

Simulations of Cryogenic Line Chillo down with Advanced Sub-Grid Wall Boiling Models

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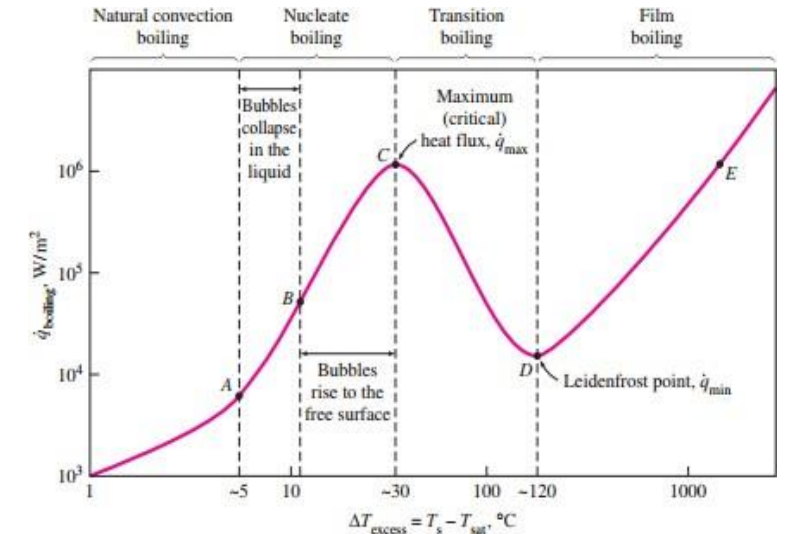
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Motivation

- Predictions of chilldown in cryogenic transfer lines requires improved understanding of boiling process and surface heat transfer
 - Due to operation close to the Critical Point; Large Variability in Properties including Specific Heat and Thermal Conductivity
 - Physics of Nucleation/Microlayer and bubble dynamics not well understood
- Accurate modeling of critical heat flux and departure from nucleate boiling critical to estimating surface temperature history and quenching
 - Difficult to characterize heat flux directly with correlations; predictions come with large error bands and uncertainty
 - Data for water does not correlate well due to much larger thermal effects of phase change
 - Higher Reynolds number results in increased sensitivity of heat transfer to roughness



Boiling Curve

Motivation (Contd.)

- In collaboration with Prof. Emilio Baglietto at MIT as part of a NASA funded program, advanced boiling sub-models for cryogenics are being developed
 - Experimental test program at MIT in liquid nitrogen to generate data for cryogenic fluids
 - New boiling correlations for cryogenics being developed from test data
- Present effort employs earlier models developed for water that have been adapted for cryogenic fluids by employing thermodynamic similarity scaling
- Sub-grid models with thermodynamic scaling have been tested and demonstrated for line chilldown in both liquid nitrogen and liquid hydrogen
 - Quenching prediction in liquid nitrogen for Test 40 of experiments by Darr et al.
 - Quenching prediction in liquid hydrogen for Test 8b of experiments by Hartwig et al.

Darr, S.R., Hong Hu, Glikin, N.G. Hartwig, J.W. et al. "An experimental study on terrestrial cryogenic transfer line chilldown I. Effect of mass flux, equilibrium quality, and inlet subcooling", *Intl Journal of Heat and Mass Transfer*, 103, December 2016.

Hartwig J.W., Styborski, J. et al. "., "Liquid Hydrogen line chilldown experiments at high Reynolds Numbers II. Analysis " *Intl Journal of Heat and Mass Transfer*, 156, 2020.

Outline

- Overview of boiling sub-models and thermodynamic scaling modifications for boiling parameters in cryogenic fluids
- Overview of CRUNCH CFD[®] numerical framework and implementation of boiling model
- Simulations of line chilldown in liquid nitrogen and comparisons with data for Test 40 of experiments by Darr et al.
- Simulations of line chilldown in liquid hydrogen and comparisons with data for Test 8b of experiments by Hartwig et al.
 - Sensitivity studies to various physical parameters conducted to better understand the rapid chilldown in liquid hydrogen
- Conclusions

Cryogenic boiling model development

Pool Boiling Test Data in Liquid Nitrogen

Florian Chavagnat and Prof. Baglietto
Massachusetts Institute of Technology

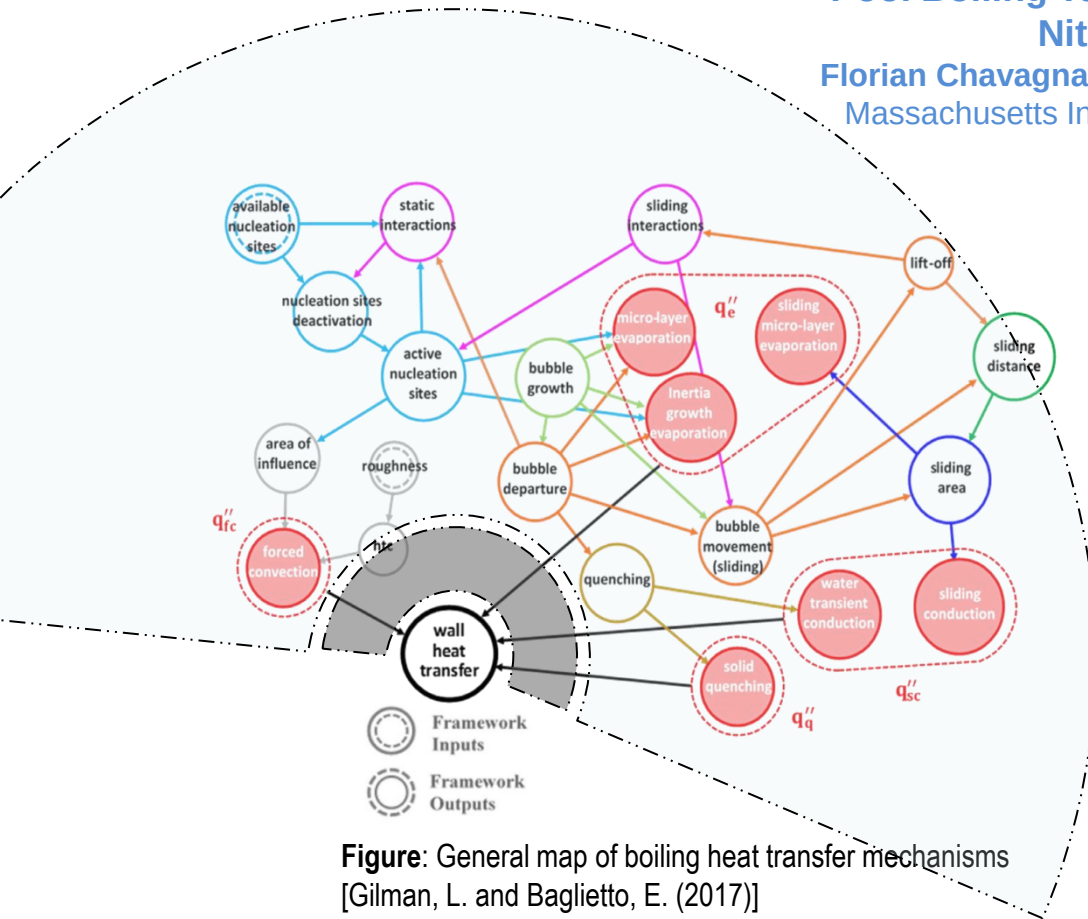
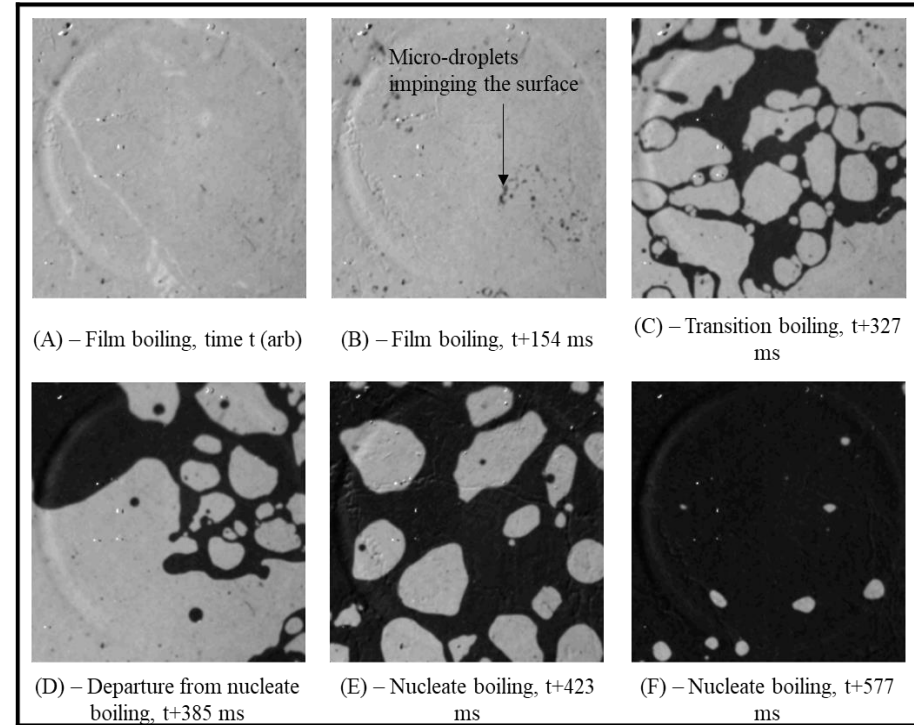


Figure: General map of boiling heat transfer mechanisms
[Gilman, L. and Baglietto, E. (2017)]



Objectives:

- Efficient and flexible Cryogenic Boiling Implementation
- Focus is to “reduce” complexity in favor of numerical efficiency
- Allow for rapid evolution with availability of new Cryogenic data

From NASA Phase II SBIR 80NSSC20C0195 Final Report “Simulation of Chillardown Process with a Sub-Grid Boiling Model” July 2023

Baseline Boiling Sub-Model for Water

Wall Heat Flux Partitioning at Solid Surface

$$q''_{tot} = q''_c + (1 - VOF)(q''_q + q''_e) \leftarrow \text{Evaporative}$$

Computed From CFD
Computed From Boiling Model

Quenching Heat Flux Term

$$q''_q = h_q (T_w - T_q)$$

Del Valle
Kenning
Model

$$h_q = 2K_q f \sqrt{\frac{\rho_l c_{pl} k_l t_w}{\pi}}$$

$$K_q = F_A \frac{\pi D_d^2}{4} N'' \quad t_w = \frac{C_w}{f}$$

Evaporative Heat Flux Term

$$q''_e = N'' f \frac{\pi D_d^3}{6} \rho_g h_{lg}$$

$$f = \sqrt{\frac{4g(\rho_l - \rho_g)}{3D_d \rho_l}}$$

Bubble Departure Frequency
(Cole, 1983)

$$D_d = d_1 \theta \left(\frac{\sigma}{g \Delta \rho} \right)^{0.5} \left(\frac{\Delta \rho}{\rho_g} \right)^{0.9}$$

Bubble Departure Diameter
(Kocamutafaogullari, 1983)

$$N'' = \left(m \Delta T_{sup} \right)^p$$

Nucleation Site Density
(Lemmert-Chawla Model, 1977)

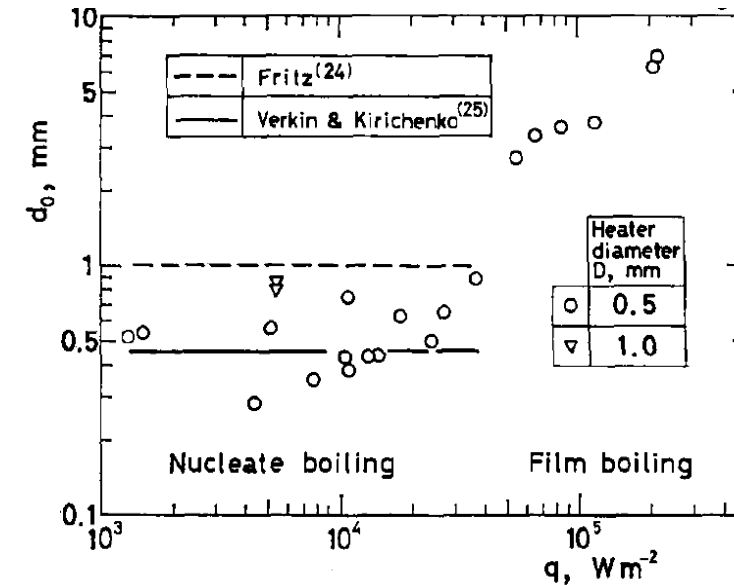
- Accurate prediction of wall heat flux depends on sub models for bubble departure frequency and diameter as well as bubble nucleation site density
- Key parameter that requires calibration is the parameter d_1 in the model for bubble departure diameter
- Constants used for boiling in water are inadequate for cryogenics and result in bubble departure diameters that are orders of magnitude lower

Evaluation of Baseline Sub Model for Cryogenics

- Test data from pool boiling data for liquid nitrogen (Kida et al, 1981) shows bubble diameters of 0.5-1 mm
- Boiling correlations for water yield bubble diameter values of 0.05 mm (an order of magnitude lower)
- Thermodynamic effects due to proximity to critical point may be the cause of this discrepancy
- Large disparity in liquid to vapor density ratio results requires recalibration of parameter in bubble departure diameter formulation

$$D_d = d_1 \theta \left(\frac{\sigma}{g \Delta \rho} \right)^{0.5} \left(\frac{\Delta \rho}{\rho_g} \right)^{0.9}$$

Constant d_1 needs to be recalibrated for cryogenics



Property	Water at 0.12 MPa	Nitrogen at 0.12 MPa
Surface Tension (N/m)	0.058	0.008
Liquid Density (kg/m ³)	954.8	800
Vapor Density (kg/m ³)	0.7	5.35
Density Ratio	1,364	149.5

Large Disparity in Density Ratio of Vapor to Liquid between Water and Nitrogen

Thermodynamic Similarity Scaling for Cryogenics

Step 1:

Get equivalent “reduced” pressure in water to evaluate

$$P_{Eq} = P_{c-w} \frac{P_{n2}}{P_{c-n2}}$$

Step 2 :

Evaluate constant d_1 in water using test data or correlations for bubble departure diameter at this pressure

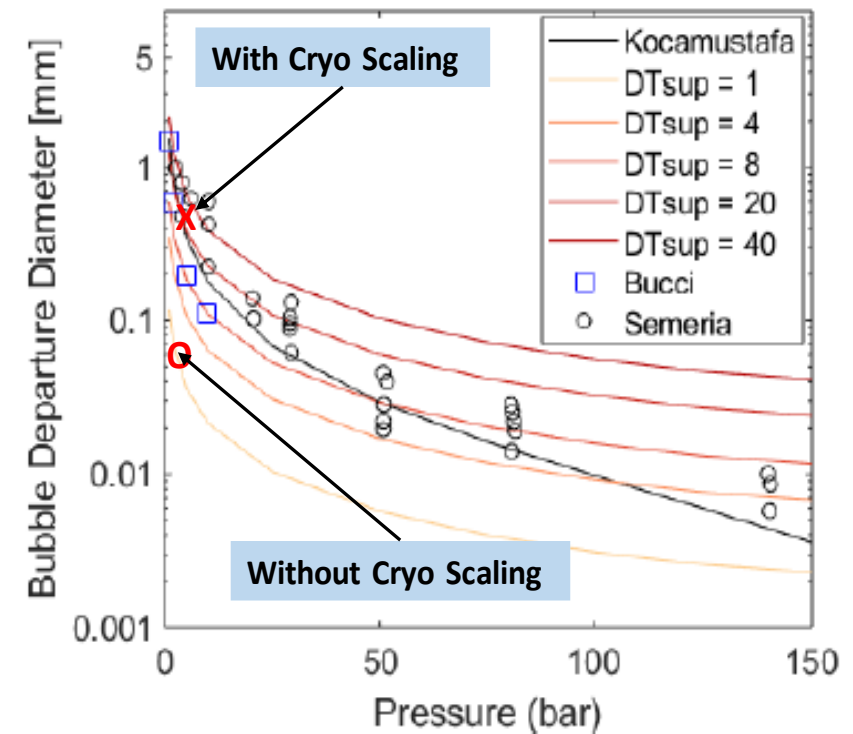
$$d_{1,w} = \frac{D_{d,w}}{\theta \left(\frac{\sigma}{g \Delta \rho} \right)^{0.5} \left(\frac{\Delta \rho}{\rho_g} \right)^{0.9}}$$

Step 3 :

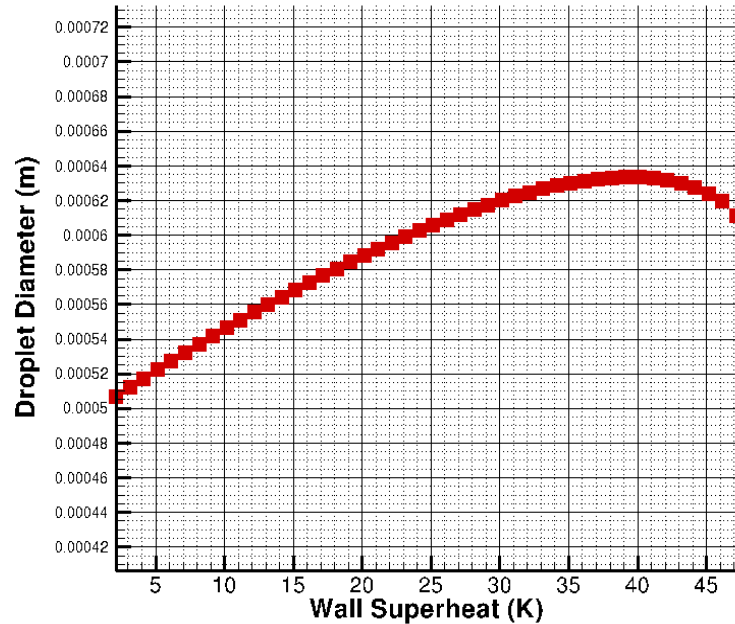
Scale Evaluate constant d_1 in water with ratio of liquid to vapor density

$$\left(d_{1w} \frac{\rho_L}{\rho_v} \right)_{water} = \left(d_{1n} \frac{\rho_L}{\rho_v} \right)_{Cryogenic}$$

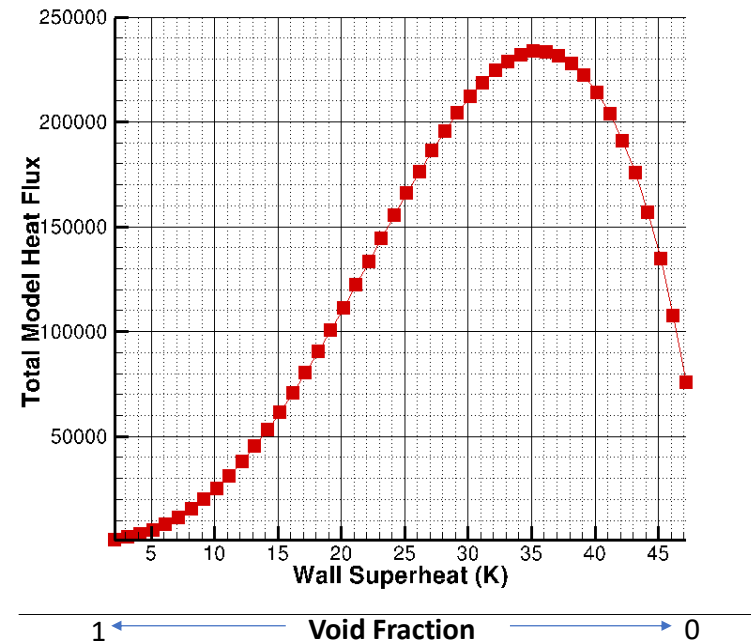
Bubble Departure Diameter :
Comparison of value for water and cryogen



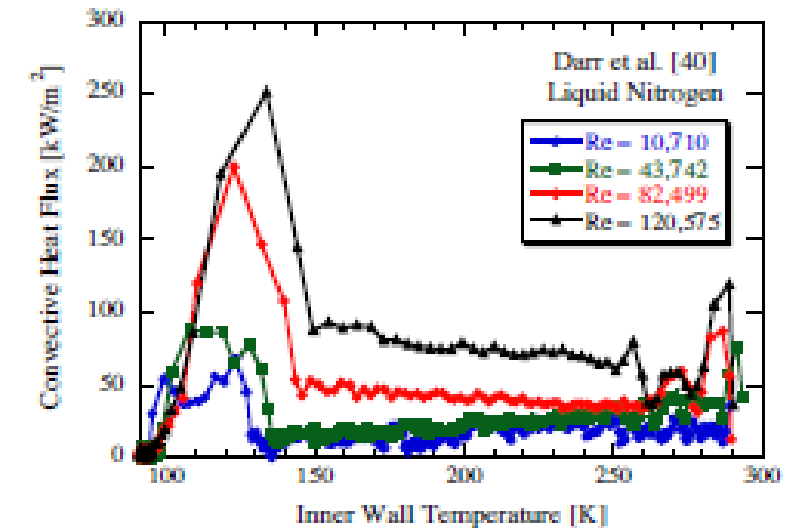
Sub-Model Behavior with Cryogenic Scaling: Liquid Nitrogen



Bubble Departure Diameter from Boiling Model ~ 0.5 mm



Total Heat Fluxes from Boiling Model



Measured Heat Fluxes from Darr et al.

CRUNCH CFD® Multi-Physics Framework

Compressible Solver (CRUNCH COMP)

- Generalized “all-speed” preconditioned flow solver for compressible fluids
- *Robust* Non-ideal/real fluid equations of state with utility for NIST table generation
- Advanced turbulence models with *accurate* roughness modeling
- Chemistry manager allows reaction mechanisms specified in Chemkin/Cantera formats
- Non-equilibrium dispersed phase via Eulerian formulation
- Grid motion for moving bodies

Incompressible Solver (CRUNCH INCOMP)

- Incompressible/weakly compressible multi-phase flow solver for cavitating liquids
- Cryogenic fluids: thermal effects modeled
- Grid motion for moving bodies

Thermal Solver (CRUNCH THERMAL)

- Heat conduction module
- Coupled COMP/THERMAL calculations via heat transfer BC

CRISP CFD

- Grid adaptation tool for unstructured grids with error quantification
- Adaptation for mesh deformation due to moving boundaries
- Adaptation based on flow features

Preconditioned All-Speed Compressible Formulation

• Generalized Preconditioned Formulation

- Solves for pressure and temperature instead of density and internal energy to overcome stiffness issues. Pressure and temperature are always well-defined even for stiff systems
- Techniques used for traditional “density” based codes can be used for this formulation now by casting it in time-marching form

• Versatile Thermodynamics

- Matrices retain derivatives in generalized form
- **Allows specification of generalized EOS routines without modifying the code numerical formulation**
- Specifically, enthalpy can be a function of pressure and temperature e.g., cryogenic fluids
- Speed of sound of generalized fluid determined by the eigenvalues of matrix [A]

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

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

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

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

$$\rho = F(P, T, Y_i),$$

$$h = G(P, T, Y_i)$$

Thermodynamic Property Evaluation cont.

- EoS specification can either be through analytical formulations (e.g. SRK) or through NIST table look-up
 - Ability to handle real fluid properties and large “spiky” gradients near critical point
- Phase change models for cryogenic fluids with thermodynamic effects rigorously accounted for
 - Equilibrium framework: Robust, inexpensive and well validated for near critical condensation and cavitation. Phase change with finite-rate driving fluid to equilibrium
 - Non-Equilibrium: dispersed Lagrangian phase with velocity and temperature non-equilibrium. Hertz-Knudsen phase change formulation
- Extensive validation for both cavitation and condensation phase change for liquid nitrogen, hydrogen, oxygen and near critical CO₂

Hosangadi, A. and Ahuja, V., “Numerical Study Of Cavitation In Cryogenic Fluids,” Journal of Fluids Engineering, Vol. 127, pp. 267-281, March 2005

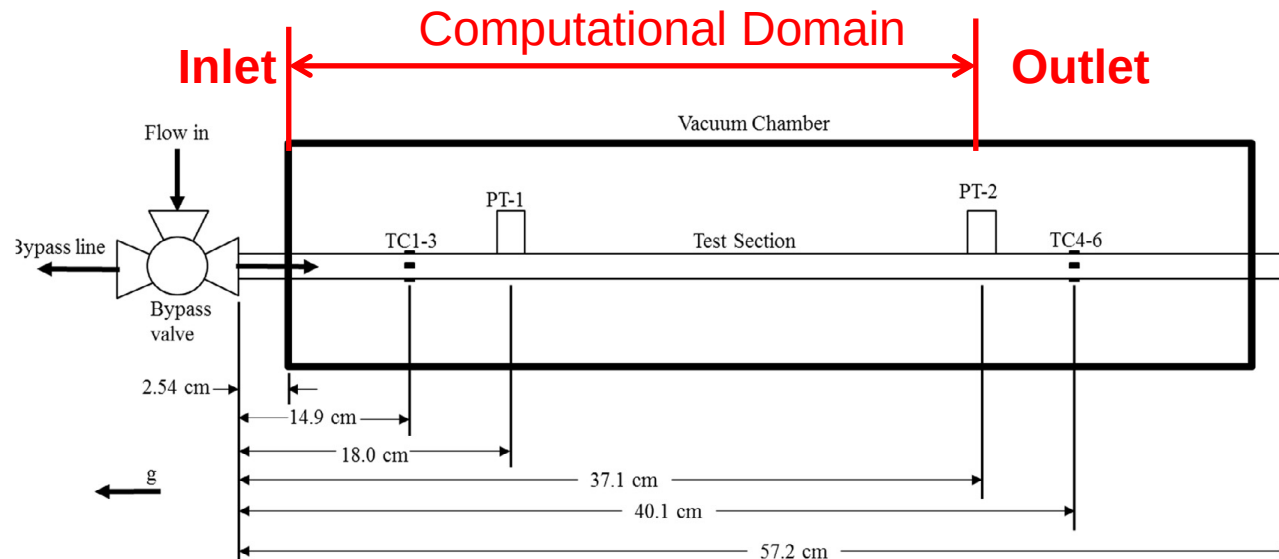
Hosangadi, A., Ahuja, V., and Ungewitter, R.J., “Simulations of Rotational Cavitation Instabilities in the SSME LPFP Inducer,” Paper No. AIAA-2007-5536, 43rd AIAA/ASME/SAE/ASEE Joint Propulsion Conference & Exhibit, Cincinnati, OH, July 8 – 11, 2007.

Hosangadi, A., Liu, Z., Weathers, T, Ahuja, A., and Busby, J., “Modeling Multiphase effects in CO₂ Compressors at Subcritical Inlet Conditions”, *J. Eng. Gas Turbines Power*, August 2019, 141: 081005-1

Quenching in Liquid Nitrogen Flows

Quenching in Liquid Nitrogen Under Terrestrial Conditions

- Chillydown with Tube in Vertical Upward Configuration
- Liquid Nitrogen Fed From a Dewar; Test Section in Vacuum chamber
- Saturated and Sub-cooled Conditions at the Inlet
 - Darr, S. R., et al., "An experimental study on terrestrial cryogenic transfer line chillo down I. Effect of mass flux, equilibrium quality, and inlet subcooling," *Intl J. of Heat and Mass Transfer*, Vol. 103, 2016.
- Used Precooler to Condition Flow before Injection in Test Section
- Test 40 from Darr Test Matrix Simulated



AVERAGE INLET CONDITIONS

$$G_{\text{inlet}} \text{ (mass flux)} = 327.82 \text{ kg/m}^2\text{s}$$

$$P_{\text{inlet}} = 325.9357 \text{ kPa}$$

$$T_{\text{inlet}} = 86.61 \text{ K}$$

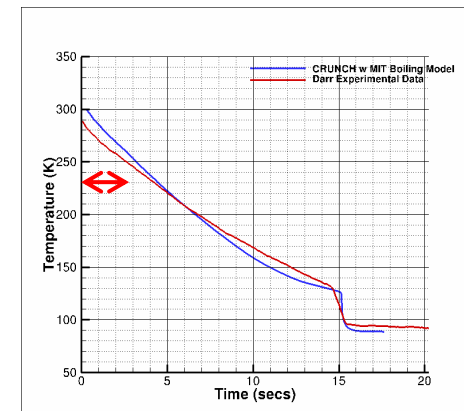
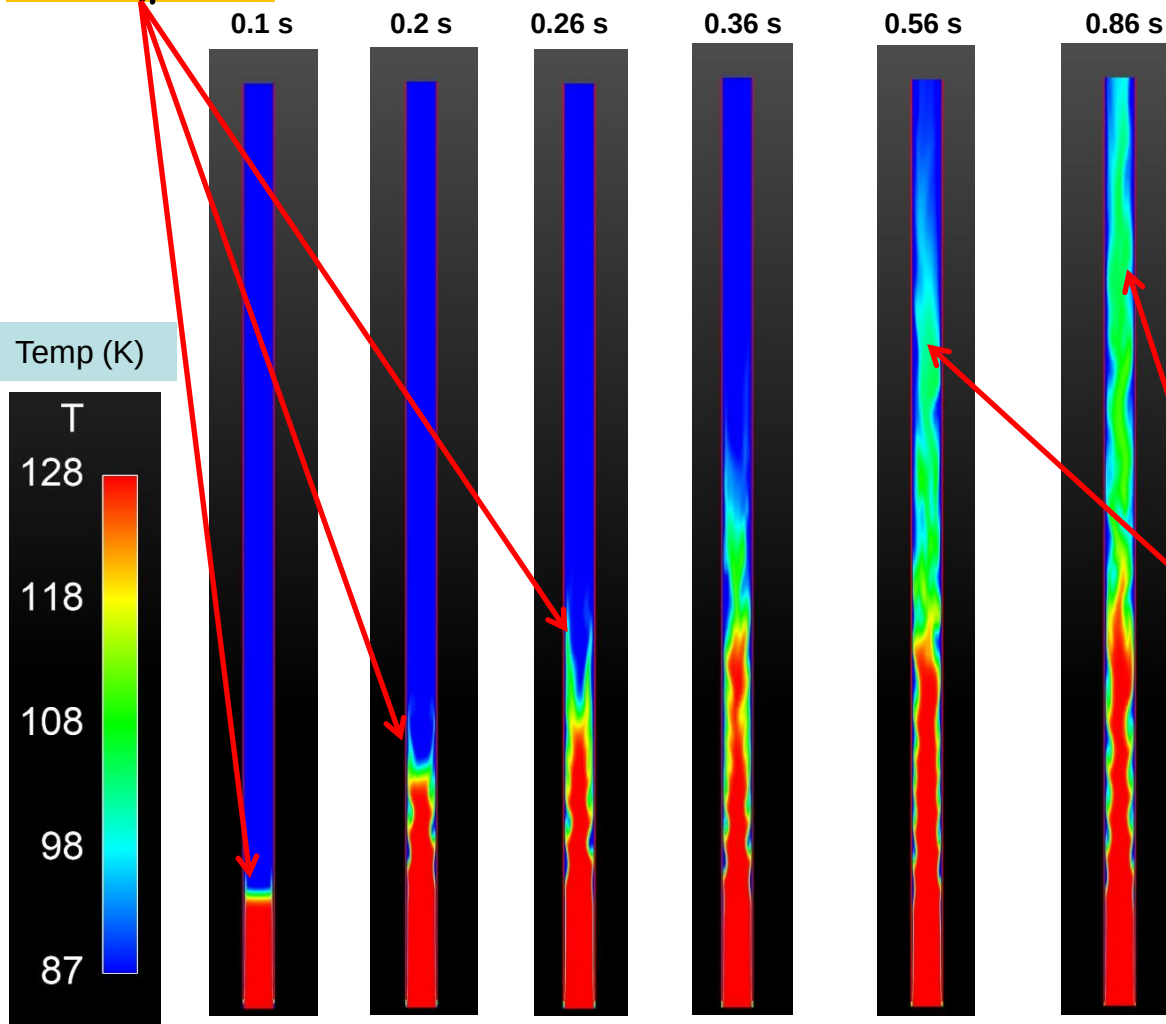
$$T_{\text{sub}} = T_{\text{sat}}(P_{\text{inlet}}) - T_{\text{inlet}} = 2.23$$

$$\alpha_{\text{inlet,liq}} = 1.0$$

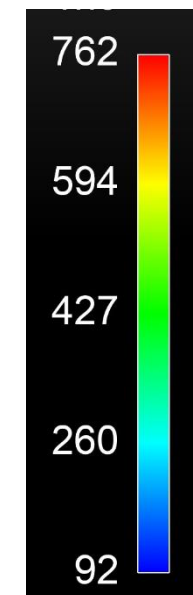
Early Evolution of Flow in Vertical Tubes

Low Inflow Velocity and Sub-Cooled Inlet leads to an Annular Front

Walls show Temperature distribution; Tubes show density distribution



Mixture Density kg/m^3



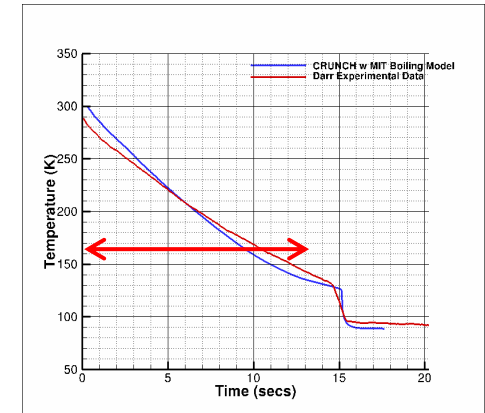
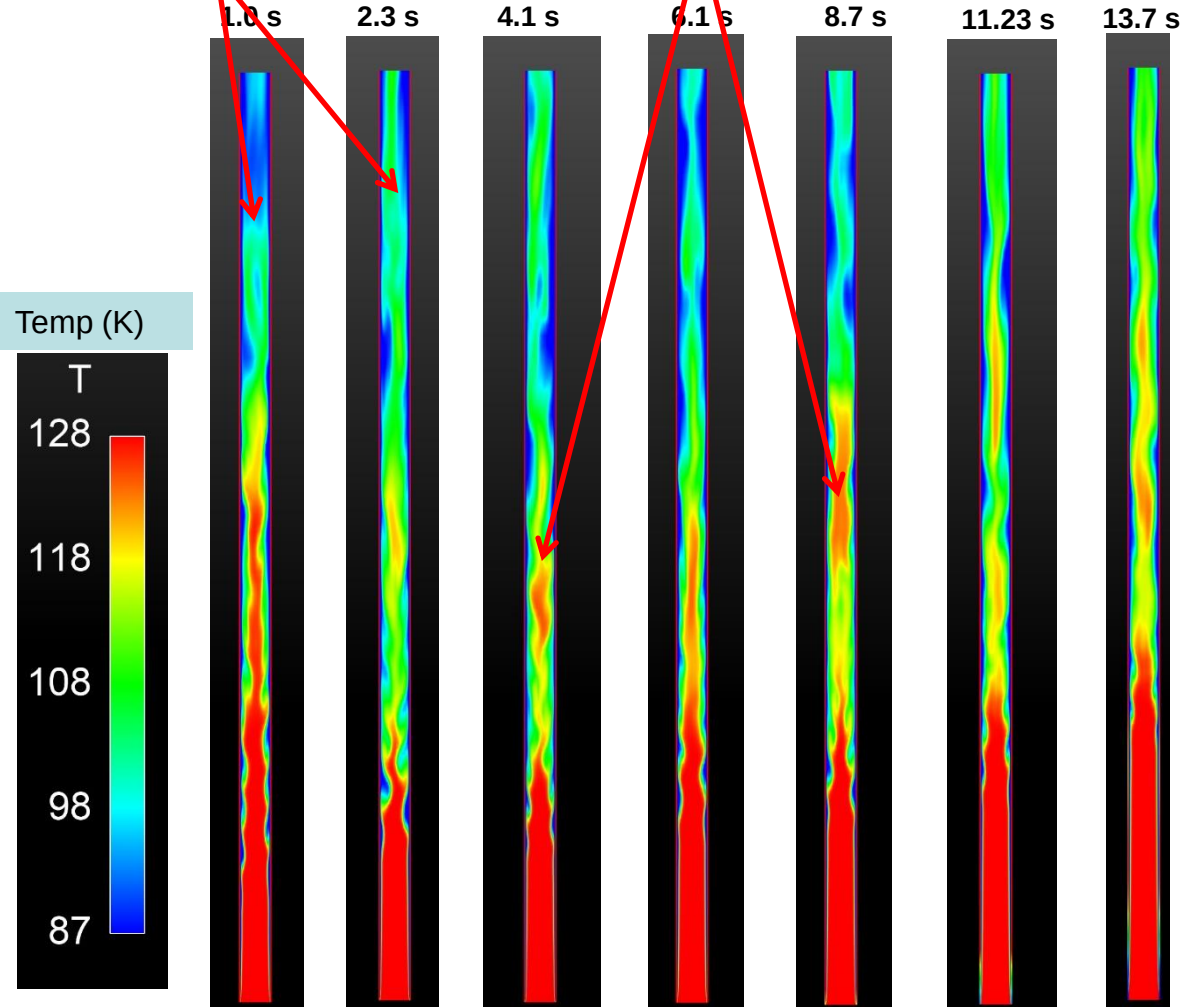
Strong Instability leads to two-phase flow. Misty Appearance of Flow in most of the tube

Evolution of Flow in Vertical Tubes After Initial Stages

Walls show Temperature distribution; Tubes show density distribution

Dispersed Flow in Most of Tube Characteristic of Cryogenic Flows

Ligaments break off

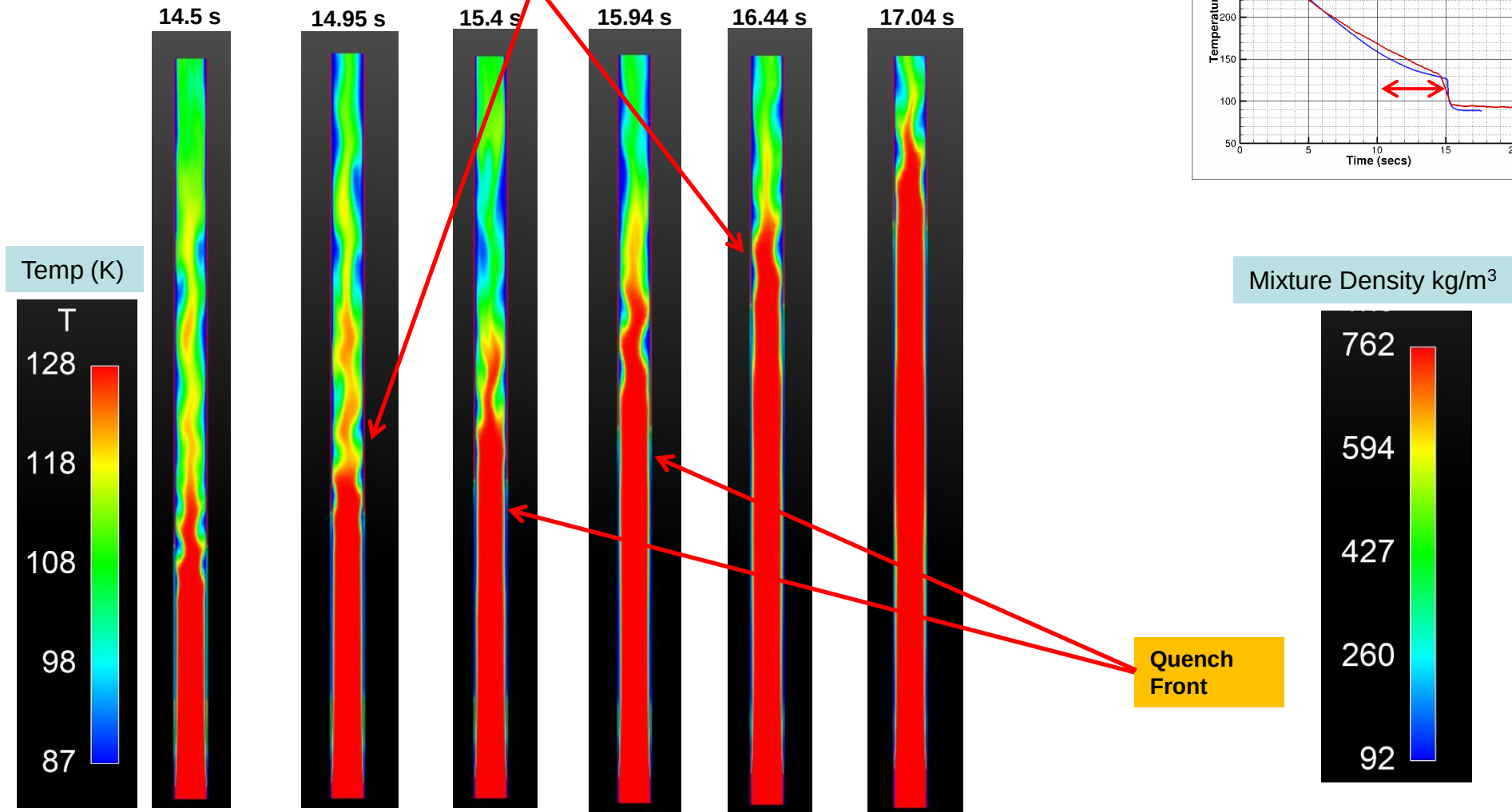


Innovative solutions to complex problems

Late-Stage Evolution of Flow in Vertical Tubes

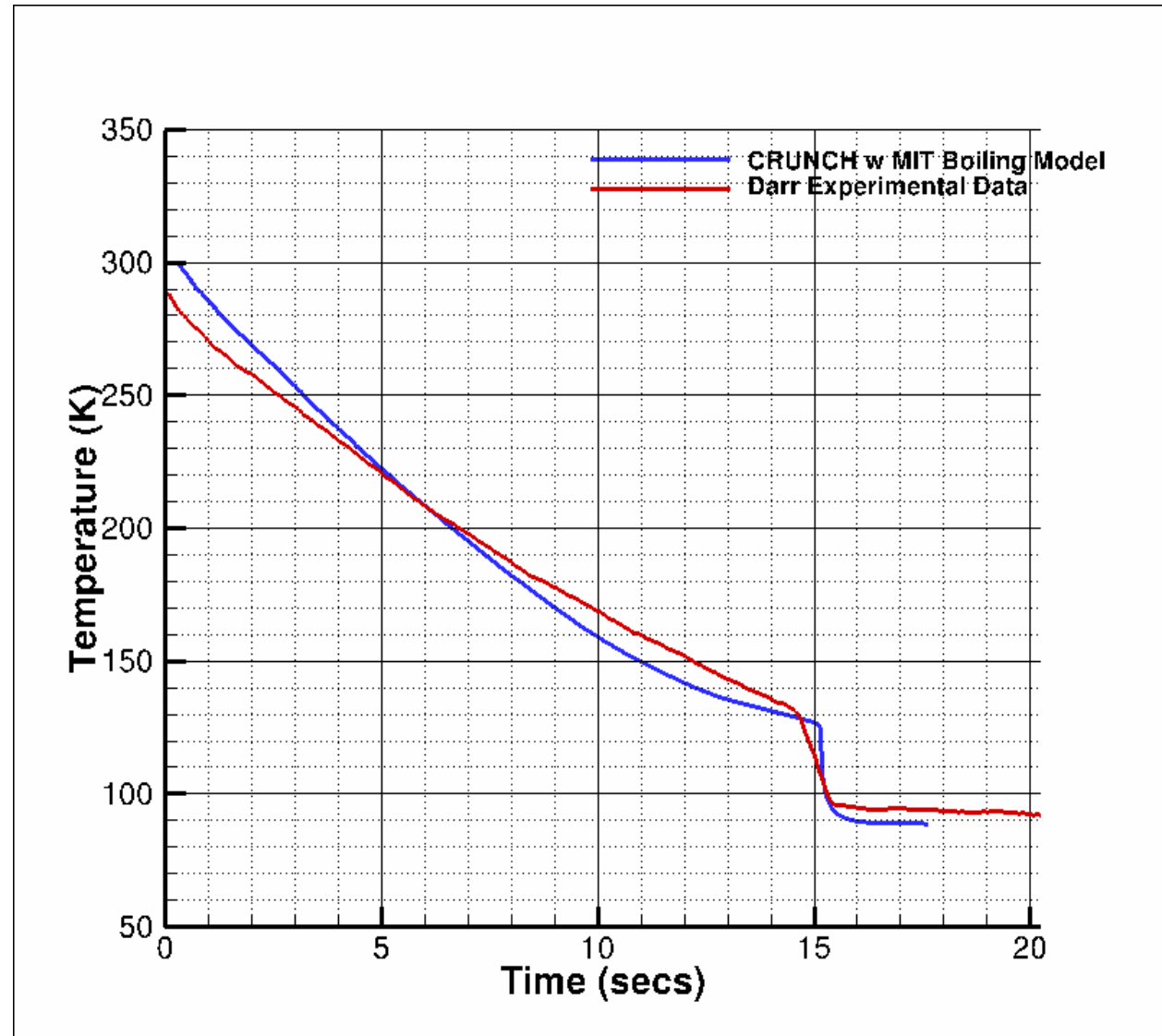
Walls show Temperature distribution; Tubes show density distribution

Rapid Shrinkage of Dispersed Phase Region



Innovative solutions to complex problems

Prediction of Quenching by Boiling Model



Averaged TC1 Data
from Experiment
being Compared with
CFD Trace Values

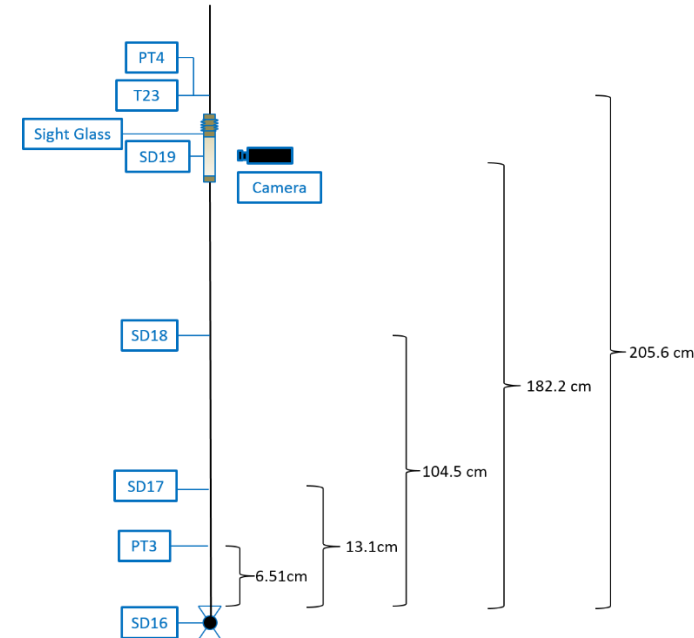
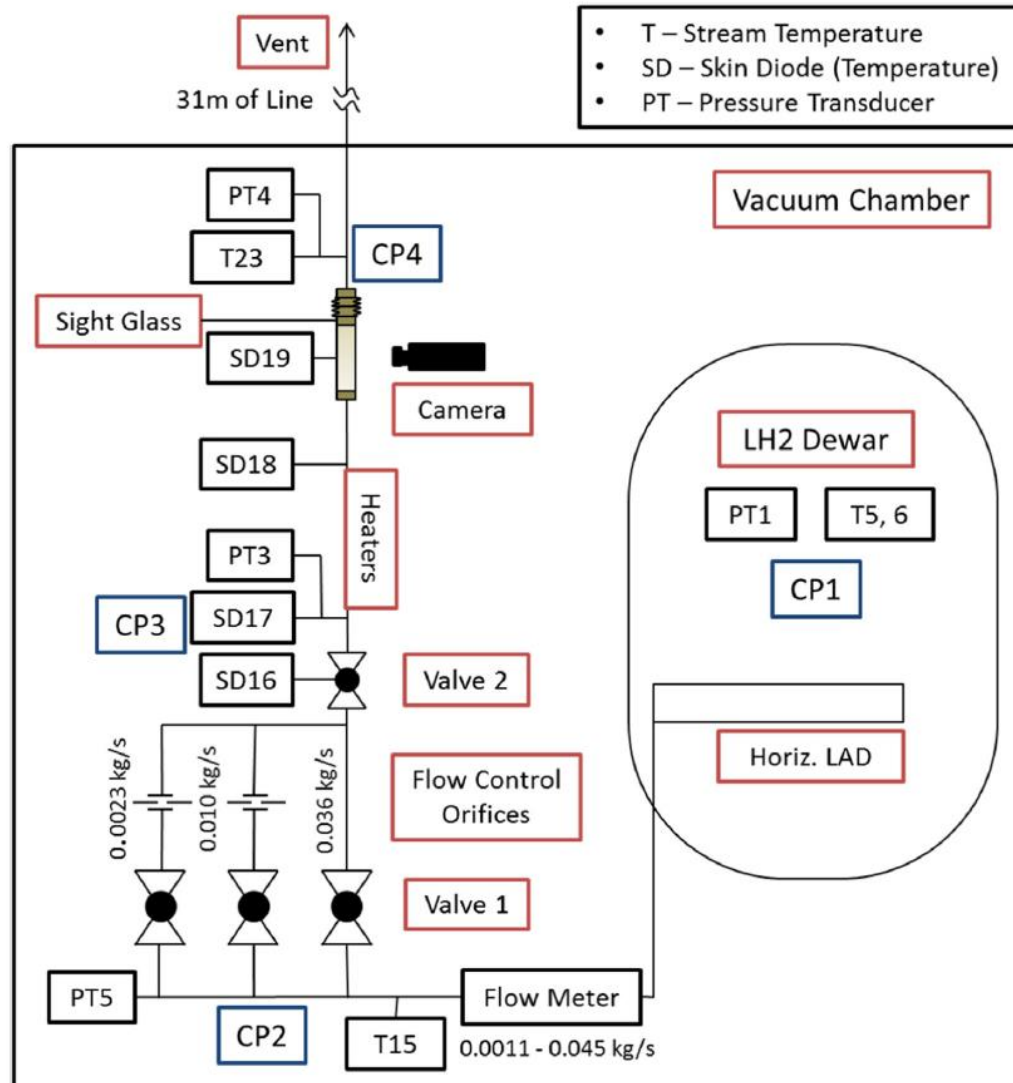
Quenching in Liquid Hydrogen Flows

Overview of Issues with Hydrogen Boiling

- There is a need for improved understanding of hydrogen boiling characteristics for more efficient storage and transfer
- Hydrogen behaves very differently than other cryogenics such as liquid nitrogen
 - Chillover in liquid hydrogen is very rapid and the traditional “knee” in surface temperature curve is not prominent
 - Hydrogen exhibits annular flow with liquid later on the wall and two-phase flow in core as opposed to inverted annular flow in liquid nitrogen
- Simulations of liquid hydrogen line chillover experiments conducted at NASA (Hartwig et al.) were simulated to understand numerical sensitivities and improve understanding of physics

Hartwig J.W., Styborski, J. et al. “., “Liquid Hydrogen line chillover experiments at high Reynolds Numbers II. Analysis ” *Intl Journal of Heat and Mass Transfer*, 156, 2020.

Hydrogen Chillo down Test



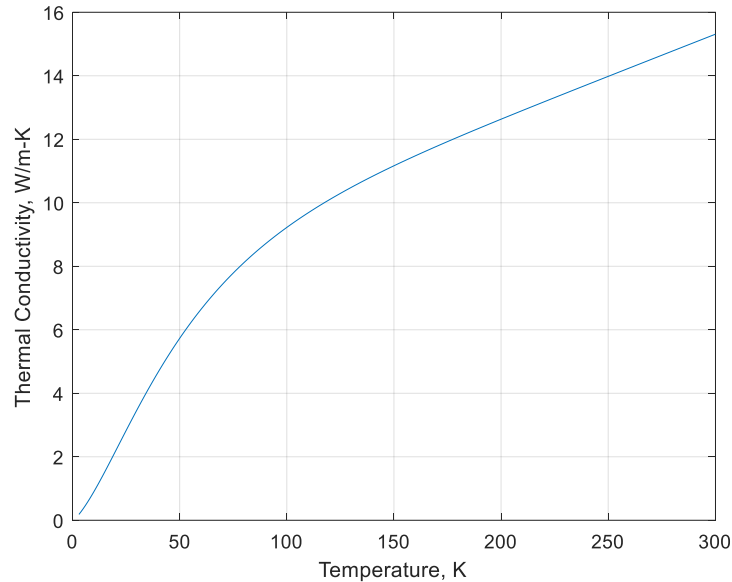
Computational domain: PT3 to SD18 (98 cms)

Mass flux : 400 Kg/m²-s

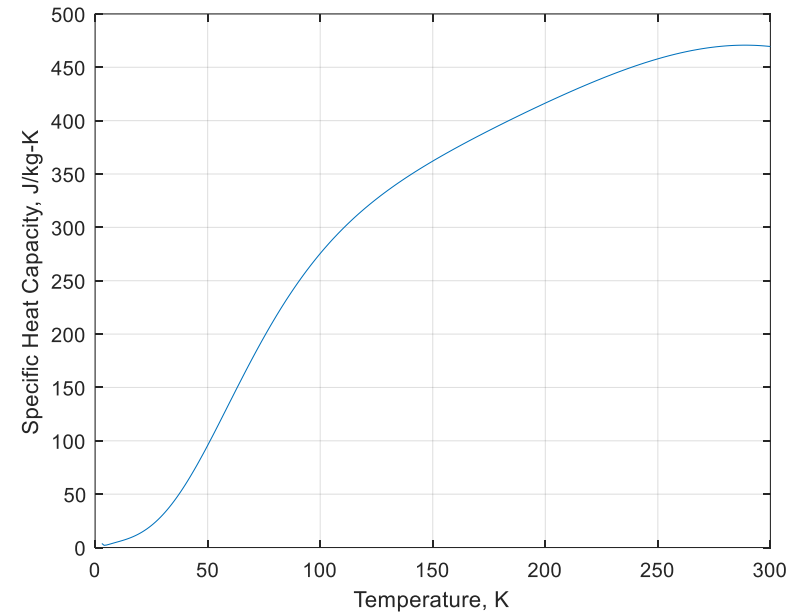
Average Pressure: 0.2 MPa

Liquid Inflow temperature: 23.61 K (0.25 K sub-cooling)

Thermal Properties of Stainless Steel



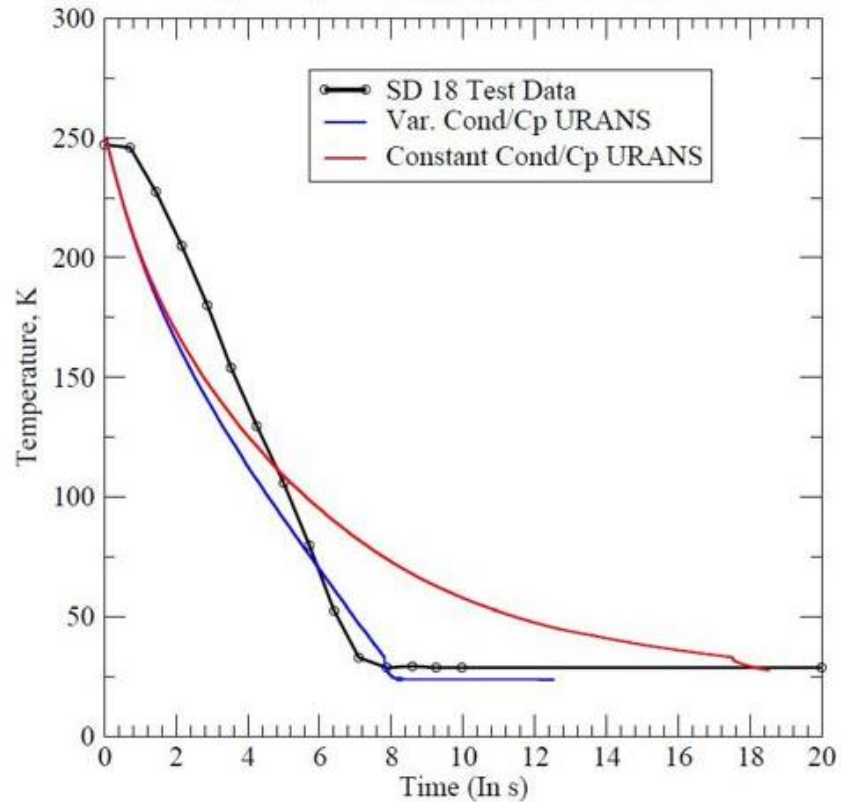
Thermal Conductivity



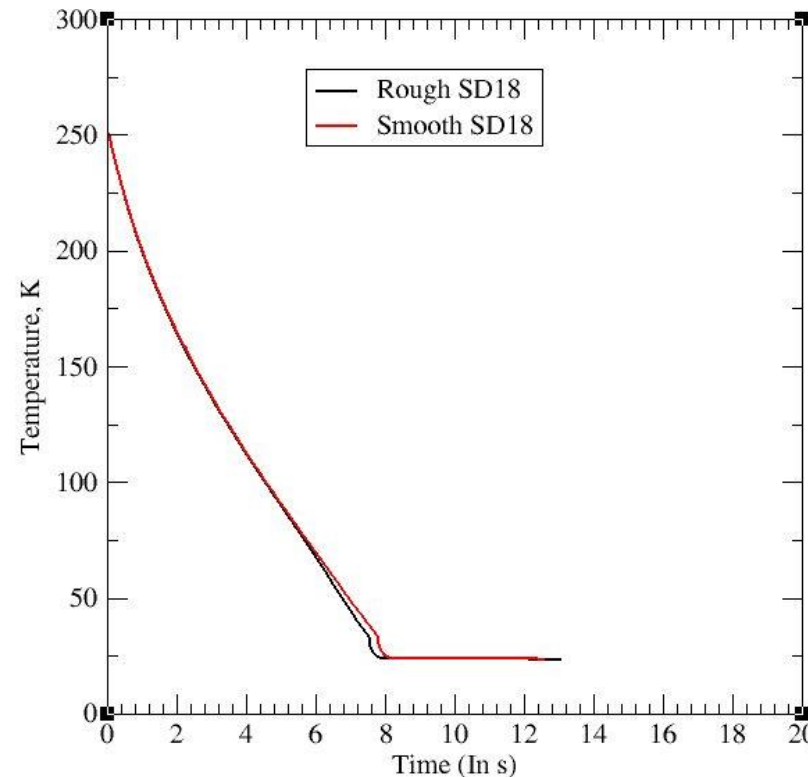
Specific Heat

- Lower thermal conductivity sustains large temperature gradient in solid for the same heat flux
- Similarly lower specific heat leads to larger temperature drop with time
- Combination of these effects leads to more rapid rate of temperature drop

Chiltdown Temperature History: Sensitivity Studies



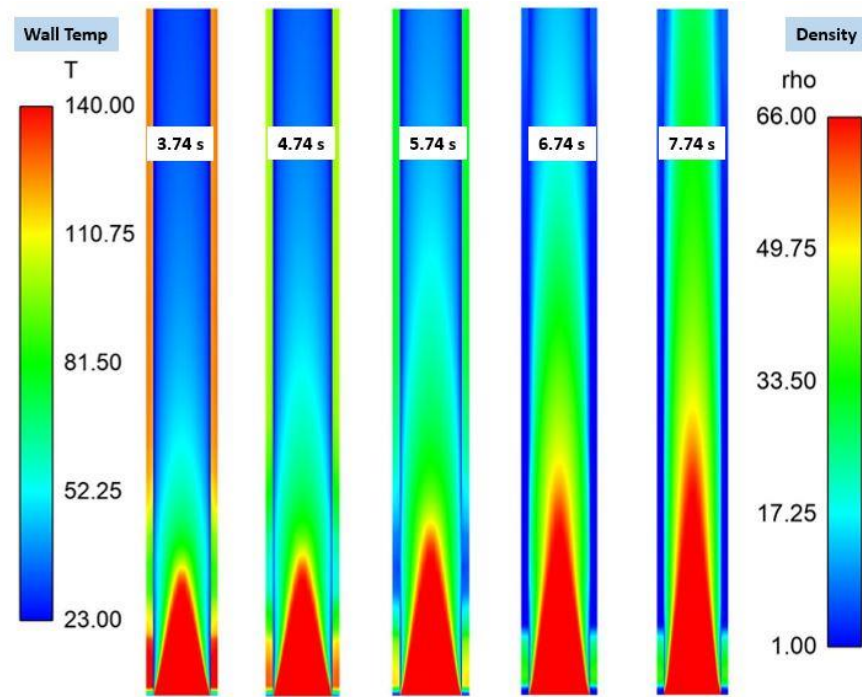
**Effect of Variable Material Properties
For Stainless Steel Compared with
Constant Material Properties**



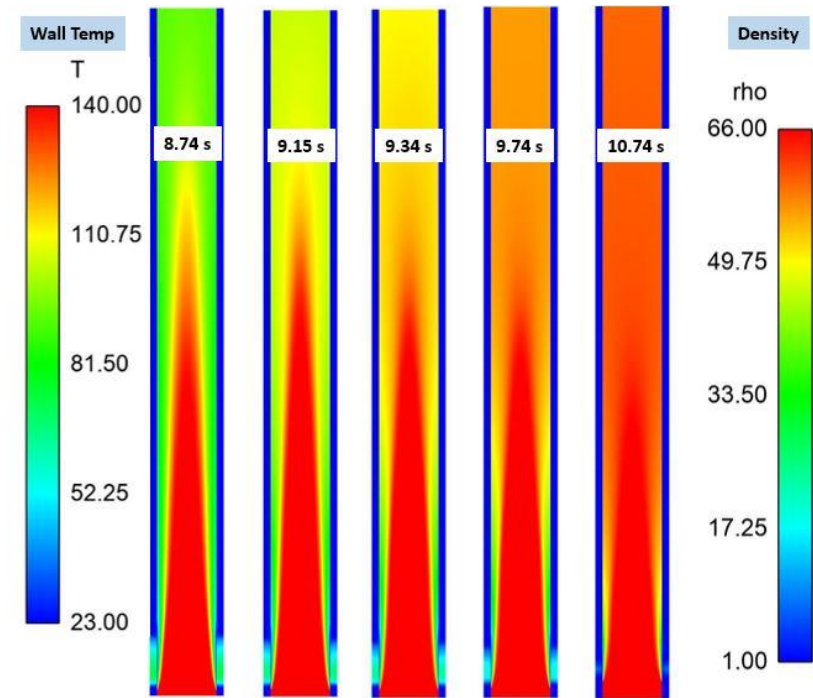
**Effect of Surface Roughness for Inner
Wall**

- Specifying variable thermal properties for solid material critical for obtaining accurate chiltdown profile
- Due to rapid slope in film cooling, “knee” from quenching has very small drop in temperature

Fluid Density and Wall Temperature



Flow Evolution Before Quenching



Flow Evolution after Onset of Quenching

- Unlike in liquid nitrogen where a liquid front advances, here we observe a two-phase core in the pipe close to equilibrium. Quenching proceeds with the density in the core rising rather than an advancing liquid front
- Present simulations were done with a sub-cooled liquid at inlet. For annular flow we likely will require a two-phase saturation inflow at inlet

Conclusions

- Advanced boiling sub-models developed in collaboration with MIT have been implemented in CRUNCH CFD®
 - Adapted for cryogenic fluids with thermodynamic scaling concepts based on reduced pressures and temperature relative to critical point
 - Mechanistic representation of physics at the boiling wall that explicitly tracks bubble parameters
- The boiling sub-model was tested in liquid nitrogen for Test 40 of experiments by Darr et al.
 - Temperature history at TC1 showed good comparison with test data
 - Wall temperature at which quenching occurs matches well with test data

Conclusions (Cont..)

- Demonstration for quenching in liquid hydrogen performed for Test 8b of Hartwig et al.
 - Flow turbulence effects substantially increase film heat transfer
 - Modeling variable thermal properties of solid particularly at lower temperatures are critical
 - The hydrogen core flow at quenching onset presents as a two-phase mixture in equilibrium as opposed to an advancing liquid front observed in liquid nitrogen flows. After onset of quenching density rises rapidly due to condensation of vapor,
 - More studies are needed to understand how annular quench fronts observed in some liquid hydrogen tests evolve; may require modeling of saturated two-phase flow at inlet as opposed to sub-cooled liquid as currently modeled.

Acknowledgements

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