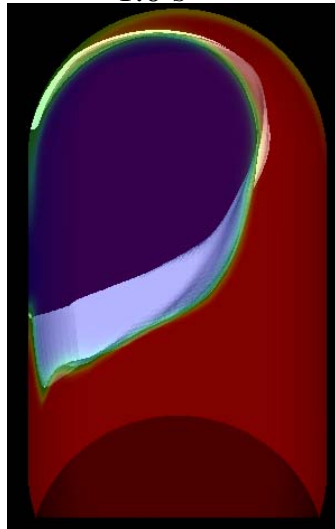
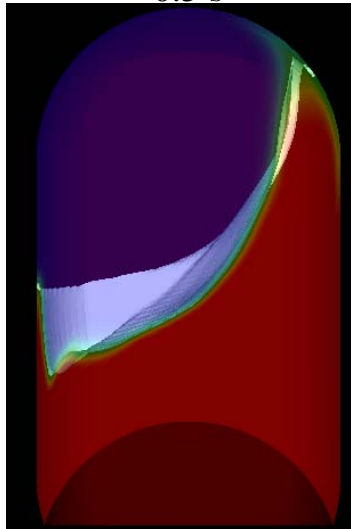
0.5 s

1.0 s

2.0 s

2.5 s

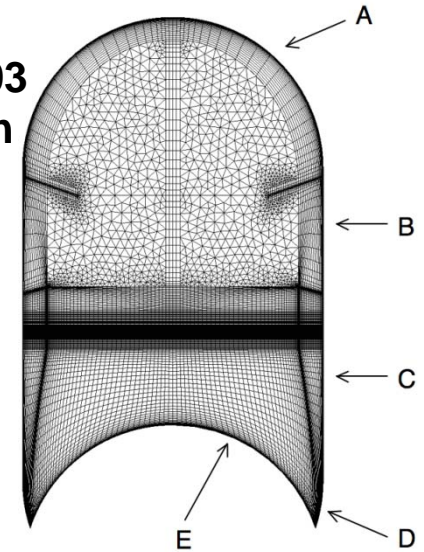
4.0 s



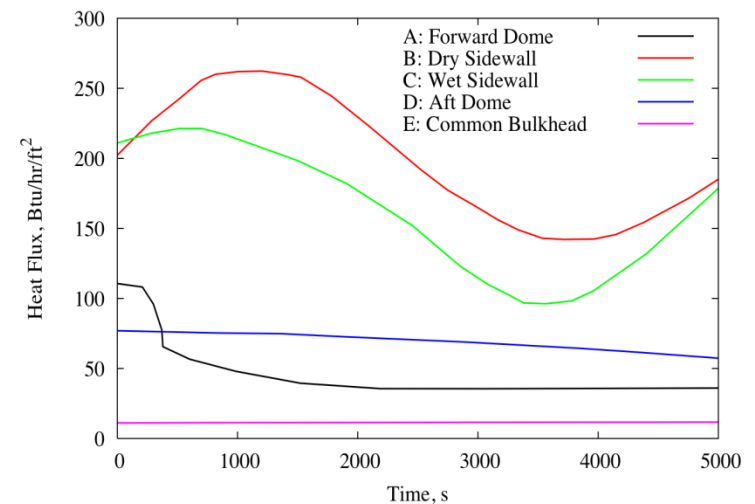
VALIDATION FOR PHASE CHANGE – AS-203 SELF-PRESSURIZATION EXPERIMENT

- Simulations of Saturn AS-203 Self-Pressurization Fuel Tank Experiment
- Fuel Tank Modeled with its Slosh Deflector and Baffle
- Tank was instrumented for pressure and temperature measurements during orbiting SIV-B stage
- Variable Heat Flux Distribution on various segments of Tank
- Tank contained 16,000 lbm of liquid Hydrogen and had an initial pressure of 12.4 psia

Liquid Hydrogen Fuel Tank in AS-203 Self-Pressurization Experiment



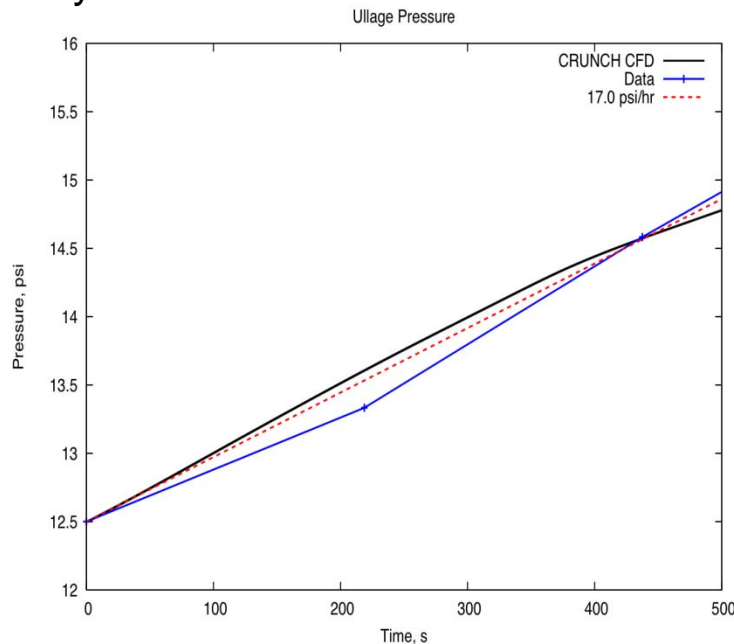
Heat Flux Distribution



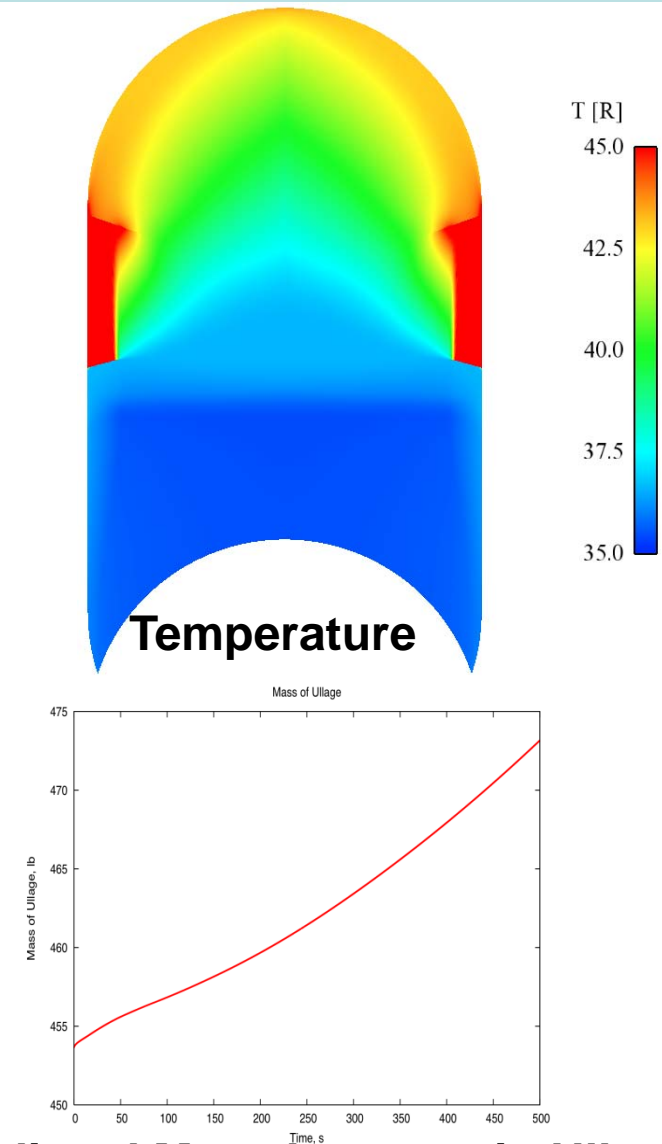
Measured Heat Flux Distribution in Tank

COMPARISONS OF CFD PREDICTIONS and EXPERIMENTAL MEASUREMENTS/DEDUCTIONS

- During Experiment conditions recorded during first 600 secs before Telemetry Blackout
- Increase in Pressure combination of heat transfer from walls and propellant boil-off
- Development of Thermal Boundary Layers and convective cells in Tank



Predicted and Measured Ullage Pressure Rise during Self-Pressurization



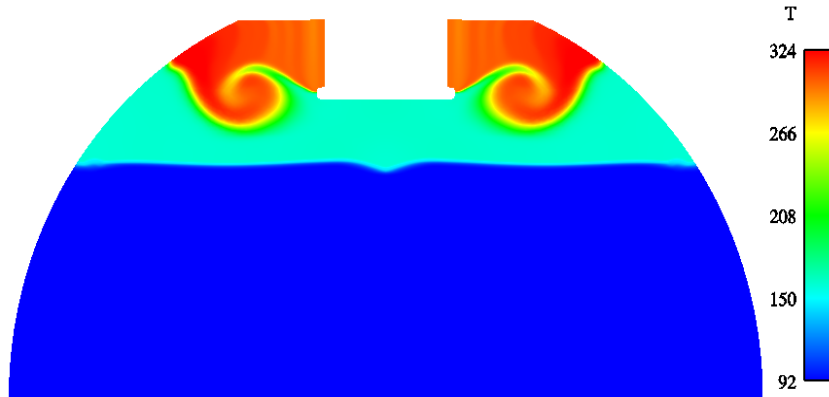
Predicted Mass Increase in Ullage

PRESSURIZATION OF LOX TANK

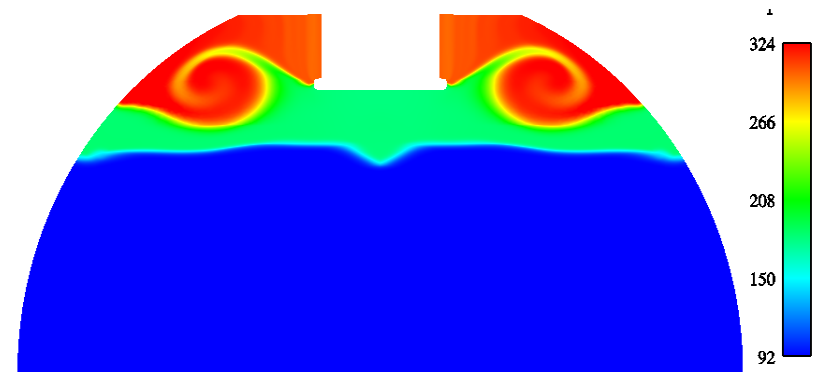
- Simulations of High Pressure Lox System in E-1 Test Complex at NASA SSC
 - System Comprises of 2600 Gallon LOX Dewar Run Tank
 - High Pressure Source of Pressurant Gas(Nitrogen) substituted for Oxygen in Simulation
 - Constant Mass Flow of Gas injected into Tank at 1158 lbm/s
 - Flow Enters Tank Radially through Diffuser
 - Individual Holes of Diffuser not modeled
 - Simulation Started at Pre-pressurization conditions
 - 90% liquid 10% ullage
 - Ullage at 325 psia, 135.16 K
 - Liquid Sub-cooled at 90.18 K
 - System Encompasses entire spectrum from compressed liquid, supercritical to superheated compressible
 - System pressurizes from 325 psia to 1350 psia in 0.3 secs.

PRESSURIZATION OF LOX TANK

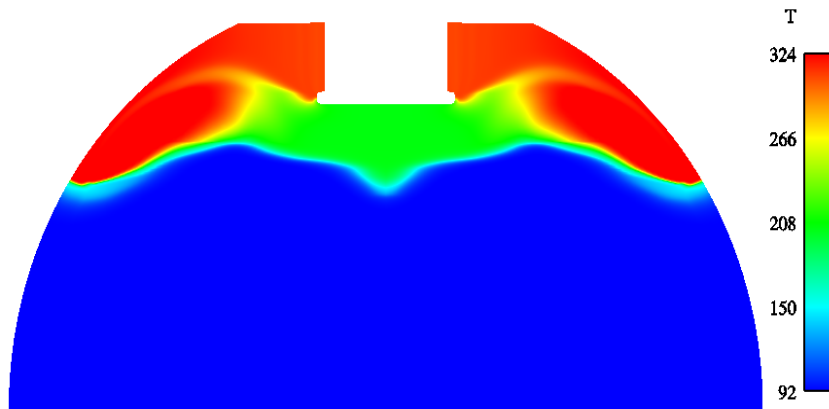
Temperature Distribution



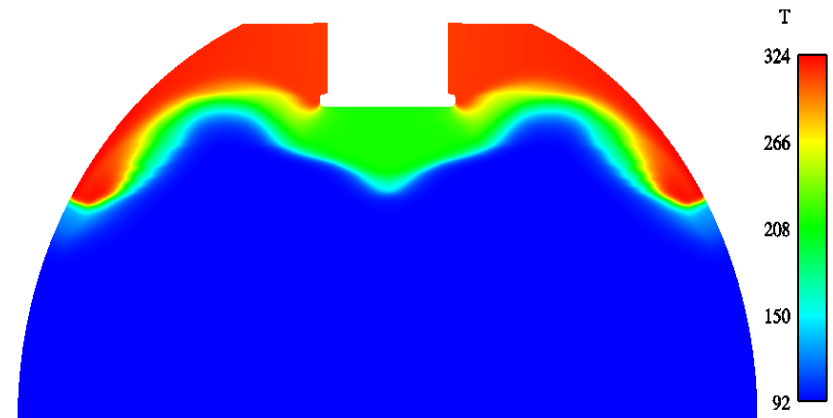
$T = 0.05$ secs



$T = 0.1$ secs



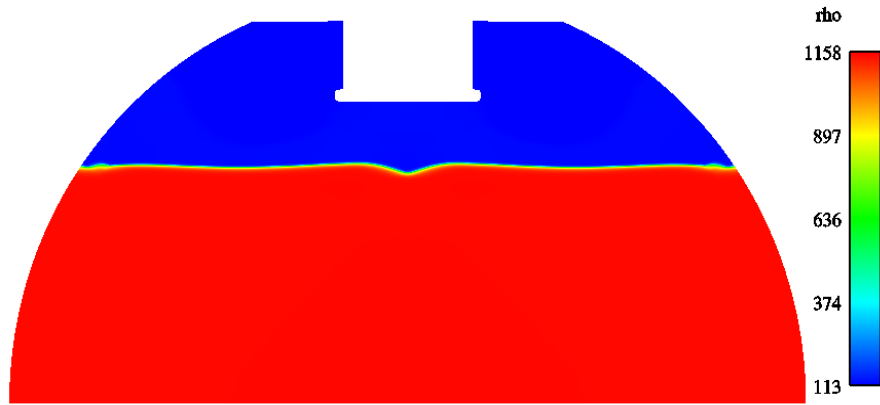
$T = 0.2$ secs



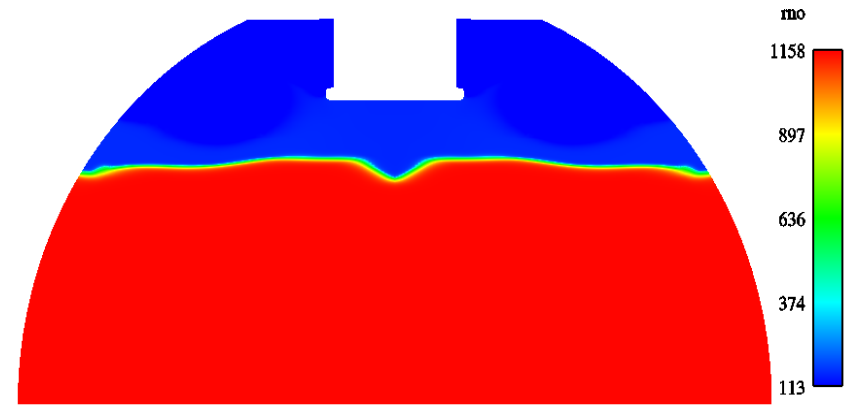
$T = 0.3$ secs

PRESSURIZATION OF LOX TANK (cont)

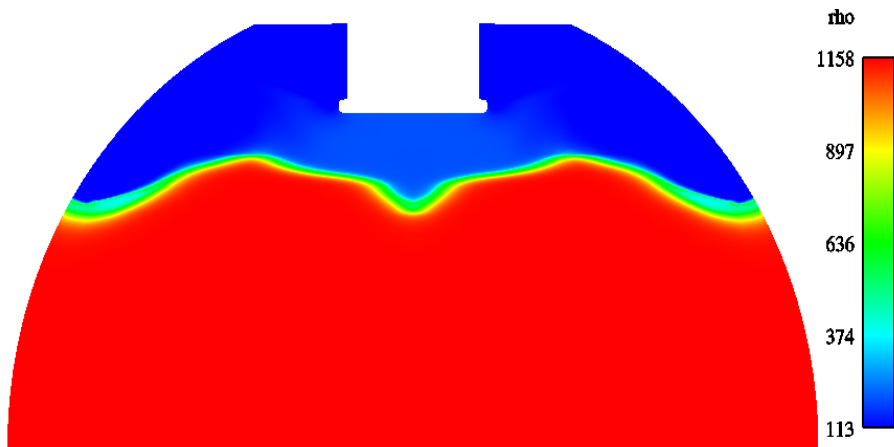
Density Distribution



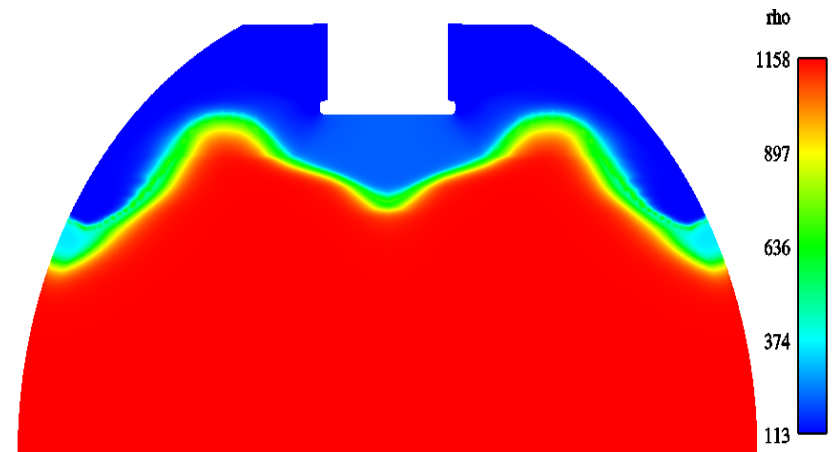
T = 0.05 secs



T = 0.1 secs



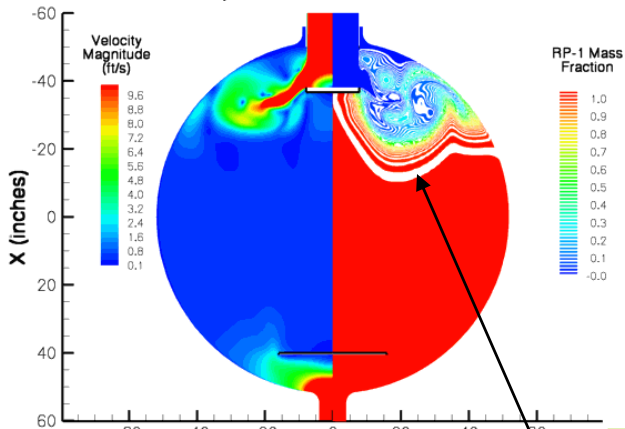
T = 0.2 secs



T = 0.3secs

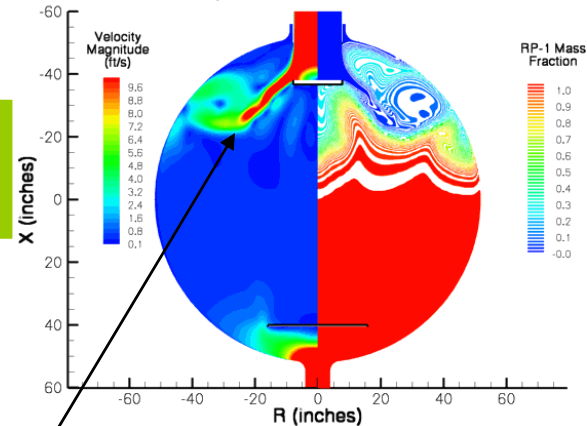
Propellant Drain Tank Modeling

E1 High Volume High Pressure RP-1 Tank
RP-1 Mass Flow Rate = 1050 lb/sec
N2 Mass Flow Rate = 550 lb/sec
Tank Pressure = 8500 psi
Elapsed Time = 1150 milliseconds



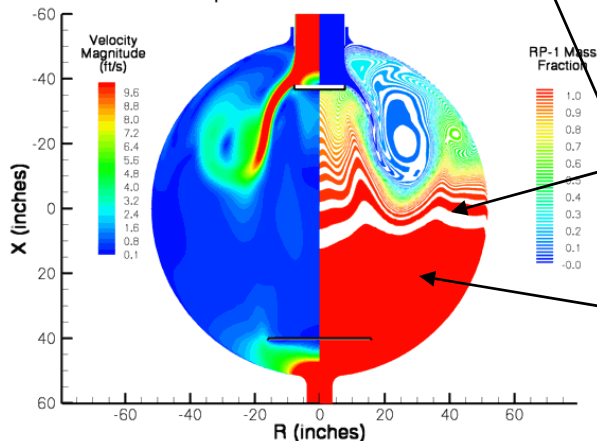
Evolution of RP-1
pressurization
with nitrogen

E1 High Volume High Pressure RP-1 Tank
RP-1 Mass Flow Rate = 1050 lb/sec
N2 Mass Flow Rate = 550 lb/sec
Tank Pressure = 8500 psi
Elapsed Time = 2275 milliseconds



Velocity Distribution

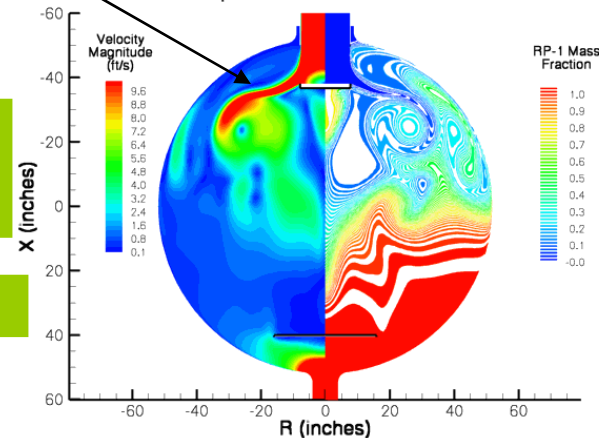
E1 High Volume High Pressure RP-1 Tank
RP-1 Mass Flow Rate = 1050 lb/sec
N2 Mass Flow Rate = 550 lb/sec
Tank Pressure = 8500 psi
Elapsed Time = 3400 milliseconds



Nitrogen
contamination
front

RP-1 mass fraction

E1 High Volume High Pressure RP-1 Tank
RP-1 Mass Flow Rate = 1050 lb/sec
N2 Mass Flow Rate = 550 lb/sec
Tank Pressure = 8500 psi
Elapsed Time = 5650 milliseconds



7/15/2008

SUMMARY

- Advanced Gas/Liquid Framework with Real Fluids Property Routines
 - A multi-fluid formulation in the preconditioned CRUNCH CFD® code developed where a mixture of liquid and gases can be specified
 - Various options for Equation of state specification available (from simplified ideal fluid mixtures, to real fluid EOS such as SRK or BWR models)
 - Vaporization of liquids driven by pressure value relative to vapor pressure and combustion of vapors allowed
 - Extensive validation has been undertaken
 - Currently working on developing primary break-up models and surface tension effects for more rigorous phase-change modeling and interfacial dynamics
- Framework Applied to Run-time Tanks at Ground Test Facilities
- Framework Used For J-2 Upper Stage Tank Modeling
 - NASA MSFC tank pressurization
 - Hydrogen and oxygen tank pre-press, repress and draining being modeled at NASA MSFC.
 - NASA AMES tank safety effort
 - liquid hydrogen and oxygen are separated by a baffle in the J-2 tank. We are modeling pressure rise and possible combustion if a hole develops in the baffle and liquid hydrogen leaks into the oxygen tank. Tank pressure rise rates simulated and risk of combustion evaluated.