

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

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A meso-scale model developed at MIT [2][11] for boiling processes in water was adapted for cryogenics and demonstrated for chillover of propellant transfer lines in both liquid nitrogen and hydrogen. The sub-grid boiling model accurately captures the contributions to heat transfer from the generation of bubble nuclei, growth, and interaction of the bubbles in the microlayer as well as quenching of the boiling surface following bubble departure. It was adapted for cryogenic fluids using thermodynamic scaling concepts taking into account non-dimensional pressures and temperatures that are scaled by the corresponding critical values for the fluid. The boiling model was demonstrated for line chillover in liquid nitrogen (Darr et al. [6]). The predicted wall temperature at which quenching occurs was close to the test data while the slope of the temperature curve after quenching is initiated, showing a steeper variation than the test data. Simulations were also performed for liquid hydrogen by simulating experiments of Hartwig et al. [7]. Chillover times in liquid hydrogen are much more rapid due to higher heat transfer in the film boiling regime and accounting for the higher turbulence levels were found to be important. Furthermore, at the much lower fluid temperatures in liquid hydrogen flows, accounting for the variable thermal properties of the solid material is critical and has a dramatic impact on the quench times. The need for additional studies to better understand the evolution of the quench front in liquid hydrogen was noted.

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1.0 Introduction

Efficient chilldown in liquid rocket engines/engine components and tankage is critical to ensure high quality cryogenic propellant devoid of two-phase content delivered to the engines before ignition. To develop high-fidelity design support tools, accurate predictions of transient heat flux to solid surfaces as the fluid transitions through the various boiling regimes is critical. Over the past few decades, several experiments related to the quenching of heated tubes in a cryogenic environment have been carried out to understand and classify the phase change process and the resulting complex two-phase regimes. These studies have established that the phase change process evolves through different stages of film, transition, and nucleate boiling before the walls are quenched and single-phase convective heat transfer between the wall and the cryogenic liquid is restored.

The boiling process has been studied extensively in water due to the broad range of industrial applications including notably the nuclear industry. However, it's unclear if the data for water is directly applicable to cryogenics. The disparity with cryogenics arises from the fact that the thermodynamic regime is much closer to their critical point resulting in higher vapor /liquid density ratios, substantial thermal effects from phase change, and rapid thermodynamic/transport property variations with temperature. Nevertheless, there have been several efforts at developing empirical correlations of the heat transfer coefficient/heat flux for cryogenic fluids (see Hartwig et al. [1] for a review). Popular system level fluid/thermal codes such as GFSSP and SINDA/FLUINT have embedded such correlations with varying levels of sophistication. Hartwig et al. [1] compared predictions from simulations with both codes to cryogenic experimental data sets of liquid nitrogen and liquid hydrogen and found the mean absolute errors (MAE) to be well in excess of acceptable engineering practices and indicating a need for tools that provide much higher fidelity.

The goal of the present effort is to demonstrate a high-fidelity, numerical framework for predictions of quenching and boiling in different cryogenic fluids. In this framework advanced sub-grid scale boiling models derived at MIT from mechanistic principles (Baglietto and coworkers [2]) have been modified and scaled for cryogenic fluids. These models have been incorporated into the CRUNCH CFD[®] [3]-[5] code which has been validated extensively for phase change in cryogenic fluids operating near critical conditions. The sub-grid boiling model will be evaluated for their ability to accurately capture the contributions to heat transfer from the generation of bubble nuclei, growth, and interaction of the bubbles at the wall as well as quenching of the boiling surface following bubble departure. The integrated framework will be demonstrated for line chilldown in liquid nitrogen using the test data of Darr et al. [6]. The framework will subsequently be applied to chilldown in liquid hydrogen by simulating the experimental configuration of Hartwig et al. [7] and additional work needed to further improve predictions particularly for liquid hydrogen discussed.

In the sections to follow, we will give a brief overview of the numerical framework in CRUNCH CFD[®] followed by a discussion of the sub-grid boiling model (Baglietto and coworkers [2]) and the modifications implemented for cryogenic fluids. Simulations of chilldown in liquid nitrogen for the Darr tests [6] will be discussed in detail followed by results for chilldown in liquid hydrogen for the test configuration of Hartwig et al. [7]. Sensitivity studies identifying the effect of variable thermal properties of the stainless-steel pipe wall on the chilldown curve for liquid hydrogen curve are also discussed and our conclusions are summarized.

2.0 Summary of Cryogenic Fluid Framework in CRUNCH CFD[®]

The numerical framework of the CRUNCH CFD[®] software features a preconditioning framework for real fluid systems [8]. One of the key attributes of this numerical formulation is that it alleviates the numerical stiffness resulting from strong thermodynamic property variations both near the critical point, as well as at subcritical conditions where phase change can result in sharp variations in acoustic speed and density. Specifically, it allows for sharp variations in the derivatives of density and enthalpy near the critical point to be modeled faithfully leading to improved results with more robustness near the critical point.

The numerical formulation requires the specification of density, enthalpy, and their derivatives ρ_p, ρ_T, h_p, h_T as a function of local pressure and temperature. As an alternative to analytical equation of state models, a table look-up procedure generated from NIST database [9] has been implemented to obtain thermodynamic properties, their derivatives, as well as transport properties i.e., viscosity μ , and thermal conductivity k , as a function of input pressure and temperature using bilinear interpolation. Extensions of the table look-up procedure for subcritical conditions where liquid and vapor properties must be evaluated independently are described in Hosangadi et al. [5].

Phase change is modeled within a “two-fluid” framework (see Ref [3]-[5] for details) wherein separate mass conservation transport equations for liquid and vapor are solved. However, the two components are assumed to have the same local conditions and hence only mixture conservation equations for momentum and energy are solved. Phase change is driven by local conditions; a finite rate phase change model that is based on the difference between the fluid pressure relative to the saturation pressure at the local temperature is implemented. In Eqn. (1) below the net mass transfer is given by m_i and is comprised of vaporization and condensation terms that drive the solution to pressure equilibrium:

$$m_i = K_f \rho_L \phi_L + K_b \rho_g \phi_g$$

$$K_s = \begin{cases} 0 & p < p_v \\ \frac{1}{\tau_s^*} \left[\frac{p - p_v}{\frac{1}{2} \rho_\infty V_\infty^2} \right] & p > p_v \end{cases} \quad (1)$$

where τ_f^* is the non-dimensional time scale for vapor formation in seconds and τ_b^* is the non-dimensional time scale for liquid condensation in seconds.

The numerical framework for real fluids in CRUNCH CFD® has been validated extensively for phase change in a wide range of near critical cryogenic fluids including liquid nitrogen, hydrogen as well as as sCO_2 applications operating very close to the critical point. Fundamental validation including temperature and pressure profiles due to phase change and associated thermodynamic effects due to latent heat effects have been presented for vaporization/cavitation [3] as well as condensation in nozzles [5] for near critical fluids.

3.0 Sub-Grid Boiling Model

A meso-scale model developed at MIT [2][11] originally for boiling processes was adapted for cryogenics and implemented in the CRUNCH CFD® framework. One of the primary objectives is to provide an accurate representation of the physics at the boiling wall, with the specific aim of delivering a sub-grid scale mechanistic representation with the largest generality. The model aims at introducing all necessary mechanisms, and explicitly tracks: (1) the size and dynamics of the bubbles on the surface; (2) the amount of microlayer and dry area under each bubble; (3) the amount of surface area influenced by sliding bubbles; (4) the quenching of the boiling surface following a bubble departure and (5) the statistical bubble interaction on the surface. While insights from recent experiments performed at MIT ([14][15]) have driven the formulation of a physically consistent mechanistic wall heat flux partitioning model [11], the model was originally developed for nuclear applications with water being the working fluid. As described in the discussion below, this model was adapted for cryogenic fluids using thermodynamic scaling concepts taking into account reduced pressures and temperatures that are scaled by the critical values.

3.1 Heat Flux Partitioning Model for Water

The wall boiling phenomena is incorporated in the CFD formulation through a mechanistic formulation for the heat flux partitioning ([12][13]), where the total heat flux is computed as the sum of the three partitioned components.

$$\dot{q}_{tot} = \dot{q}_c + (1 - VOF)(\dot{q}_q + \dot{q}_e) \quad (2)$$

where q_c'' , q_q'' , and q_e'' represent the heat flux of liquid convective heat transfer, quenching heat transfer and the evaporation, respectively. Among them, the convection term, q_c'' , represents the convective heat flux which describes the removal of heat by convection on the region of the wall that is not affected by boiling. The quenching heat transfer and evaporation relate to only the wetted area and therefore are multiplied by the amount of liquid void fraction existent at the wall. The convective contribution to the heat flux, q_c'' , is derived by the gas-liquid mixture conductivity and the temperature difference between the fluid and the wall. The quenching term, q_q'' , describes the enhancement of heat transfer due to the replacement of a departing bubble by an influx of cooler liquid further away from the wall. Quenching heat transfer is the component of heat flux that is used in heating this replacement liquid, as modeled by Del Valle and Kenning [16].

$$q_q'' = h_q (T_w - T_q) \quad (3)$$

where T_q is the temperature of the fresh liquid influx brought to the wall by the departure of a bubble. In smaller bubbles, typical of cryogenic fluids or with conventional fluids at high pressures, the saturation temperature is considered a good approximation for T_q . h_q is the quenching heat transfer coefficient. The quenching heat transfer coefficient is defined as using the Del Valle Kenning model [16] as:

$$h_q = 2K_q f \sqrt{\frac{\rho_l C_{pl} k_l t_w}{\pi}} \quad (4)$$

where f is the bubble departure frequency. k_l is the conductivity of the liquid phase; t_w is the wait time between bubble departure and the nucleation of the next bubble and defined as follows:

$$t_w = \frac{C_w}{f} \quad (5)$$

where C_w is the wait coefficient and the default value is 0.8. This value comes from an assumption by Kurul and Podowski [13] that quenching occurs between the departure of one bubble and the nucleation of next. This period is 80% of the departure cycle. K_q in the Eq. (6) is the bubble influence wall area fraction, and is expressed as follows:

$$K_q = F_A \frac{\pi D_d^2}{4} N'' \quad (6)$$

where F_A is a scaling coefficient and usually set as 2. D_d is the bubble departure diameter. N'' is the nucleation site density on the solid wall. The evaporation term, q_e'' , represents the energy required to produce bubbles from nucleation to departure. This term is a strong function of wall superheat $T_w - T_{sat}$. In fixed heat flux applications, once boiling starts this term is responsible for maintaining a wall temperature that is slightly higher than the saturation temperature. An evaporation heat flux is constructed for the nucleate boiling mechanism: bubbles nucleate and grow on suitably sized cavities on the wall; bubbles reach a critical size, at which point the forces holding the bubble to the wall are no longer balanced. The evaporation heat flux is expressed as

$$\dot{q}_e = N'' f \frac{\pi D_d^3}{6} \rho_g h_{lg} \quad (7)$$

where h_{lg} is the latent heat. N'' is the nucleation site number density. f is the bubble departure frequency. D_d is the bubble departure diameter as also noted above. In this mechanistic formulation, the accurate prediction of the wall boiling phenomena relies on the individual models of bubble departure diameter, bubble departure frequency, nucleation site density, which are discussed below.

3.1.1 Bubble Departure Frequency

The bubble departure frequency formulation by Cole [17] is specified here. This formulation uses the Departure diameter to evaluate the frequency, smaller bubbles depart faster.

$$f = \sqrt{\frac{4g(\rho_l - \rho_g)}{3D_d\rho_l}} \quad (8)$$

3.1.2 Bubble Departure Diameter

The quantification of the bubble departure diameter model plays an important role on the wall boiling model since both evaporation and quenching heat transfer rely on the bubble departure diameter model. A correlation that accounts for the effect of pressure proposed by Kocamustafaogullari [18] is specified here. The correlation relates the bubble departure diameter non-dimensionalized by the capillary length, to a modified by a density ratio, which makes it useful for a wide range of pressure. the model is given as follows:

$$D_d = d_1 \theta \left(\frac{\sigma}{g\Delta\rho} \right)^{0.5} \left(\frac{\Delta\rho}{\rho_g} \right)^{0.9} \quad (9)$$

where d_1 is a calibration constant, with a default value of 1.5126×10^{-3} m/radian. θ is a wall contact angle for the working fluid, with a default value of 0.722 radians, which is suitable for water but needs to be re-evaluated for a cryogen. σ is the surface tension.

3.1.3 Nucleation Site Density Model

The nucleation site density model requires particular attention, as it drives the rapid growth in boiling heat transfer with wall superheat. In this effort, two nucleation site density models were evaluated for conditions representative of liquid nitrogen; a) Lemmert-Chawla' model [21] and b) Data driven nucleation site density model by Li et al. [24]. The Lemmert-Chawla' active nucleation site density correlation is a commonly adopted model, and the formulation is shown below:

$$N'' = (m\Delta T_{sup})^p \quad (10)$$

The default values for m and p are 185.0 sites/m² and 1.805, respectively. An important point to note is that this model does not have any pressure effects built in.

The data-driven nucleation site density model developed by Li et al. [24] has been applied to CFD simulations of subcooled boiling in a vertical heated tube. The new model is based on a parametric analysis of existing experimental data in water and is a function three crucial parameters relevant to the nucleation site density: wall superheat, system pressure, and contact angle. However, in our preliminary stand-alone evaluation of both the Lemmert-Chawla and Li models for conditions representative of chilldown in liquid nitrogen lines, the Lemmert-Chawla model gave better comparisons of heat flux compared to test data for liquid nitrogen compared to the Li model (as is discussed later below). Hence for subsequent coupled CFD simulations the Lemmert-Chawla model was the default option.

3.2 Modification of Boiling Coefficients for Cryogens

To understand the behavior of the boiling model, a series of stand-alone calculations were performed for liquid nitrogen at a pressure of 0.12 MPa representing the chilldown experiments of Antar and Collins [26]. The coefficients used in the closure model were the values derived for that in water while using the thermodynamic properties of liquid nitrogen. These simulations provided bubble departure diameter of 50 microns which is several orders of magnitude lower than experimental data for bubble diameters of ~0.5 mm in liquid nitrogen nucleate boiling as shown in Figure 1.

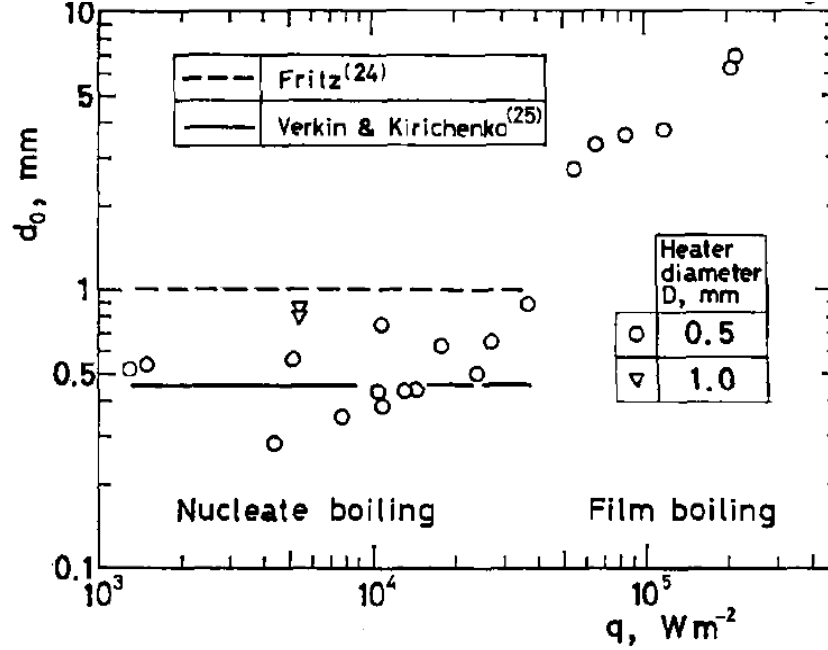


Figure 1: Data from Pool Boiling Experiments of Kida et al. [25] showing droplet diameters around 0.5 mm in liquid Nitrogen.

To understand the source of the discrepancy between the predicted and measured bubble sizes we compare the thermodynamic properties of water and nitrogen at 0.12 MPa in Table 1. We observe that there the liquid to vapor density as well as surface tension is an order of magnitude smaller for Nitrogen relative to water reflecting the fact that it has a much higher reduced pressure (normalized by critical pressure) value of (P/P_c) . Using the thermodynamic similarity principles, the departure diameter coefficient used in Eqn. (9) is determined by taking the value for water calibrated with test data and scaling it by the ratio of liquid to vapor densities for water and nitrogen as shown below in:

$$\left(d_{1w} \frac{\rho_L}{\rho_v} \right)_{\text{water}} = \left(d_{1n} \frac{\rho_L}{\rho_v} \right)_{\text{Nitrogen}} \quad (11)$$

Table 1. Comparisons of Properties of Water and Nitrogen at 0.12 MPa

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

Using the thermodynamic scaling of Eqn. (11) in d_1 being larger by approximately an order of magnitude than that used for water. The predictions for the bubble departure diameter as a function of wall superheat are shown below in Figure 2 and we observe that the range of bubble diameter (~ 0.5 - 0.64 mm) is roughly consistent with the test data of Kida et al. [25]. Furthermore, we also note that while comparing test data for water and cryogen the system pressure needs to be scaled by the ratio of critical pressures as shown below in Eqn. (12):

$$P_{eq}^w = P_{n_2} \left(\frac{P_c^w}{P_c^{n_2}} \right) \quad (12)$$

Here P_{n_2} is the pressure for the nitrogen system while P_{eq}^w would be the equivalent pressure for water at which comparisons can be done or test data for water can be used. Lastly, the total heat flux is plotted in Figure 3 as a function of superheat and we note that the peak heat flux of 200 kW/m^2 is approximately consistent with the heat flux predictions for liquid nitrogen chilldown in the Darr test [6]. This provides confidence that the thermodynamic scaling to convert boiling sub-model coefficients in water for use in cryogen fluids is providing physically consistent and accurate results.

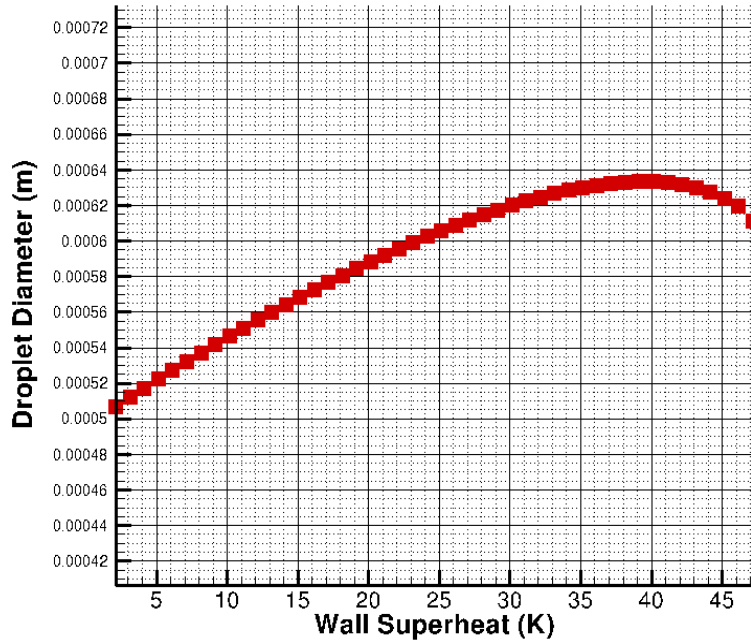


Figure 2: Bubble Departure Diameter After Applying Thermodynamic Scaling to Boiling Model Coefficients.

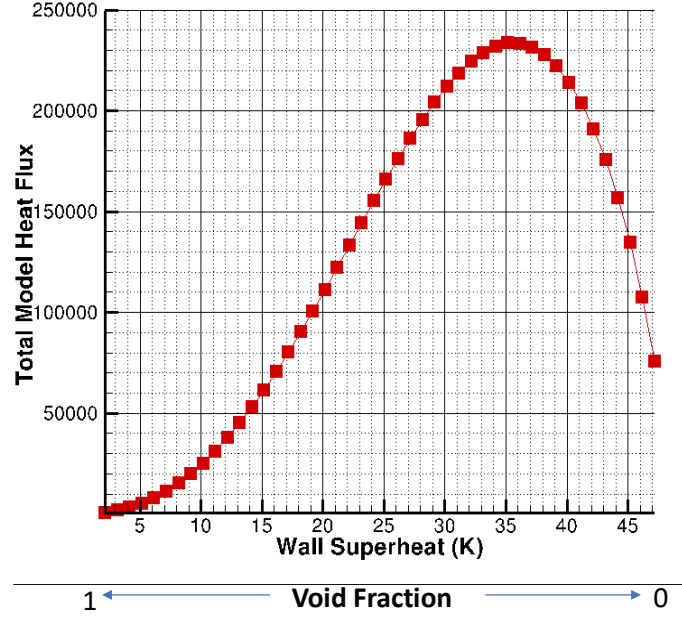


Figure 3: Estimated Total Heat flux as a Function of Wall Superheat with Thermodynamic Scaling to Boiling Model Coefficients.

4.0 Simulations of Line Chillover in Liquid Nitrogen

In this section, we present simulation results for line chillover in liquid nitrogen and simulate Test 40 of the Darr et al. [6] experiment. The test section is shown in Figure 4: the tube has a length of 57.2 cm from the exit of the bypass valve. The tube is made of 304SS material and has an ID 1.168 cm and an OD of 1.27 cm. The thermocouples are placed 14.9 cm and 40.1 cm from the inlet of the test section and the pressure transducers are located at 18 cm and 37.1 cm respectively. The computational domain was truncated at 37.1 cm from the inlet to allow for better boundary condition in the CFD by using the pressure measurements at this location as a back pressure condition.

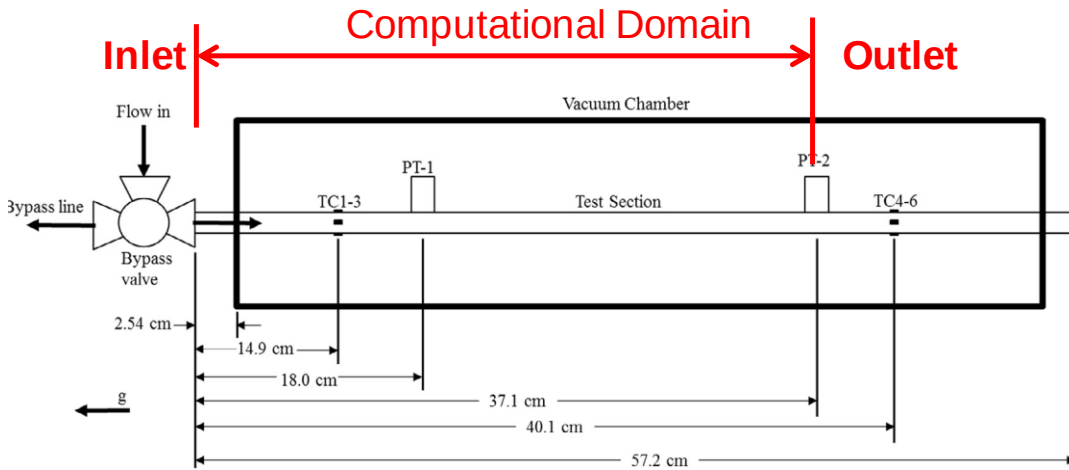


Figure 4: Details of the Experimental Test Section and the Computational Domain for the Experiment by Darr et al. [6].

The conditions at the inlet are shown in Table 2. At the inlet the simulations specified the mass flux and the inlet temperature. We note that the inlet temperature is subcooled by 2.23K relative to the inlet pressure and this results in pure liquid composition at the inlet. The solid walls were initialized with a temperature of 300K. A high resolution NIST table for nitrogen was generated to cover the expected conditions in the simulations. The simulation is performed at 1-G conditions with gravity acting vertically down (towards the bypass valve).

Table 2. Inlet Conditions for Test 40: Liquid Nitrogen Simulation

Inlet Pressure	325.93 kPa
Inlet Temperature	86.61 K
Degree of Subcooling	2.23 K
Inlet Mass Flux	327.82 kg/m ² s

The simulation was performed on a fully 3-D configuration. The fluid grid has approximately 100,000 vertices while the solid domain grid had approximately 85,000 vertices. Figure 5 shows the inlet plane and zoomed-in side view of the grids; the fluid grid is in blue and solid domain grid is in red. Strongly coupled fluid-thermal boundary conditions that enforce continuity in temperature and heat flux were enforced at the interface between the fluid and solid grid. The remaining boundaries of the solid domain were adiabatic. For the simulations with liquid nitrogen, constant thermal properties for the solid wall were specified since the variation in properties above 100K is not as dramatic as that at temperatures below 50K as would be the case for liquid hydrogen. Transient simulations were carried out without specifying a turbulence model (i.e., unsteady laminar) with three inner iterations at each time step. The time step specified was of the order of 5.e-5 secs.

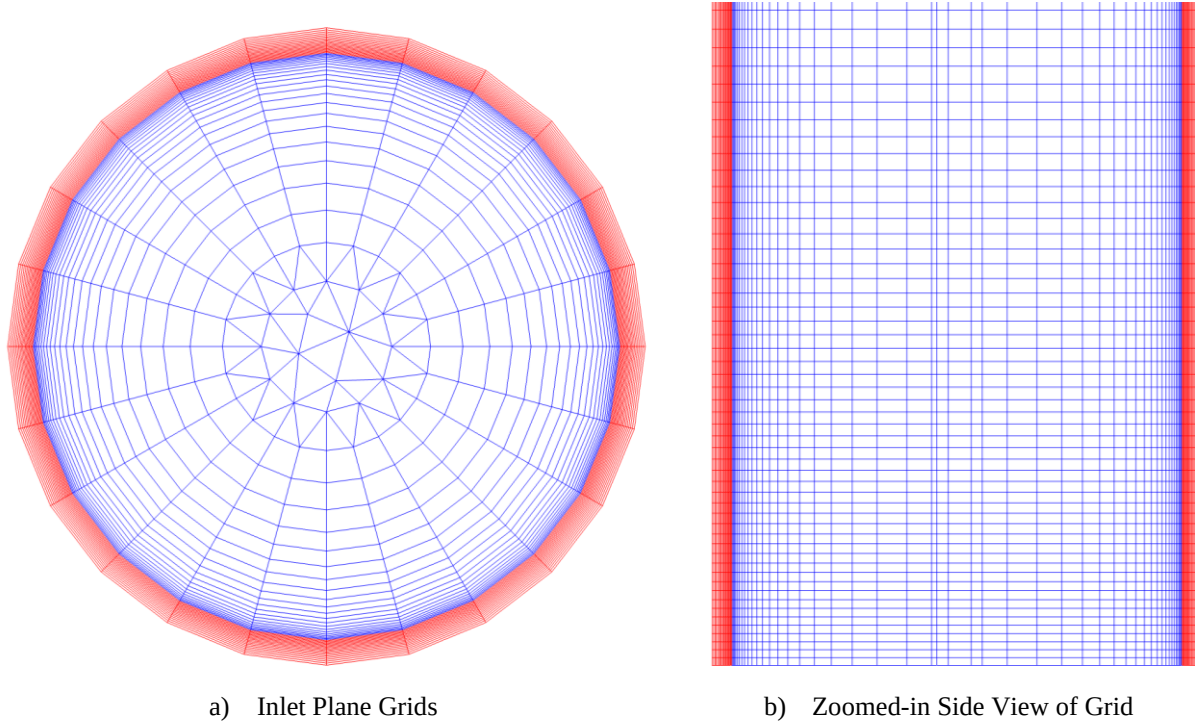


Figure 5: Fluid and Solid Module Grids for Liquid Nitrogen Simulation (Darr et al. [6]): Blue; fluid Domain, Red; Solid Domain

The evolution of the liquid front at early times in the process is shown below in Figure 6. As the liquid is injected into the vertical tube with warm nitrogen vapor at 300 K, the front assumes an annular shape initially with a mixture of liquid and gas climbing up against the walls of the tube (Figure 6). The contours in the tube in the figure are colored by mixture density while the thin walls surrounding the tube are shown by the temperature distribution. The initial formation of an annular front was unexpected and was not observed in simulations for the Antar experiment [26] that we have performed. It is hypothesized that since the momentum of the injected front is an order of magnitude smaller in the Darr experiment, the effect of gravity may be more pronounced and is possibly the reason for the difference in the front shape early in process. By 0.86 secs the tube is filled with dispersed two-phase mixture and the vapor film is formed throughout the length of the tube. Furthermore, in the early evolution phase, the thermal boundary layer becomes destabilized due to flashing close to the wall resulting in increased unsteadiness of the liquid front.

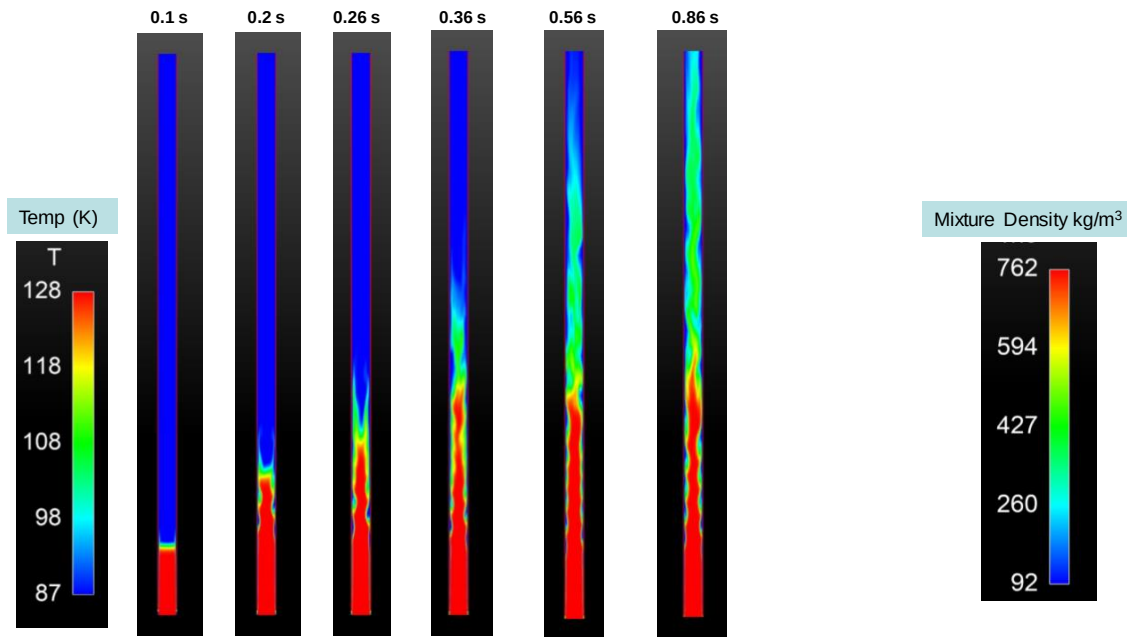


Figure 6: Early Evolution of the Flow in the Vertical Tube.

Later in the cycle, the liquid core advances slowly (Figure 7), as film cooling takes place at the walls. The thin vapor film is sustained for a long period of time while liquid ligaments continually tear out of the core and travel vertically upward. Subsequently, around 14 secs, quenching is observed (Figure 8) in the inner wall and the quench front and the liquid core subsequently propagates rapidly in the tube.

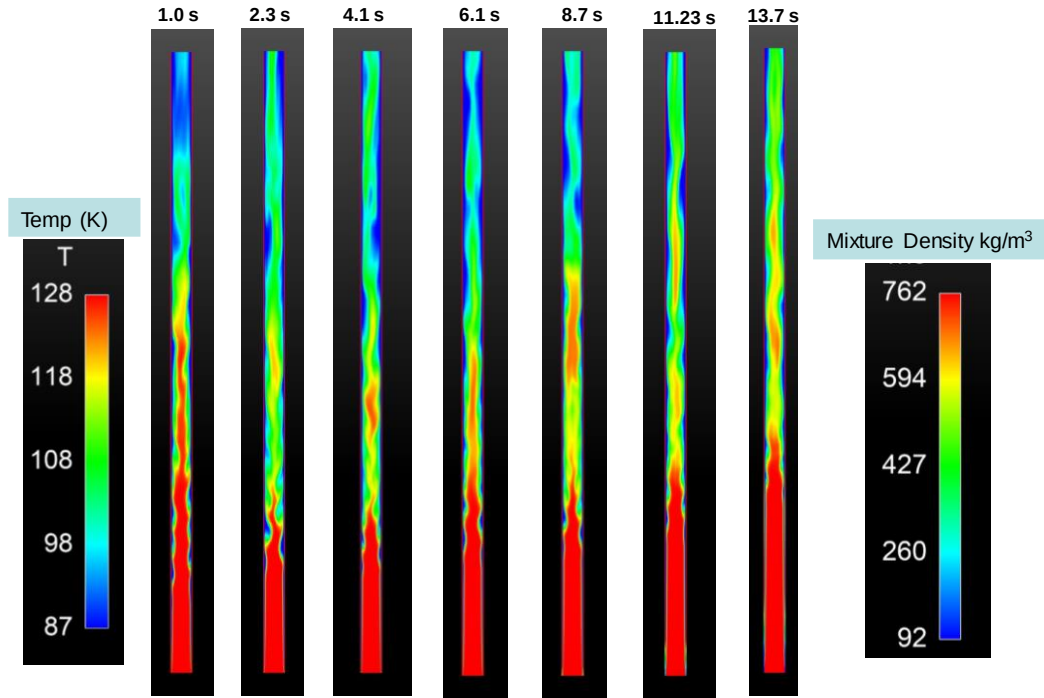


Figure 7: Flow Patterns in the Vertical Tube during the Film Boiling Phase.

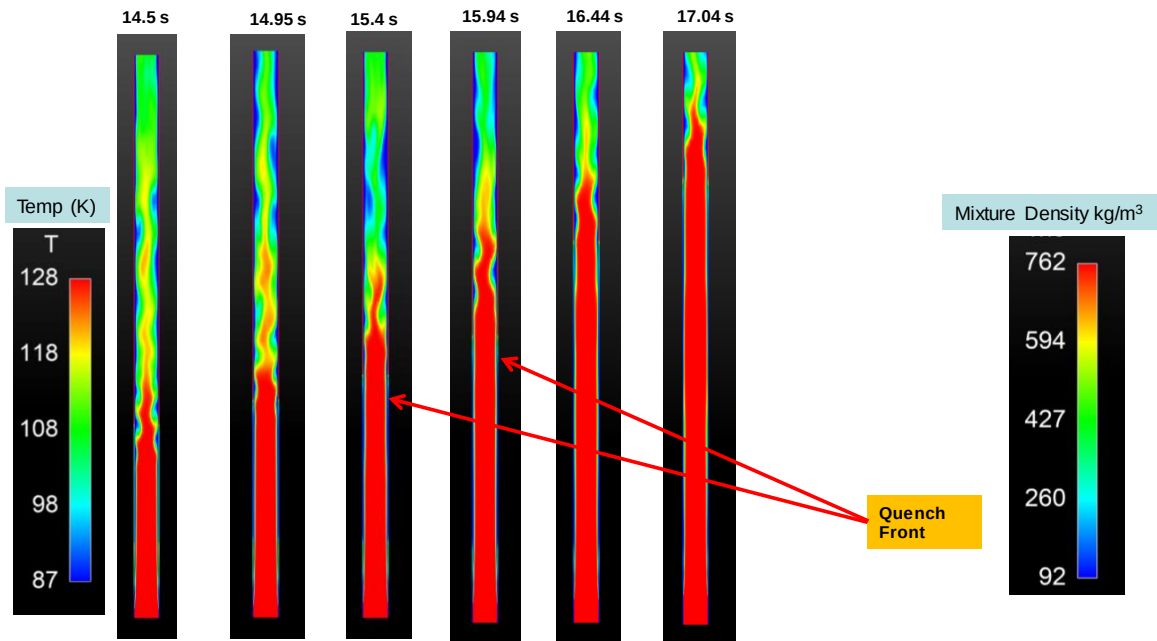


Figure 8: Flow Patterns in the Vertical Tube during the Quenching Phase.

Temperature comparisons on the inner wall with the readings from the TC-1 thermocouple show good agreement between the CFD calculation and the experiment (Figure 9). In the film boiling regime, the comparison of the slope between the simulation and test data is reasonable. We note that matching the slope in the film boiling regime is quite challenging since the temperature evolution is both a function of the

phase change rates as well as the local evolution of the mixture front which can be sensitive to a variety of parameters including grid resolution, unsteady turbulence effects, as well as the non-uniform solid thermal properties. The sharp change in the temperature slope where the film boiling transitions to nucleate boiling is captured very well. The increase in the heat flux during the transition to nucleate boiling is provided by the MIT sub-grid boiling model that has been implemented here. *We note that the wall temperature at which the transition occurs comes close to the test data and is reflection of the good performance of the MIT sub-grid boiling model.* The slope of the temperature curve after quenching is initiated, showing a steeper variation and furthermore the final equilibrium value of temperature is slightly lower than the test data. The reason for the difference in the final equilibrium value is not entirely known and may be due to parasitic heat loss in the test. In summary, the performance of the MIT sub-grid boiling model quenching in liquid nitrogen was good with transition to nucleate boiling occurring close to what the test data indicated.

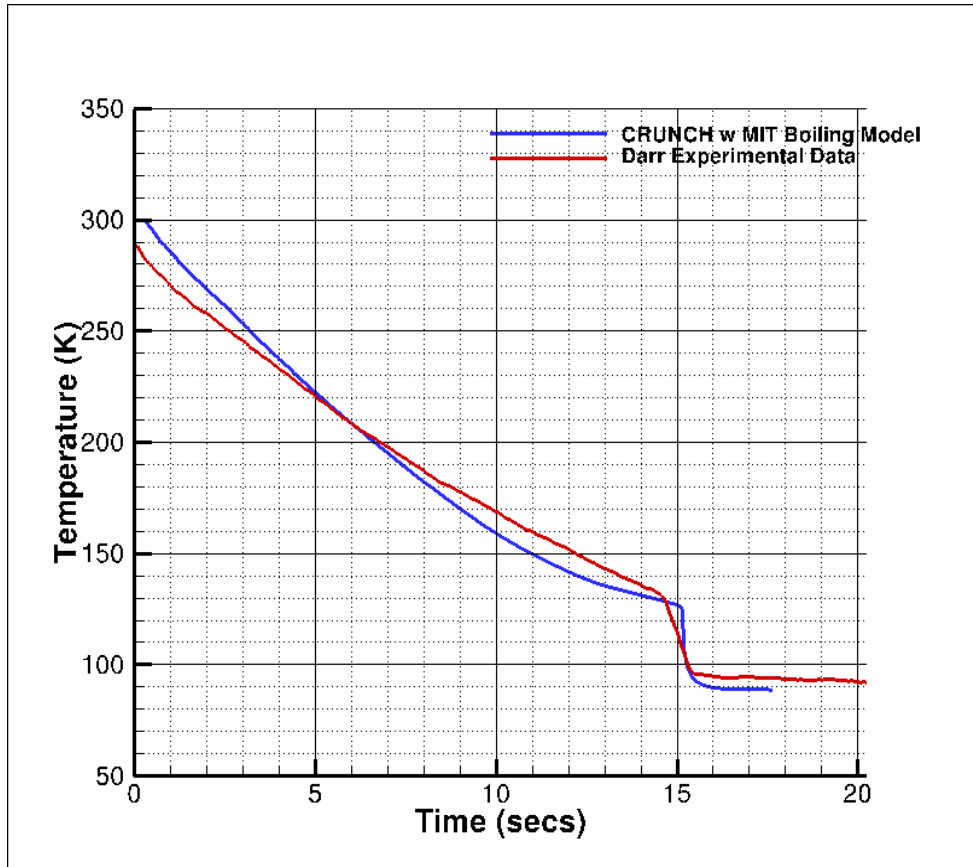


Figure 9: Temperature Comparisons Between the CFD Calculations and the Experimental Data at the TC-1 Thermocouple Location.

5.0 Simulations of Line Chillover in Liquid Hydrogen

In this section, we discuss preliminary simulations of liquid hydrogen chillover in vertical tubes under 1-G conditions and compare with test data published by Hartwig et al. [7]. The chillover experiments were carried out at the Small Multi-Purpose Research Facility at NASA GRC at different conditions including pulsatile flow and trickle flow at different mass flow rates and operating pressures in liquid hydrogen. The computational domain modeled in the simulations was for a total length of 98 cm starting 6.51 cm downstream of the bypass valve. In the simulations here we model Test8b at a high flow rate and

the test measurements including inlet mass flow and temperature are shown below in Figure 10. We note that the quenching time scales in hydrogen are quite rapid (order of $\sim 7\text{-}10\text{ s}$) and in this short time scale the mass flow through the line is still rising. This illustrates both the challenges in testing liquid hydrogen as well as the difficulty in accurately modeling liquid hydrogen tests. For the simulations here an average mass flux value of $138.5\text{ kg/m}^2\text{-s}$ was specified. The average pressure in the line is 0.25 MPa , the saturation temperature corresponding to this pressure is 23.86 K . For the calculations here, we assume pure liquid inflow with a sub-cooled temperature of 23.61 K (corresponding to 0.25 K sub-cooling). It is not clear if a sub-cooled liquid inflow is the correct inlet boundary condition for hydrogen and it is possible that the test may have had either saturated liquid or more likely two-phase inflow entering and more data as well as additional sensitivity studies may be required to resolve this issue.

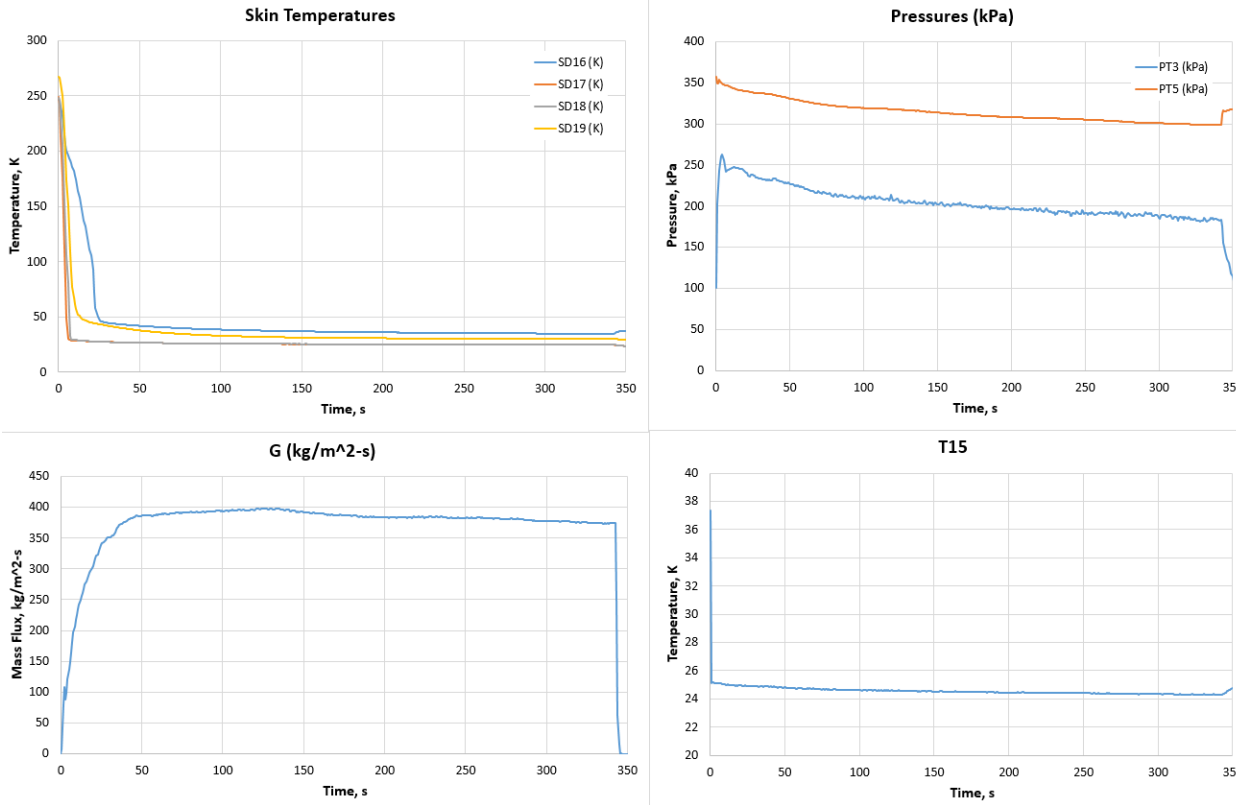


Figure 10: Test Data for Duration of Liquid Hydrogen Chillardown Test8b.

The pipe test section in the experiment has an outer diameter of 1.27 cm and an inner diameter of 1.02 cm and this region was modeled as the solid walls of the pipe were initialized with an ambient temperature of 250 K . The properties of the stainless steel drop significantly at temperatures corresponding to liquid hydrogen (Marquardt et al. [27]) as shown below in Figure 11 and Figure 12 for thermal conductivity and specific heat respectively. The thermal conductivity drops from 14 W/m-K at 250 K to 2.6 W/m-K at 23.6 K while the specific heat drops from 457 J/kg-K to 17.5 J/kg-K which is more than an order of magnitude. Therefore, modeling the variation in properties is critical to obtaining the correct thermal response for the solid in liquid hydrogen flows. We note that while variable solid thermal properties will also affect liquid nitrogen chilldown simulations the impact was less significant due to the higher temperatures of liquid nitrogen. We also note that the boiling parameters for the quenching model had to be calibrated for liquid hydrogen using thermodynamic similarity rules described earlier.

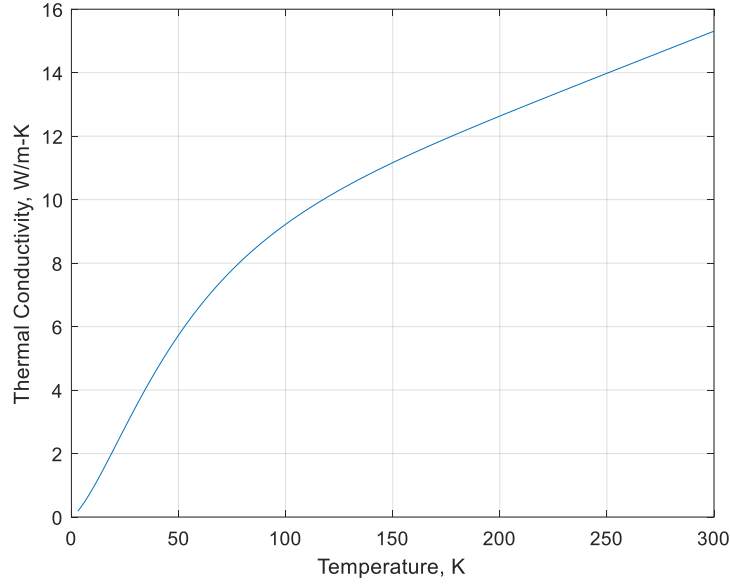


Figure 11: Variation of Thermal Conductivity with Temperature for Stainless Steel 304 (Marquardt et al. [27]).

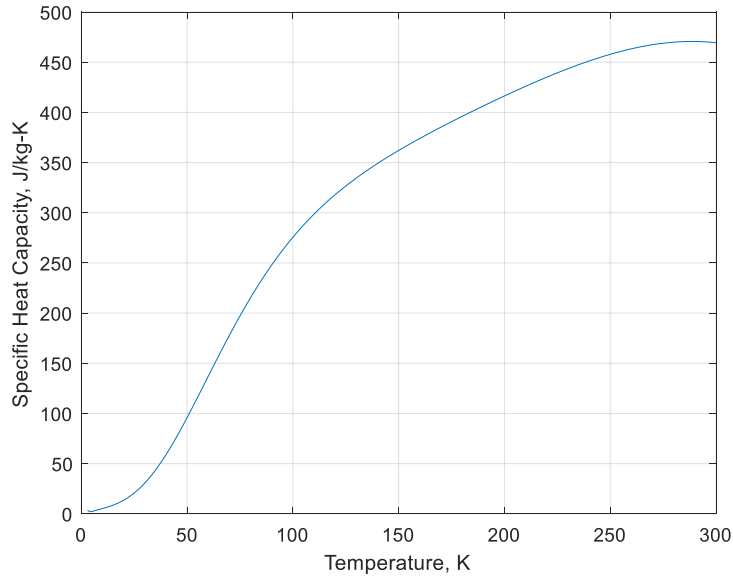


Figure 12: Variation of Specific Heat with Temperature for Stainless Steel 304 (Marquardt et al. [27]).

Chilldown in liquid hydrogen lines shows rapid cooldown of the solid wall temperature compared to liquid nitrogen. Therefore, multiple calculations were performed to better the chilldown physics and sensitivity of the chilldown curves to different parameters. The baseline calculation was performed with the LES framework which performed very well in the previous liquid nitrogen simulations. However, the LES framework does not resolve the turbulent boundary layer very well and as we shall discuss below for the hydrogen case, we had to go to an unsteady RANS formulation due to the higher Reynolds number for this case. Both the baseline LES and unsteady RANS cases were computed with the variable thermal properties for stainless steel as shown in Figure 11 and Figure 12.

In Figure 13, the temperature history at SD18 for the test data (black curve) is compared with the simulation results for the LES calculation (red curve) as well as the unsteady RANS simulation (blue curve). Both calculations have been performed with variable conductivity and specific heat specified for the stainless steel. We note that the LES simulation (red curve) results provide a slow rate of temperature drop indicating that the heat transfer rate from a laminar boundary layer solution is inadequate since the turbulent boundary layer promotes more mixing. This calculation was stopped before chilldown due to the unrealistically slow drop in temperature. The turbulent unsteady RANS solution provides a much faster initial rate of temperature drop which is reasonably close to the slope of the test data. The turbulent solution shows quenching occurring after the temperature becomes subcritical below 34 K and reaching a final temperature of roughly 24 K which is slightly below the test data temperature of 28 K. The chilldown times are reasonably well predicted with the simulation showing quenching at 7.45 while the test data shows equilibration at 6.45-7 s. We note that if surface roughness effects are included the chilldown may become slightly faster and show an even better match. These results identify turbulent boundary layer heat transfer as an important parameter for liquid hydrogen chilldown unlike liquid nitrogen where the LES calculation and laminar boundary layer were adequate. Furthermore, we note that it is difficult to determine when quenching occurred in the test because the data was only obtained every 0.71 sec.

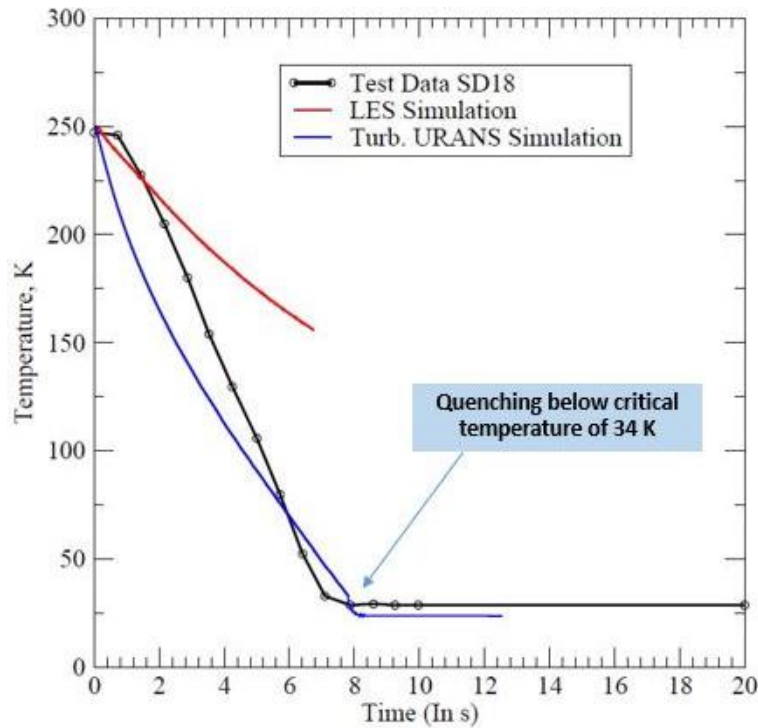


Figure 13: Temperature History at SD18 for Test Data Compared with LES and URANS Simulation.

The effect of variable thermal properties for stainless steel were investigated next by keeping all numerical parameters the same (i.e., turbulent unsteady RANS and phase change rate) but making the stainless-steel properties to be constant at their 250 K values. The comparison at SD18 location is shown below in Figure 14 where the red curve corresponds to the constant thermal properties while the blue curve is the baseline case with variable properties. We observe that there is a dramatic slowdown in the chilldown rate when the thermal properties are made constant. The quenching at the wall now occurs at roughly 17.5 s compared to the baseline time of 7.45 s. Interestingly the equilibrium temperature after quenching comes closer to the experimental data of 28K for reasons that are not entirely clear.

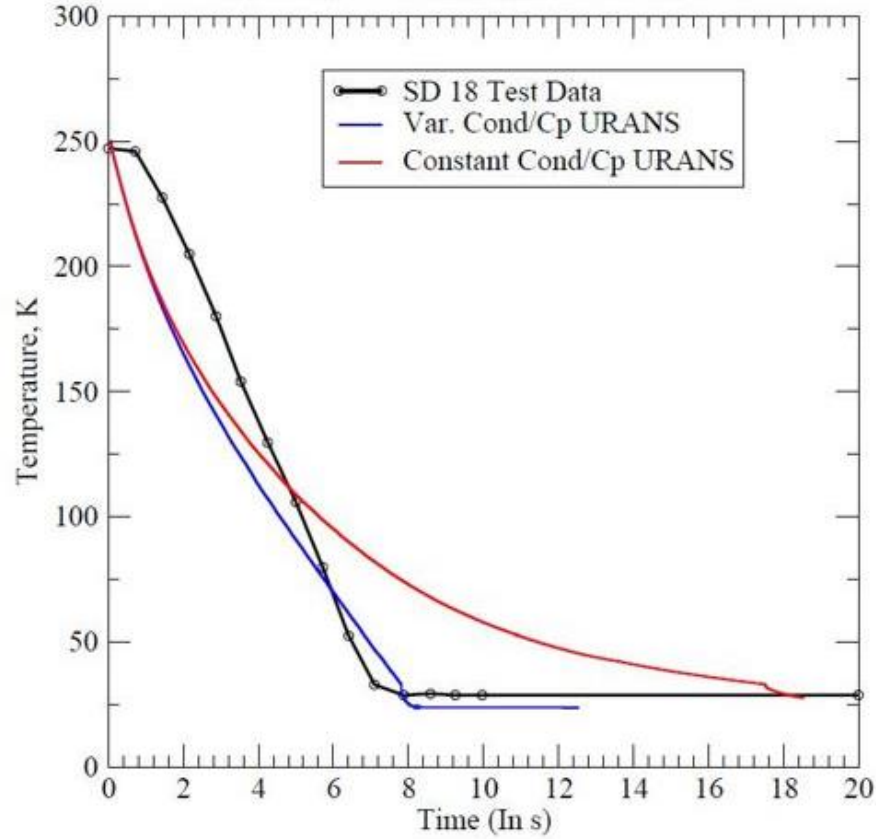


Figure 14: Temperature History at SD18 for Variable Thermal Properties for Stainless Steel Compared with Constant Property Solution.

The flow contours for the time period until quenching occurs are plotted in Figure 15; the density contours are shown for the fluid while the stainless-steel walls are colored by the solid temperature. We observe a liquid front advancing from the inlet in an inverted annular fashion. However, downstream of the liquid front, two phase liquid-vapor mixture at cold temperature is observed in the core with significant vapor content making the density low. Indeed, when quenching occurs at 7.74 s at SD18, we observe that fluid at this location is a two-phase mixture in the core and the liquid front has not yet advanced to this location. We note that the liquid front in liquid hydrogen tests is believed to have an annular behavior with liquid climbing up at the wall and the core progressing slower. The inverted annular behavior observed here numerically may be an artifact of the subcooled inlet temperatures specified here. Additional work would be needed to model saturated or two-phase inflow whose vapor volume fraction can dynamically change as the inlet pressure increases. Despite the phase distribution discrepancy, the chilldown curve agrees reasonably well with the test data.

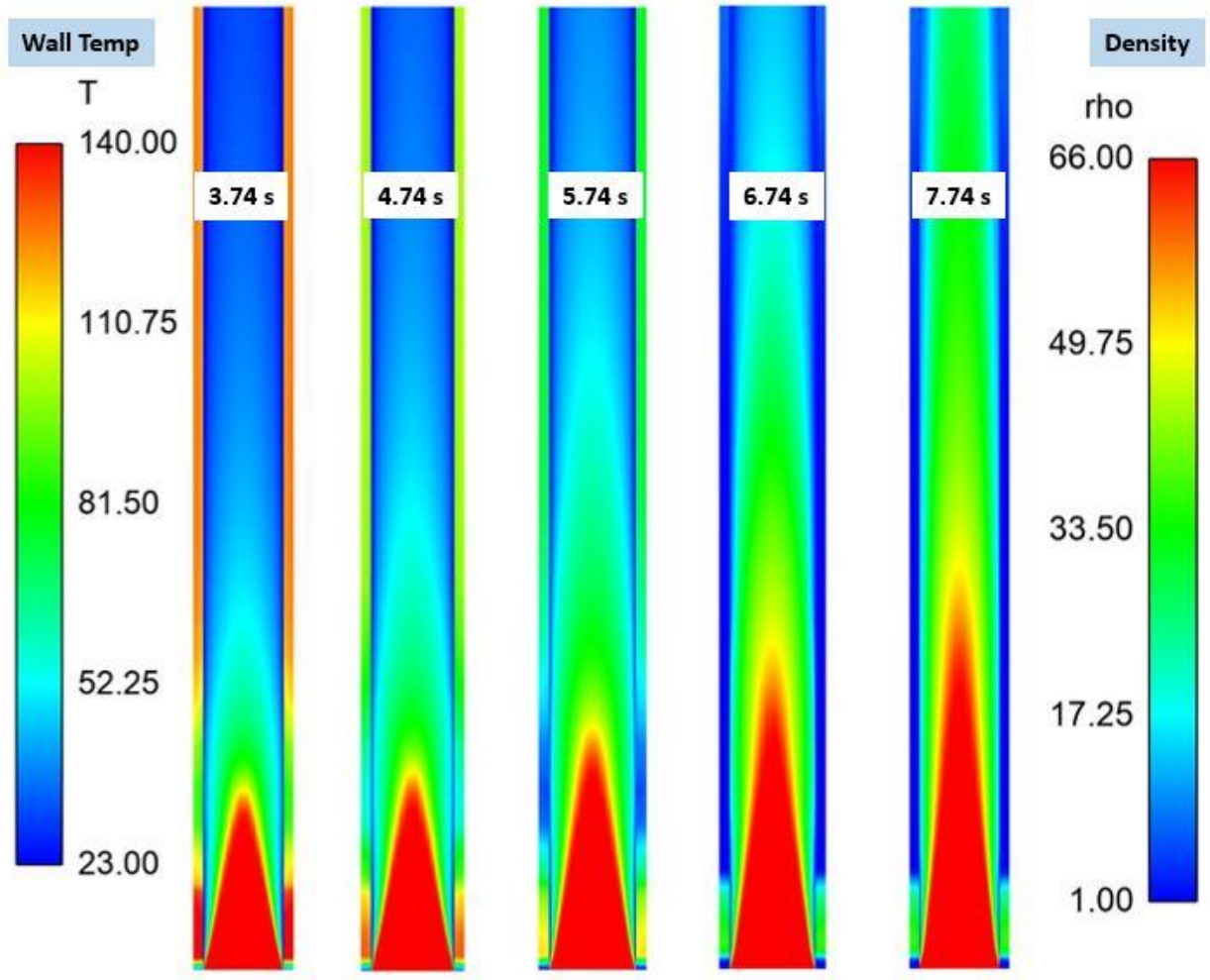


Figure 15: Fluid Density and Wall Temperature Contours Until Onset of Quenching.

The corresponding fluid contours after quenching are shown in Figure 16. The fluid density contours show that rather than having a pure liquid front advance, condensation in the cold two-phase mixture as the pressure rises results in the density rising and the composition becoming nearly all liquid very rapidly. This behavior is very different from that observed in liquid nitrogen where a more conventional flow field is observed with an advancing liquid front indicating quenching. More effort would be needed to understand this behavior along with flow visualization data to characterize the experimental behavior more rigorously for the same flow conditions.

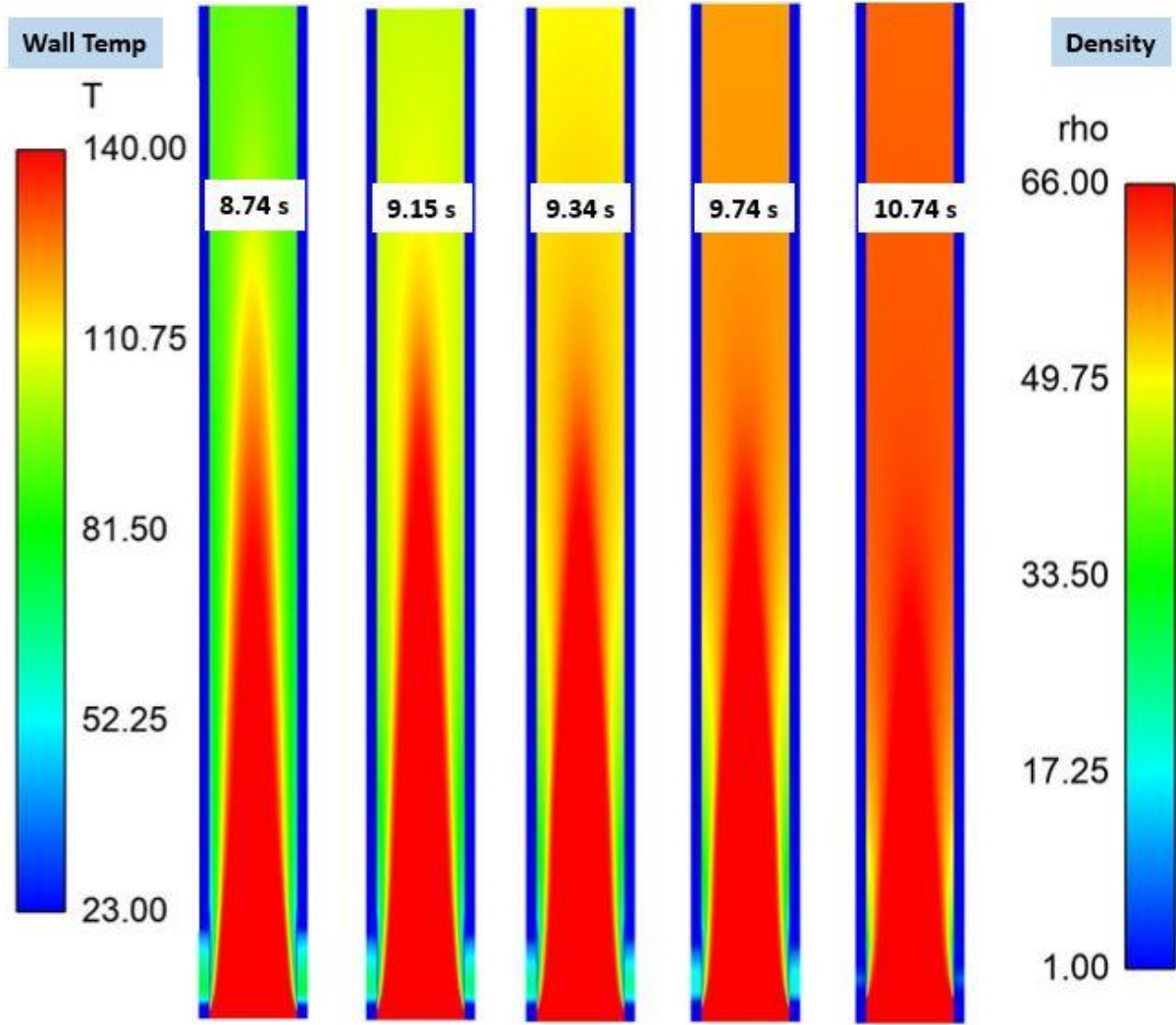


Figure 16: Fluid Density and Wall Temperature Contours After Quenching at Wall.

6.0 Conclusions

A meso-scale boiling model developed at MIT [2][11] originally for water was adapted for cryogenic fluids. The model is designed to provide a mechanistic representation of the physics at the boiling wall and explicitly tracks: (1) the size and dynamics of the bubbles on the surface; (2) the amount of microlayer and dry area under each bubble; (3) the amount of surface area influenced by sliding bubbles; (4) the quenching of the boiling surface following a bubble departure and (5) the statistical bubble interaction on the surface. The model was adapted for cryogenic fluids using thermodynamic scaling concepts taking into account non-dimensional pressures and temperatures that are scaled by the corresponding critical values for the fluid and a detailed procedure to scale the parameters in the model was developed.

Chilldown physics for liquid nitrogen under terrestrial conditions were validated by comparing with test data from the experiments by Darr et al. [6]. Temperature comparisons on the inner wall with the readings from the test thermocouple showed good agreement between the CFD calculation and the experiments. In the film boiling regime, the comparison of the slope between the simulation and test data is reasonable. The sharp change in the temperature slope where the film boiling transitions to nucleate

boiling is captured very well. We note that the wall temperature at which the transition occurs comes close to the test data and is reflection of the good performance of the original MIT sub-grid boiling model.

Chilldown in liquid hydrogen lines under terrestrial conditions was also modeled and compared with test data of Hartwig et al.[7]. Good comparison was obtained for the temperature history on the wall when variable thermal properties of stainless steel were specified and turbulence effects in the boundary layer were modeled. The simulations indicate that chilldown in liquid hydrogen has very different characteristics compared to liquid nitrogen as has also been noted in the experiments. Sensitivity studies conducted identified the following important physics: 1) Modeling variable properties of stainless-steel conductivity and specific heat as a function of temperature is critical. Use of constant properties at the higher temperature value leads to more than doubling in the chill down time, 2) Flow turbulence effects in liquid hydrogen are significantly more important than in liquid nitrogen. Turbulent boundary layers result in higher film cooling heat transfer rates, and 3) More studies are needed to understand how the annular quench fronts observed in some liquid hydrogen tests evolve.

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8.0 References

- [1] Hartwig, J., Darr, S., Asencio, A., “Assessment of Existing Two Phase Heat Transfer Coefficient and Critical Heat Flux Correlations for Cryogenic Flow Boiling in Pipe Quenching Experiments,” *Intl J. of Heat and Mass Transfer*, Vol 93, pp. 441-463, 2016.
- [2] Gilman, L., Baglietto, E., A self-consistent, physics-based boiling heat transfer modeling framework for use computational fluid dynamics, *Int. J. Multiph. Flow* 95, 35–53, 2017.
- [3] Hosangadi, A. and Ahuja, V., “Numerical Study of Cavitation in Cryogenic Fluids,” *Journal of Fluids Engineering*, Vol. 127, pp. 267-281, March 2005.
- [4] Hosangadi, A., Ahuja, V., and Ungewitter, R.J., “Simulations of Rotational Cavitation Instabilities in the SSME Low Pressure Fuel Pump,” JANNAF 54th JPM / 3rd LPS / 2nd SPS / 5th MSS Joint Meeting, Denver, CO, May 14-17, 2007.
- [5] Hosangadi, A., Liu, Z., Weathers, T., Ahuja, V., Busby, J., “Modeling Multiphase Effects in CO2 Compressors at Subcritical Inlet Conditions,” *J. Eng. Gas Turbines Power*, Aug 2019, 141: 081005-
- [6] Darr, S.R., et al., “An experimental study on terrestrial cryogenic transfer line chilldown I. Effect of mass flux, equilibrium quality, and inlet subcooling,” *Intl J. of Heat and Mass Transfer*, Vol. 103, 2016.
- [7] Hartwig, J., Styborski, J., Stiegemeier, B., Chung, J.N., Rame, E., McQuillen, J., “Liquid Hydrogen line chilldown experiments at high Reynolds Numbers. II. Analysis,” *Intl Journal of Heat and Mass Transfer*, 156 (2020) 119805.
- [8] Hosangadi, A., Sachdev, J., and Venkateswaran, S., “Improved Flux Formulations for Unsteady Low Mach Number Flows,” Seventh International Conference on Computational Fluid Dynamics, Paper No. ICCFD7-2202, Big Island, Hawaii, July 2012.
- [9] NIST: Thermophysical Properties of Fluid Systems. Online Access at <https://webbook.nist.gov/chemistry/fluid>

- [10] Hosangadi, A., Lee, C.P., Kannepalli, C., and Arunajatesan, S., "Three Dimensional Hybrid RANS/LES Simulations of a Supercritical Liquid Nitrogen Jet," Joint Propulsion Conference & Exhibit, Hartford, CT, Paper No. AIAA-2008-5227, July 2008.
- [11] Gilman, L.A., "Development of a General Purpose Subgrid Wall Boiling Model from Improved Physical Understanding for use in CFD," Ph.D. dissertation, MIT, 2014.
- [12] Judd, R. L., & Hwang, K. S. (1976). A comprehensive model for nucleate pool boiling heat transfer including microlayer evaporation. *Journal of Heat Transfer*. Vol. 98 (4), pp. 623-629.
- [13] Kurul, N. & Podowski, M. (1990). Multidimensional effects in forced convection sub- cooled boiling. In: *Proceedings of the Ninth International Heat Transfer Conference*. Vol. 2, pp. 21-26.
- [14] Phillips, B.A., "Experimental Investigation of Subcooled Flow Boiling Using Synchronized High Speed Video, Infrared Thermography, and Particle Image Velocimetry," Massachusetts Institute of Technology, 2014.
- [15] Richenderfer, A., et al., Investigation of subcooled flow boiling and CHF using high-resolution diagnostics, *Experimental Thermal and Fluid Science* 99 (2018) 35–58.
- [16] DelValle, V.H., and Kenning, D., "Subcooled flow boiling at high heat flux," *International Journal of Heat and Mass Transfer*, vol. 28, no. 10, pp. 1907 - 1920, 1985.
- [17] Cole, R., "A photographic study of pool boiling in the region of the critical heat flux," *American Institute of Chemical Engineering Journal*, vol. 6, pp. 533-542, 1960.
- [18] Kocamustafaogullari, G., Ishii, M., "Interfacial area and nucleation site density in boiling systems," *Int. J. Heat Mass Transf.*, Vol. 26, No. 9, pp. 1377– 1387, 1983.
- [19] Zuber, H., "Hydrodynamic Aspects of Boiling Heat Transfer", PhD Thesis, University of California, 1959.
- [20] Semeria, H., J. de L'Hydraulique de la Société. Hydrotechnique de France (1962).
- [21] Lemmert, M., Chwala, J.M., *Heat transfer in boiling*, Academic Press and Hemisphere, New York and Washington, Chapter 11, 1977.
- [22] Hibiki, T. and M. Ishii, Active nucleation site density in boiling systems, *Int. J. Heat Mass Transfer*, Vol. 46, No. 14, pp. 2587-2601, 2003.
- [23] Tolubinsky, V., and Kostanchuk, D., "Vapour bubbles growth rate and heat transfer intensity at subcooled water boiling," *Heat Transfer 1970: Reprints of papers presented at the 4th International Heat Transfer Conference*, Paris, 1970.
- [24] Li, Q., Y. Jiao, M. Avramova, P. Chen, J. Yu, J. Chen and J. Hou, Development, verification and application of a new model for active nucleation site density in boiling systems, *Nucl. Eng. Des.*, Vol. 328, pp. 1-9 2018.
- [25] Kida, M., Kikuchci, Y., Takahashi, O., & Michiyoshi, I., "Pool-Boiling Heat Transfer in Liquid Nitrogen," *Journal of Nuclear Science and Technology*, 501-513, 1981.
- [26] Antar, B.N., and Collins, F.G., "Flow Boiling During Quench in Low Gravity Environment," *Microgravity Science and Technology X/3*, pp. 118 – 128, 1997.
- [27] Marquardt et al., "Cryogenic material properties database," 11th International Cryocooler Conference, Keystone, CO, 2000.
- [28] Hartwig, J.W., and Styborski, J., "Flow Visualization and Stream Temperature Measurement of Liquid Hydrogen Line Chill Down Experiments", *ASME J. Heat Transfer*, 137(2), p 020904, 2015.