VENTLESS PRESSURE CONTROL OF CRYOGENIC STORAGE TANKS

by

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Submitted in partial fulfillment of the requirements
For the degree of Doctor of Philosophy

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January, 2011
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Dr. Donald Feke

(date) August 2, 2010

*We also certify that written approval has been obtained for any proprietary material contained therein.
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ACKNOWLEDGEMENTS

First, I would like to acknowledge the financial support from the National Defense Science and Engineering Fellowship for the first year of this undertaking and the support of the Ohio Space Grant Consortium for the following three years. I would like to thank Dr. Mohammad Kassemi for giving me the opportunity to work on this project and allowing me the latitude to explore various aspects of this problem that I thought were interesting. I would also like to thank Dr. Iwan Alexander. Our meetings, where we ground through some of the finer points of this problem, were helpful. The gratitude of Dr. Charles Panzarella cannot be understated. His rigorous approach to problem solving is something I’ve tried to emulate during the course of this research effort.

My thanks are also extended to Dr. Feke and Dr. Kamotani for their thoughtful comments and questions.

With regard to the ground-based experiment, several individuals deserve mention. First, the engineering team of Mr. Scott Meyer, Mr. Frank Kmicik, and Mr. Robert Butcher did an excellent job of transforming experimental concepts and requirements into hardware. The efforts of Mr. John Juhas in the initial build up and Mr. Frank Lam in subsequent modifications to the test rig is also greatly appreciated. I would also like to acknowledge the help of Ms. Amy Wu in calibrating some of the instrumentation. Thanks are also due to Dr. Nasser Rashidnia for helping me to x
diagnose and troubleshoot various aspects of the experiment that weren’t behaving as expected. Our lunchtime chats definitely made the time I spent in the lab more enjoyable.

Computationally, the resources provided by the National Center for Space Exploration Research, Case Western Reserve University, NASA Glenn Research Center, and the Ohio Supercomputing Center are all greatly appreciated. The IT support provided by Mr. David Thompson has also been helpful.

Finally, I would like to extend my appreciation to all my colleagues and friends at Case Western Reserve University, the National Center for Space Exploration Research, and the NASA Glenn Research Center. My years in Cleveland have been some of my favorite.
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<td>$A_o$</td>
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<td>Baffle spacing</td>
</tr>
<tr>
<td>$C$</td>
<td>Tube clearance</td>
</tr>
<tr>
<td>$c_p$</td>
<td>Specific heat at constant pressure</td>
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<tr>
<td>$c_p^o$</td>
<td>Ideal gas specific heat capacity</td>
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<td>$c_v$</td>
<td>Specific heat at constant volume</td>
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<td>Hydraulic diameter</td>
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<tr>
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<tr>
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<td>$I_{meas}$</td>
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<tr>
<td>$j$</td>
<td>Condensation mass flux</td>
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<td>$J$</td>
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Nomenclature
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<td>$J_e$</td>
<td>Total energy flux</td>
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<td>$J_q$</td>
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<tr>
<td>$K$</td>
<td>Stiffness matrix</td>
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<td>Thermal conductivity</td>
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<tr>
<td>$l$</td>
<td>Interface thickness</td>
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<tr>
<td>$L$</td>
<td>Characteristic length, latent heat</td>
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<tr>
<td>$(L_1, L_2)$</td>
<td>Area coordinates</td>
</tr>
<tr>
<td>$m$</td>
<td>Mass</td>
</tr>
<tr>
<td>$\dot{m}$</td>
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</tr>
<tr>
<td>$M$</td>
<td>Evaporation rate</td>
</tr>
<tr>
<td>MLI</td>
<td>Multilayer insulation</td>
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<td>$M_w$</td>
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<td>$(\hat{n}, \hat{t})$</td>
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<tr>
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</tr>
<tr>
<td>$N_t$</td>
<td>Number of heat exchanger tubes</td>
</tr>
<tr>
<td>Nu</td>
<td>Nusselt number</td>
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<tr>
<td>$p$</td>
<td>pressure</td>
</tr>
<tr>
<td>$P$</td>
<td>Power</td>
</tr>
<tr>
<td>PEEK</td>
<td>Polyether ether ketone</td>
</tr>
<tr>
<td>$P_T$</td>
<td>Tube pitch</td>
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Pr Prandtl number

$q''$ Heat flux

$\dot{Q}$ Heat power

$\dot{Q}_w$ Total heat power

$R$ Gas constant, Radius

$Ra$ Rayleigh number

$Re$ Reynolds number

$S$ Viscous stress tensor

$s$ Specific entropy

$S$ Entropy

$T$ Temperature

$T$ Stress tensor

$T$ Nodal temperatures

$u$ Specific internal energy

$U$ Internal energy, total heat transfer coefficient

$v$ Velocity

$V$ Volume, velocity

$V_{source}$ Source voltage

$W_i$ Weighting coefficients

$X$ Mole fraction

$(Z, R)$ Nodal coordinates
\((z, r)\) Coordinate directions

**Greek**

\(\beta\) Coefficient of thermal expansion

\(\xi\) Coordinate along 1D finite element

\(\delta\) Dirac function

\(\Delta t\) Time increment

\(\partial \Omega\) Interfacial region

\(\kappa\) Bulk viscosity

\(\rho\) Density

\(\sigma\) Accommodation coefficient, surface tension

\(\omega\) Mass fraction, accentric factor

\(\Omega\) Bulk phase region

\(\mu\) Dynamic viscosity

\(\nu\) Specific volume

**Subscripts and Superscripts**

\(\text{avr}\) Average

\(\text{bulk}\) Bulk liquid or vapor phase

\(c\) Critical

\(E\) Elemental
<table>
<thead>
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<td>$g$</td>
<td>Gas</td>
</tr>
<tr>
<td>$I$</td>
<td>Interface</td>
</tr>
<tr>
<td>$il$</td>
<td>Liquid side of the interface</td>
</tr>
<tr>
<td>$in$</td>
<td>Inlet</td>
</tr>
<tr>
<td>$iv$</td>
<td>Vapor side of the interface</td>
</tr>
<tr>
<td>$jet$</td>
<td>Jet</td>
</tr>
<tr>
<td>$l$</td>
<td>Liquid</td>
</tr>
<tr>
<td>$n$</td>
<td>Time step</td>
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<td>Nozzle</td>
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<td>$o$</td>
<td>Initial, reference</td>
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<td>out</td>
<td>Outlet</td>
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<td>$s$</td>
<td>Surface quantity, shell</td>
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<tr>
<td>$sat$</td>
<td>Saturation</td>
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<tr>
<td>$t$</td>
<td>Tank, tube</td>
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<tr>
<td>$T$</td>
<td>Transpose</td>
</tr>
<tr>
<td>$v$</td>
<td>Vapor</td>
</tr>
<tr>
<td>$wl$</td>
<td>Wetted wall</td>
</tr>
<tr>
<td>$wv$</td>
<td>Non-wetted wall</td>
</tr>
<tr>
<td>+</td>
<td>Liquid region</td>
</tr>
<tr>
<td>–</td>
<td>Vapor region</td>
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Ventless Pressure Control of Cryogenic Storage Tanks

Abstract

by

STEPHEN BARSİ

Future operations in space exploration will require the ability to store cryogenic liquids for long durations. During storage, the tanks may self-pressurize due to heat leaks from the ambient environment. When heat leaks into the tank, the cryogenic liquid vaporizes causing the ullage pressure to rise. Being able to effectively control tank pressure will make these long duration storage concepts feasible. One way to control tank pressure involves the use of a subcooled axial liquid jet to both thermally destratify the bulk liquid and remove energy from the tank. In this dissertation, the effectiveness of using subcooled jet mixing as a pressure control scheme is analyzed by performing a small-scale experiment in a normal gravity environment with a refrigerant. Following a period of self-pressurization, the jet’s speed and degree of subcooling are parametrically varied so that relevant trends can be identified. Experimental results show that mixing the bulk liquid is not sufficient to control pressure. To sustain any pressure reduction, subcooling the mixing jet is necessary. The rate of pressure reduction is greater for increased jet speeds and subcooling. Analytical and computational models were developed in order to predict the pressurization behav-
ior. Model comparisons reveal that generally a thermodynamic model underpredicts the self-pressurization and depressurization rates. The lack of agreement is primarily attributed to the homogeneity assumption inherent in the model. To improve model predictions, a zonal model is developed which relaxes the global homogeneity assumption. Comparisons between the experimental data and the zonal model predictions are excellent for moderate to high jet flow rates. For slower jet speeds, buoyant flow in the bulk liquid adversely affects the effectiveness of a subcooled mixing jet and a more detailed computational model is required to capture this intraphase phenomena.
Future operations of many space propulsion, environmental control and life support, thermal and power systems will all depend on the ability to store, process, and control a variety of single or multiphase fluids in reduced gravity environments.\textsuperscript{1} For many of these systems, cryogens are the fluids of choice and indeed, in future missions to the Moon or Mars, cryogens will play an integral role.

In a recent NASA workshop,\textsuperscript{2} the long term preservation of cryogens for life support systems was identified as a critical issue for the development of advanced human life support technologies. For the in-situ resource utilization program, the preservation of cryogens is essential, as large quantities of liquid oxygen (LOX) and liquid methane (LCH\textsubscript{4}) will have to be stored on the surfaces of the Moon or Mars.\textsuperscript{3,4} To realize a significant reduction in mission costs, NASA had envisioned placing large cryogenic propellant depots in low earth orbit (LEO) or deep space for periods of up to five years.\textsuperscript{5,6} For these large storage tanks, which should be able to contain 100,000 lb\textsuperscript{7,8} of LOX or liquid hydrogen (LH\textsubscript{2}), zero loss storage of these propellants...
is essential. Even in NASA’s Constellation program, the efficient storage of cryogens has been identified as a core technology. In the Exploration Systems Architecture Study, cryogenic fuels are currently envisioned for the reaction control system on the crew exploration vehicle, on the Earth Departure Stage (EDS) and on the Lunar Surface Access Module’s (LSAM) descent and possibly ascent stages. For both the EDS and LSAM, cryogenic fuel tanks will be loitering in LEO for several weeks. Additionally, for the LSAM ascent stage, these cryogenic fuel tanks will be required to stay on the lunar surface for up to six months. As reported by Motil and Meyer, based on preliminary design estimates, the LOX and LCH4 tanks on the lunar surface may lose up to 3% of usable propellant per month. Obviously, reducing these losses would translate into cost savings for the exploration program. This brief survey highlights the many technologies that would benefit from efficient storage of cryogenic liquids.

Storage of cryogens though presents a significant challenge. Cryogens are stored at very low temperatures and may be subjected to large heat loads while the storage tanks are loitering in LEO, in transit, or sitting on the surface of the Moon or Mars. The heat load can come from a variety of internal or external sources. The external sources can include incident solar radiation, planetary albedo, aerodynamic heating, or conduction loads from the tank’s support structure. Internally, the exothermic reaction of ortho/para conversion of LH2 and the kinetic energy associated with liquid sloshing, which eventually dissipates as heat, can all be factors. When heat leaks into the tank, it will be carried to the liquid-vapor interface by conduction and natural convection. Once this thermal energy reaches the surface, the liquid may
start vaporizing. Since vaporization occurs in a closed tank, the tank pressure will increase. Design constraints regarding the tank’s maximum operating pressure and requirements regarding tolerable liquid losses make controlling both the phase change process and the tank pressure a necessity.

Various strategies have been identified as possible mechanisms to control tank pressure. The simplest strategy involves periodically venting the vapor overboard to reduce the pressure. Venting is a straightforward operation in a normal or partial gravity environment where the lighter vapor sits atop the heavier liquid. In a reduced gravitational environment, where the position of the vapor is less certain, venting only vapor becomes more challenging. While venting does reduce tank pressure, it does nothing to mitigate boil-off losses. That is, venting over time will still lead to considerable propellant losses.

Other strategies involve storing the liquid as a bulk subcooled phase\textsuperscript{10} or using combinations of MLI blankets to insulate the tank and sunshades to shield the tank from solar radiation or planetary albedo.\textsuperscript{10,12–14} Bulk liquid subcooling can increase the amount of energy the liquid can hold before vaporization and boiling takes hold thus delaying the tank’s pressure rise. Sunshades serve to reduce the heat load on the storage tank. While both of these strategies offer some benefits, both lack the robustness of an active pressure control system.

When heat leaks into the tank from the surroundings, the temperature field inside often stratifies. Mixing the fluid inside the tank can destratify the thermal field; reducing temperature gradients near the liquid-vapor interface and bringing the cooler
INTRODUCTION

fluid that had settled out closer to the surface - both of which promote condensation and a reduction in tank pressure. Mixing strategies alone have been the subject of much research. Passive mixing has been shown to have a significant effect on fluid behavior in low gravity environments. Gebhart showed that random disturbances can result in transport rates much greater than would be expected in the absence of all disturbances.\textsuperscript{15} Grodzka reports that experiments conducted during Apollo 14 and 17 and data taken from the oxygen tanks aboard Apollo 15 revealed that natural convection caused by g-jitter can be significant.\textsuperscript{16} Passive mixing however lacks the robustness necessary for active pressure control. Active mixers such as axial or radial liquid jets or spray bars have also been studied. Axial jets exhibit a definite gravity dependence. Oftentimes, the liquid jet flows opposite the direction of buoyancy which tends to reduce its effectiveness. Spray bars, on the other hand, are typically gravity independent since liquid is ejected radially into both phases from a bar running the entire length of the tank. As will be discussed shortly though, which active mixing strategy is more effective remains uncertain. Regardless, active mixing alone offers only a temporary reduction in tank pressure. Because the mixing device itself adds energy to the system, the net heat load post-destratification can be larger than if no mixer were present.

Consequently, active mixers are often coupled to a refrigeration system. One of the earliest refrigeration concepts considered for cryogenic storage systems was a thermodynamic vent system (TVS).\textsuperscript{17} In a TVS, some sacrificial liquid passes through a throttling device to reduce its temperature. The colder two-phase fluid then passes...
through a heat exchanger which can be attached to the outer surface of the tank to intercept the incident heat load. Due to heat transfer into the two-phase fluid, vaporization occurs and the resulting vapor is eventually vented overboard. Alternatively, after passing through the throttling valve, the fluid can enter a heat exchanger which can be used to subcool a liquid jet or be placed internal to the tank to remove energy from the bulk liquid and vapor. A spray bar/heat exchanger TVS system designed by Rockwell Aerospace and extensively tested at the Marshall Space Flight Center has demonstrated the ability to control tank pressure within a very tight control band for a variety of cryogens and mission scenarios. Although less common, a TVS system consisting of an axial jet mixer and a heat exchanger has also been tested. In a recent review, Hastings reported TVS performance comparisons between an axial jet mixer and a spray bar. Although tank pressure decayed more rapidly during the spray bar operation, the axial liquid jet resulted in better bulk mixing. The comparisons appear to be inconclusive especially since the liquid flow rates were different in the two test cases. Regardless of the combination of mixer or heat exchanger employed, a TVS is designed to sacrifice some liquid to reduce the bulk energy of the system. Hence, operation over extensive periods of time will lead to loss of usable propellant.

Recent advances in zero boil-off (ZBO) technologies have improved the prospects of a truly zero loss storage system. The main refrigeration system used in a ZBO system is a cryocooler. The cooler can be mounted outside of the tank and mated to heat exchangers, internal condensing surfaces, heat pipes, or wall-mounted thermally
conducting sheets. While Plachta has achieved ZBO conditions during ground testing using passive mixing, because the conduction and natural convection time scales are much slower in low gravity, a ZBO cryocooler is often combined with an active mixer to enhance condensation and pressure control. Preliminary testing has been performed with both axial jet mixers and spray bars.

These preliminary proof-of-concept tests are very promising. Even a modest reduction in boil-off losses (and thus launch mass) can translate into significant mass savings. Comparing a ZBO system with a passive storage and insulation system, Plachta showed that for short duration missions a ZBO system is not as attractive as a passive storage tank due to the increased launch mass of the mixer and cryocooler. However, after a relatively short time (1 week for LOX, 2 weeks for LCH4, and 2 months for LH2) the mass and cost benefits of a ZBO system are quickly realized. Besides the cost and mass savings, ZBO adds to mission flexibility as delays in rendezvous or docking would no longer jeopardize propellant mass margins. While the benefits of a ZBO system may be substantial, more work is required before its full potential is realized. From a power consumption and reliability standpoint, it may not be practical to continuously operate an active mixer. Optimization is necessary to tune the system to maximize performance. Optimizing a ZBO system requires a better understanding of the complicated and coupled transport phenomena inside the tank which can affect thermal stratification, self-pressurization, and pressure control. These same issues were identified in past reviews as critical to cryogenic storage and remain as relevant today.
Due in part to these reviews, extensive research dating back to the Apollo program has been performed but unanswered questions still remain. To answer some of these questions, large-scale flight demonstrations are generally preferred. Large-scale flight experiments, however, can be costly and time consuming. As pointed out by Chato,\textsuperscript{39} computational tools can offer development cost savings and improved designs but these tools must be quantitatively validated. As such, the design approach currently favored by much of the cryogenic community is to develop numerical models, validate them against small-scale experiments in both normal and reduced gravity, and then use both the sub-scale experimental data and the computational models to extrapolate the ZBO design to an actual flight system. Indeed, this is the approach adopted in this dissertation.

Having established the relevance of the current research problem, before the dissertation objectives are outlined, a survey of prior research in the field will be presented.

### 1.1 Literature Survey

NASA has a rich heritage of flight testing and flight qualifying cryogenic fluid management technologies in support of past exploration programs. Beginning in the early 1960s, and continuing for several years, several experiments were conducted aboard Aerobee sounding rockets which provided approximately $4\frac{1}{2}$ minutes of low gravity. Knoll \textit{et al.}\textsuperscript{40} performed LH2 experiments in a 9" diameter partially full Dewar subjected to radiant heating. The measured self-pressurization rate was larger
than a simple thermodynamic analysis predicted. Thermal measurements indicated that during the experiment an initially wetted-wall eventually formed dry spots during the flight. The experiment sat on a de-spin platform to counter the effects of the spin-stabilized rocket. Misalignment of the de-spin platform resulted in accelerations of \( \pm 0.02 \text{g} \). In a subsequent flight, a similar experiment was performed and this time, nucleate boiling was observed. Unfortunately for this flight, the de-spin platform malfunctioned. In a similar experiment reported by Nunamaker \textit{et al.},\textsuperscript{42} temperature measurements indicated wall dry out and fluid sloshing in the tank. Once again, the self-pressurization rate was underpredicted by thermodynamics. Later in the Aerobee program, Aydelott\textsuperscript{43} conducted similar experiments but with a higher liquid fill level. Aydelott reported that the measured self-pressurization rate was approximately twice the rate predicted by thermodynamics, that ullage motion during the flight resulted in some fluid mixing, and that it took approximately two minutes for the radiant heaters to reach their set point temperature. Thus for a significant portion of the experiment, the incident heat load was not relatively constant.

Abdalla \textit{et al.}\textsuperscript{44} reported on the pressurization experiments conducted on an Atlas rocket which provided for 21 minutes of low gravity. During the flight, the experimental pod began tumbling which resulted in an acceleration of 0.001g. Consequently, the pressure rise characteristics were similar to testing done in 1g and temperature measurements exhibited cyclic behavior in phase with the external perturbations. During the Atlas/Centaur AC-8 flight, Lacovic \textit{et al.}\textsuperscript{45} studied propellant behavior during an orbital coast. Temperature measurements indicated significant thermal stratification...
1.1 LITERATURE SURVEY

in the ullage.

Bradshaw\textsuperscript{46} and Navickas \textit{et al.}\textsuperscript{47} described the self-pressurization results on the Saturn IVB-AS203 flight. Continuous venting of the O2 tanks during most of the flight provided a settling acceleration to the instrumented LH2 tank. Data was taken during an orbital coast, however a loss of signal resulted in 50\% of the data missing during the middle of the test. Allgeier\textsuperscript{48} reported on a small-scale LN2 experiment conducted on the AS-203 flight. During this experiment, the tank was allowed to self-pressurize after which a small amount of liquid was withdrawn from the tank and passed through a heat exchanger brazed to the outer wall of the test cell. This system exhibited good pressure control.

Several relevant experiments were also conducted on the LOX/LH2 Titan/Centaur upper stage\textsuperscript{49,50}. While these experiments were primarily investigating liquid orientation and engine restart capability after an orbital coast, temperature and pressure measurements were also made to study stratification and pressurization. From temperature measurements taken during these flights, Lacovic\textsuperscript{50} inferred that sections of the tank’s wall dried out during the coast.

While many of these proof-of-concept flight experiments yielded important data, unknown or uncontrolled boundary or initial conditions rendered them less useful for the purposes of validating numerical models. As Chato noted in a recent review\textsuperscript{39}, piggy-backing on the Saturn and Centaur upper stages made many of the these experiments cost effective but unfortunately prevented them from carrying more extensive instrumentation to provide detailed data for future model validations.
Besides these orbital and sounding rocket tests, cryogenic fluid management experiments have also been performed aboard aircraft. Ordin et al.\textsuperscript{51} mounted a 450 gal LH2 tank to the wing tip of a jet aircraft to investigate the effects of atmospheric turbulence on thermal stratification. As a result of significant agitation during the flight, the degree of stratification in the tank was diminished when compared to similar ground tests. Bentz\textsuperscript{52} conducted a small-scale Freon 113 self-pressurization/axial jet mixing experiment aboard a Lear jet flying parabolic profiles. The value of these particular parabolic flight experiments was limited due to their short duration exposure to low gravity (± 0.01g).\textsuperscript{53} In the experiment, Bentz reported that there was insufficient time between parabolas for the liquid to reach a quiescent state.

To obtain more long duration periods of low gravity, Bentz and colleagues\textsuperscript{52,54,55} performed tank pressure control experiments (TPCE) on three shuttle flights in the early 1990s. During the first flight, a small tank partially full of Freon 113 self-pressurized due to heaters submerged in the liquid. Heating was maintained for several minutes, after which, the heaters were turned off, liquid was withdrawn from the tank, and pumped back in through an axial liquid jet. The pressure collapse as a result of axial jet mixing was studied. On the second flight, during heating, higher local superheats were observed which apparently resulted in flashing of the liquid and a spike in tank pressure. The third experiment was similar to the first two, except now the test was performed at a lower fill level. These TPCE experiments provided useful data but unfortunately due to several shortcomings, the data is not suitable for numerical validation. First, the liquid jet was not thermally controlled
and unfortunately no jet temperature measurements were made. It’s uncertain how much heat leaked from the liquid jet to the surroundings. Any subcooling of the jet would have had a profound effect on the pressure reduction times. Second, no thermal controls existed between the tank and the ambient environment. Yet no attempts were made to quantify the amount of heat lost from the tank. Third, there was only a 20 minute wait period between experiments and it’s unclear whether 20 minutes were long enough for subsequent tests to begin from the same thermal and dynamic state. Finally, for all three TPCE experiments, contaminant species leaked into the test cell. The amount of non-condensable species was estimated from the overpressure above saturation. During the three experiments, the partial pressure of the non-condensable gases ranged between 1 kPa and 6.2 kPa. While the investigators claimed the non-condensable contaminants had no effect on the results, other theoretical and experimental studies would suggest otherwise. (see for example Rose,\textsuperscript{56} Minkowycz and Sparrow,\textsuperscript{57} and Hastings \textit{et al.}\textsuperscript{27}).

In addition to the flight experiments, surveyed so far, there have also been extensive ground tests both in support of and independent of these flight projects. While investigating thermal stratification in a ground liquid nitrogen experiment, Fan \textit{et al.}\textsuperscript{58} observed a thin thermal boundary layer near the tank walls and noted that convection heat transfer was significant. Beduz \textit{et al.}\textsuperscript{59} performed wall heating stratification studies of LOX and LN2 in small Dewars. Using temperature measurements in the liquid, they were able to map the morphology of the temperature fields. Below the interface, they observed a thin thermally conducting layer a few hundred microns
thick with a steep temperature gradient which resided on top of a convective layer with a shallow temperature gradient. Both layers sat atop a near uniform bulk liquid. Swim\textsuperscript{60} conducted stratification studies using Dewars partially full of liquid helium. He observed steep temperature gradients on either side of the interface in line with Beduz’s morphology studies. Tatam and colleagues,\textsuperscript{61} performing stratification experiments in a 500 gal LH2 tank, noted that a considerable amount of thermal energy went into raising the temperature of the bulk fluid which suggests the absence of well-defined boundary layers. Neff and Chiang\textsuperscript{62} reported on stratification experiments using both water and cryogenic fluids. They noted that an increase in the bulk liquid temperature indicated quasi-steady flow and temperature conditions in the tank. Moreover, they attempted to describe the stratification process semi-empirically by approximating the temperature profile in the liquid as a polynomial. These stratification tests were not limited to only recording temperature. Lovrich et al.,\textsuperscript{63} using a Schlieren system, performed flow visualization experiments using Freon and water with local side wall heating. They found that most of the heat remained above the heater with a sharp drop off in the temperature profile below. Anderson and Kolar\textsuperscript{64} also used a Schlieren setup to compare a side wall heating configuration with a bottom heating one. For side wall heating, they observed a stable temperature gradient below the interface. The bottom heating configuration led to better mixing of the bulk liquid which resulted in a more uniform temperature profile. More recently, Das et al.\textsuperscript{65} used a dye injection system to map out the temperature field in a side heated cavity containing water.
Nearly all of these stratification experiments were primarily concerned with thermal behavior and not the coupling between the temperature field and the vapor pressure. Ji et al.\textsuperscript{66} studied stratification and pressure rise and based on a scaling analysis, identified three dimensionless parameters in an attempt to describe and characterize the underlying physics. Several small-scale tests were performed to verify the validity of these dimensionless groups. Results indicated that the vapor pressure histories agreed reasonably well between the scaled pairs of tests but point-to-point temperature matches were not obtained indicating that the three dimensionless parameters were not sufficient at characterizing the entire system behavior. Manson\textsuperscript{67} also identified several dimensionless parameters to provide geometric, dynamic, and thermal similitude. In practice though, matching all of these parameters is difficult to achieve. Neff\textsuperscript{68} performed scaling experiments with LOX and LN2 to verify that the dimensionless parameters that he had identified were able to completely characterize the underlying physics. Comparing scaled pairs of tests, he observed similar temperature profiles although agreement between the temperature values was again lacking. Bourgarel et al.\textsuperscript{69} performed a scaling analysis without including conduction and interfacial phenomena. They also chose not to match Grashof numbers in their experimental tests. The similarity between their scaled pairs of tests was initially fair but deviations developed with time.

Blatt\textsuperscript{70} posited a function of the self-pressurization rate in terms of heat input, tank volume, and fill fraction. He used available data from ground and flight LOX/LH\textsubscript{2} self-pressurization tests in the literature to fit the constants in his func-
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The correlation however was based on only a limited number of data points and resulted in deviations as high as 89%. Scott et al.\textsuperscript{71} investigated stratification and pressurization in a partially full LHe Dewar. They initially observed a thermally stratified liquid but after placing thermally conducting copper rods in the Dewar, the temperature gradients were reduced and the recorded pressure rise agreed better with a thermodynamic analysis.

In the early 1990s, a series of self-pressurization experiments were performed with a 4.95 m\textsuperscript{3} partially full LH\textsubscript{2} tank at NASA Glenn’s Plumbrook station. In these tests, as with many experiments involving cryogens, the incident heat load was not an independent parameter but was instead computed from measured boil-off rates. A detailed description of this calculation as well as the tank’s thermal boundary conditions are outlined in Stochl and Knoll.\textsuperscript{72} It’s unclear whether the heat load estimated in this fashion was applicable to all the test points in the experiment. Regardless, Hasan et al.\textsuperscript{73} still found that the self-pressurization rate increased with increasing heat load. For the lower heat flux cases, there was less deviation between the measured and thermodynamically predicted pressurization rates than for the higher heat flux cases. Van Dresar et al.\textsuperscript{74} re-ran these experiments at lower fill levels. In all cases, thermodynamics underpredicted the self-pressurization rate. The effect of fill level on the pressurization rate was difficult to discern from the experimental data. The expected trend, as predicted by thermodynamics, was not reflected by the experimental data.

In support of the Aerobee sounding rocket tests, Aydelott\textsuperscript{75,76} performed a series
of ground self-pressurization tests in a 9” diameter spherical tank partially filled with LH2. He found the pressurization rate was affected mostly by the heating configuration (top, bottom, or uniform heating) with only a slight effect from varying the fill level. Comparisons were also made with a homogeneous thermodynamic model and a surface evaporation model which assumed all the incident energy was used to vaporize the liquid and keep the vapor in a saturated state. The experimental data was bounded by the two models with the thermodynamic model underpredicting the pressurization rate. Some tests were performed while shaking the tank. In this case, the pressurization rate approached the homogeneous model’s prediction. Aydelott and Spuckler\textsuperscript{77} also investigated the effects of tank size by comparing the previous 9” tank tests with tests in a 22” diameter spherical tank. They found similar pressure rises for equal values of the heating rate to volume ratio. Summarizing his results from both the ground and flight 9” diameter tank tests, Aydelott\textsuperscript{78} noted a reduced pressurization rate in low gravity. He attributed this effect to the increased wetted-wall area and the fact that direct heating of the vapor would result in a larger pressure rise rate.

While most of these ground self-pressurization experiments were conducted using small-scale tanks, Liebenberg and Edeskuty\textsuperscript{79} performed tests in a 55,000 gal Dewar 94.7% full of LH2. The observed pressure rise rate was greater than the prediction of a homogeneous model by nearly a factor of 10.

Ground testing was not limited to self-pressurization studies. Several pressure control tests were also performed. Huntley\textsuperscript{80} experimented with a closed LN2 De-
war and found that after mechanically stirring the liquid, the pressure temporarily decayed. However, he found that mixing the ullage resulted in an increase in the pressurization rate.

In evaluating TVS designs, Bullard\textsuperscript{81} noted that a bottom-mounted axial jet was more effective at collapsing the pressure than a side-mounted horizontal jet. In his mixing-only tests, the pressure reduction was temporary and it was noted that the minimum pressure was reached after only 20-30\% of the liquid circulated through the jet nozzle. He also observed that introducing a non-condensable gas into the system significantly increased the pressure collapse time. Dominick\textsuperscript{82} also examined the effects of jet orientation on the condensation rate in a small-scale tank partially filled with Freon. He observed higher rates of condensation and liquid destratification when the jet nozzle was oriented perpendicular to the liquid vapor interface. In Dominick’s experiment however, the pressure in the tank was constant since vapor was being supplied to the ullage at the same rate mass was condensing at the interface. Moreover, there were no thermal controls between the tank and the surroundings and it’s uncertain how much heat was being lost to the outside environment.

Lin et al.\textsuperscript{83} conducted a series of axial jet mixing experiments in a partially full LH2 tank. However it’s unclear whether the same level of stratification was attained between the different test cases. Nonetheless, they found the pressure collapsed faster for faster jet flow rates. For the lowest flow rate considered, the pressure continued to increase during mixing as the jet flow was not strong enough to counter the effects of buoyancy. Lin et al.\textsuperscript{84} later showed that buoyancy effects could be neglected for
Richardson numbers less than 0.5. Here also, two mixing times were identified. One was used to describe how fast the liquid destratified and the second was used to describe how fast the pressure collapsed.

Finally, Jones and colleagues\textsuperscript{85,86} conducted several ground-based pressure control tests in a small-scale tank partially filled with Freon 11. Self-pressurization was initiated by activating a heating coil submerged slightly below the surface. After pressurizing for a time, the heater was deactivated and an axial liquid jet was used to destratify the liquid. They found buoyancy dominated the flow for jet Reynolds numbers (Re) below 2000. The data did not correlate well with steady-state condensation or dye-mixing correlations. Later, Jones \textit{et al.}\textsuperscript{87} developed a closed form pressure collapse equation by assuming that the pressure drop was due to condensation and not vapor cooling. Here, it was also noted that the dimensionless mixing time correlated with Re for low jet Reynolds numbers. For larger values, the dimensionless mixing time was constant.

While most of the ground and flight experiments described thus far were applied in nature, there have been several investigations that have focused on more fundamental aspects of the problem. McNaughton and Sinclair\textsuperscript{88} studied the stability of liquid jets in terms of Re. Four flow regimes were characterized: dissipated laminar, fully laminar, semi-turbulent, and fully turbulent. Mollendorf and Gebhart\textsuperscript{89,90} performed stability and perturbation analyses investigating how buoyancy effects liquid jet behavior. Though primarily concerned with positive buoyancy, they noted that the effect on the temperature and velocity fields could be particularly strong if
buoyancy opposed the jet motion.

Symons et al.\textsuperscript{91} and Labus\textsuperscript{92} performed a set of ground tests to characterize the jet flow behavior for a GHe jet into a GHe medium. Symons and Staskus\textsuperscript{93} later studied the interaction of a liquid jet and a free surface and developed a critical Weber number (We) criterion that described the stability of the surface. The stability of the interface is important for the current tank problem since a jet geysering into the ullage would increase the interfacial area through which mass transfer can occur.

Berenyi et al.\textsuperscript{94} performed drop tower tests on a spherical tank with a radial jet and tried to characterize the different observed flow patterns using the jet’s velocity. Aydelott performed similar tests with an axial jet in both cylindrical\textsuperscript{95} and spherical\textsuperscript{96} containers. Several flow patterns, including jet geysering, were observed. Correlations were developed to describe the flow patterns in terms of We and Bond numbers (Bo). In Aydelott’s tests, only 70% of the incoming liquid was being withdrawn from the tank. It’s unclear what effect the accumulation of liquid in the tanks had on his conclusions.

In addition to these circulation and jet flow characterization tests, many experiments were conducted to better understand jet mixing. Fox and Gex\textsuperscript{97} used an acid/base neutralization technique to develop mixing time correlations in both laminar and turbulent jet regimes. Both correlations exhibited a dependence on Re and included a gravitational effect. Fossett and Prosser\textsuperscript{98} were able to correlate their jet mixing data independently of Re. Okita and Oyama\textsuperscript{99} used their data, obtained using a density-matched dye technique, along with the Fox and Gex data to develop
a mixing time correlation that was dependent on Re for low Reynolds numbers but independent of it for higher Re values. The mixing tests by Lane and Rice\textsuperscript{100} also observed a stronger Reynolds number dependence for laminar jets than for turbulent ones. Poth et al.\textsuperscript{101,102} evaluated several different mixing devices and found jet mixers to be superior. It was observed that the time required for the jet to reach the interface was approximately twice as long as a simple kinematic analysis would predict which highlights the retarding effects of negative buoyancy. Aydelott\textsuperscript{95,96} used his drop tower experiments to develop a mixing time correlation in terms of We and Bo. Lehrer\textsuperscript{103} attempted to derive a correlation independent of any empirical data but the results were inconclusive. Comparing against the Fox & Gex and Fossett & Prosser data, his correlation sometimes underpredicted and sometimes overpredicted the measurements. Grenville and Tilton,\textsuperscript{104} reasoned that liquid jet entrainment controlled the mixing of the entire vessel. They therefore included the path length of the jet as one of the characteristic length scales in their mixing time correlation. Patwardhan and Gaikwad\textsuperscript{105} performed several mixing tests and found their data agreed best with the Grenville and Tilton correlation. It seems unlikely though that any one correlation will fit all of the data. In a more detailed review, Revill\textsuperscript{106} notes that mixing is highly dependent on a number of factors including the relative size of the tank and jet, the protrusion of the jet into the tank, the fill level, and the shape of the tank. In addition, a comparison between the correlations is complicated by the fact that many of these investigators define mixing time differently from one another. Most of these studies were only concerned with jet mixing and not the phenomenon
of a jet interacting with a condensing/evaporating interface.

Helmick et al.\textsuperscript{107} performed a set of steady-state steam-on-water condensation experiments that employed an axial liquid jet. They noted that a turbulent liquid enhances condensation and that the condensation rate can be quantified in terms of fluid properties and the liquid-side turbulence. Thomas\textsuperscript{108} conducted similar experiments and observed as the liquid jet penetrated the interface, the condensation rate, which he characterized in terms of a heat transfer coefficient, increased. Chun et al.\textsuperscript{109} observed that if the jet subcooling was significant (30-80 K) mass transport can become unstable resulting in condensation bursts and rapid pressure decay. Sonin et al.\textsuperscript{110} developed a turbulent condensation correlation assuming steady state mass transfer, isotropic turbulence, small surface waviness, and negligible buoyancy. His correlation required the r.m.s. value of the turbulent velocity at the free surface which he estimated from a simple k-\(\epsilon\) analysis. Brown et al.\textsuperscript{111} extended this work by including buoyancy effects through a Richardson number dependency. Brown\textsuperscript{112} also extended Sonin’s correlation by developing another expression for the r.m.s. turbulent velocity at the free surface which was valid for smaller jet submergence depths. It remains to be seen, however, whether these steady state condensation correlations are applicable to the transient situation that prevails during the pressure control of cryogenic storage tanks.

This comprehensive experimental review pertaining to thermal stratification, self-pressurization, and pressure control underscores the degree of uncertainty in many of these experimental investigations. Additionally, the experiments themselves provide
little detailed data that is conducive to a comprehensive model validation and ver-
ification effort. Detailed measurements of the flow field are typically not made and
oftentimes the bulk of the data is compressed into a simple engineering correlation.\textsuperscript{113}
Unfortunately, this level of uncertainty and lack of more detailed data can cloud the
comparisons between model and experiments making validation efforts more difficult
and less systematic.

In parallel to the experimental efforts outlined above, numerous theoretical and
computational models of varying levels of sophistication have also been developed
to both interpret and predict experimental behavior. Historically, a homogeneous
thermodynamic model was one of the earliest analytical means to predict the self-
pressurization rate in a cryogenic tank partially full of liquid. Here, a First Law energy
balance is performed over the entire liquid-vapor system. To close the problem, the
homogeneity assumption is invoked. That is, the temperature of both the liquid and
vapor phases are equal and at saturation. There have been many versions of the
homogeneous thermodynamic model over the years. If the functional form of the in-
ternal energy of the two-phase fluid is known, then the energy derivative appearing in
the energy balance can be computed explicitly and the vapor pressure can be evolved
in time.\textsuperscript{76,114–116} Assuming constant specific heats, others\textsuperscript{117–119} have represented the
time derivative of energy as the product of specific heat and the time derivative of
temperature. Still others,\textsuperscript{120} avoid the rate form of the First Law, and use a thermo-
dynamic balance to determine the final thermodynamic state of the two phase system
after knowing the net energy input. Naturally the thermodynamic analysis assumes
that the average energy of the liquid and vapor phases changes at the same rate as the energy of the two phase mixture defined at the saturation temperature. Because this condition is not met during the initial phases of self-pressurization experiments, when thermal boundary layers are developing and temperature gradients in the liquid and vapor are not stationary, the agreement between thermodynamics and experiments has generally been poor. Moreover, because the homogeneous thermodynamic model forces the energy of each phase to change at the same rate, and the thermal inertia of the liquid is typically the largest contribution to the energy balance, thermodynamics usually underpredicts measured self-pressurization rates. Recognizing this, Aydelott\textsuperscript{76} developed a surface evaporation model which assumed the sensible energy of the liquid is constant and all of the incident energy is used for vaporization or maintaining the ullage at a saturation state. Since this model neglects the contribution of the liquid’s sensible energy to the net energy balance, it generally overpredicts measured self-pressurization rates.

In order to obtain better agreement with experimental data, transport effects should be included. A number of investigators have developed models which include energy and mass transport. These models are most easily classified as zonal methods whereby the liquid-vapor system is divided into zones at constant temperature and engineering correlations are used to model the energy and mass transport between the zones. The number of zones is completely arbitrary. Riemer developed a two zone model, one for each phase.\textsuperscript{116} Estey \textit{et al.}\textsuperscript{121} included a separate zone bounding the interface. Epstein and Georgius\textsuperscript{122} divided the tank wall, liquid phase, and
vapor phase into many axial zones. Schallhorn et al.\textsuperscript{123} partitioned the liquid into annular boundary layer zones and axial zones in the bulk. Riemer, comparing his two zone model to the homogeneous thermodynamic model, noted that the zonal model did a better job of reproducing experimental data. Hedayat et al.,\textsuperscript{124} compared the zonal model of Nguyen\textsuperscript{125} against a self-pressurization experiment and found that the model overpredicted the self-pressurization rate. The results of these models are unfortunately not unique and can vary depending on the correlations used to model heat and mass transport between the different zones.

Instead of relying on correlations, many investigators have tried to explicitly account for transport effects. In an early stratification analysis, Knuth\textsuperscript{126} modeled only the liquid phase and treated it as a semi-infinite solid. For a change in the interfacial temperature, he was determining the response of the temperature field in the liquid. Knuth\textsuperscript{127} and Thomas et al.\textsuperscript{108} extended this analysis by modeling the liquid and vapor phases as two semi-infinite media coupled at the interface. Schmidt et al.\textsuperscript{128} performed a subcooled stratification experiment and compared his results with the semi-infinite conduction solution. He found there was some agreement initially, but as time progressed, deviations increased. Segel\textsuperscript{129} performed his own pressurized stratification tests and found for low heat fluxes, there was good agreement between the measured temperature profiles in the liquid and the semi-infinite conduction solution. For higher heat fluxes, however, deviations were observed and attributed to increased convection in the liquid.

To improve on the conductive analyses, a number of investigators have used ap-
proximate integral methods to resolve natural convection in the liquid. Bailey *et al.* developed a model to study stratification in the liquid. He assumed that all of the incident energy appears as sensible heat to the free convection boundary layer, that the energy in the boundary layer is carried to an upper stratum layer where it remains, and that there is no mixing between the upper stratum and the bulk liquid. With these severe restrictions, and assumed boundary layer temperature and velocity profiles, integral heat and mass balances were performed. Comparisons between the model’s predictions and empirical stratification data was poor. In the stratification experiment, Bailey *et al.* observed mixing between the upper stratum and the bulk which was not accounted for in the model. Bailey and Fearn compared their approximate integral model to a 70 ft$^3$ LH2 stratification experiment but were again unable to accurately predict the temperature profiles in the liquid. Tellep and Harper performed a similar analysis but included an interfacial energy contribution in the integral balance and assumed a time-invariant temperature profile in the upper stratum. This resulted in a better agreement between the predicted and measured temperature profiles. Ruder and Robbins *et al.* developed similar models but noted modifications were necessary to include the effects of bottom heating and phase change. Vliet extended the analysis by including the effects of bottom heating but neglected the interfacial energy contribution in the integral balance. Barnett *et al.* included a parameter that allowed for energy exchange with the bulk liquid but still observed poor agreement between the measured and predicted surface temperature rise. More recently, Kirk *et al.* used these approximate methods to study a rotat-
ing upper stage. They assumed the liquid to be in solid-body rotation with a static paraboloid interface. They noted that the rotation had an effect on the heat transfer due to the increase in wetted-wall area, but no comparisons with experiments were made.

Eventually these approximate integral methods grew into more sophisticated boundary layer type analyses. Barnet et al. applied correlations for the boundary layer thickness, the growth of the upper stratum, and the natural convection speed at the edge of the boundary layer. He obtained reasonable agreement with measured temperature profiles after including a term that accounted for the heat of compression in the liquid. Arnett and Millhiser included both the liquid and vapor phases in their analysis and accounted for inter-phase energy and mass transport. They assumed turbulent free convection boundary layer profiles for velocity and temperature but posited the functional form of the boundary layer thickness and velocity at the edge of the boundary layer. Arnett and Voth used integral balances to compute these parameters at every location along the boundary layer. Comparing their results with Atlas/Centaur pressurization data they observed poor agreement between measured and predicted temperature profiles and underpredicted the pressurization rate by as much as 15%. Venkat and Sherif extended the Arnett and Voth model by including variable fluid properties, bottom heating, and an ortho/para conversion routine. Most of these changes resulted in only marginal differences with Arnett and Voth’s predictions. For the ortho/para concentrations analyzed, there was no discernible effect on the results. Gursu et al. tested several free convection boundary layer profiles
and found no significant effect on the results. Their ortho/para conversion routine showed clearly, and quite intuitively, that the boil-off rate increases with increasing ortho concentration. Most of these boundary layer analyses assume a stationary well-developed free convection boundary layer and a relatively simple tank geometry both of which may not be realistic in a real storage tank setting.

To obtain more meaningful predictions, these approximate techniques have given way to more sophisticated computational models. Before accounting for the more complicated interfacial heat and mass transfer, several numerical studies were conducted which investigated thermal stratification in the liquid phase due to some external heating. Nikitin and Polezhaev\textsuperscript{144} considered a partially filled sphere in microgravity. Assuming a static, insulated, and spherically-shaped free surface, they studied the interaction between buoyancy and Marangoni convection for different ullage locations inside the tank. Cherkasov\textsuperscript{145} assumed a static, flat, and shear-free surface and computed the time evolution of the temperature field for different wall and interface heating configurations. Lin and Hasan\textsuperscript{146} numerically studied the steady-state flow and temperature fields that developed as a result of buoyancy in a tank with a flat shear-free interface. They tried to characterize the thermal behavior in terms of the liquid subcooling - the interfacial temperature was assumed fixed at the saturation temperature and the temperature at the bottom of the tank was fixed at some subcooled value. Sengupta\textsuperscript{147} performed similar numerical stratification studies by enforcing an adiabatic temperature condition along the interface. His computed temperature profiles below the interface deviated from the experimental values but
the deviations decreased in the bulk liquid. Tanyun *et al.*\textsuperscript{148} also forced the surface to be adiabatic and noted that the computed surface temperature was higher than experimental measurements. Barakat and Clark\textsuperscript{149} set the interfacial temperature equal to the saturation temperature and were able to obtain some agreement with experimental temperature profiles. Navickas\textsuperscript{150} numerically studied the effect of baffles on the thermal stratification in a partially full rectangular cavity with a flat interface. His results indicated that through judicious placement of baffles, thermal stratification can be suppressed.

All of these preceding computational studies lacked a gas-phase model and treated the interface as a static surface. Grayson *et al.*\textsuperscript{151, 152} removed the second limitation by allowing the interface to freely evolve and deform. They studied how the interface and the thermal field respond to different gravitational accelerations. They, too, however neglected gas-phase transport and assumed an adiabatic interface.

In addition to the numerical stratification studies, a number of numerical studies on jet mixing has been performed. Hasan and Lin\textsuperscript{153} performed isothermal steady-state computations of axial jet mixing and its interaction with a flat interface. They compared the computed turbulent r.m.s. velocity profile with Sonin’s expression\textsuperscript{110} and noted an increased deviation close to the interface. They attributed the discrepancy to the Neumann boundary conditions placed on the turbulent kinetic energy and dissipation rate at the free surface. Later, Lin and Hasan\textsuperscript{154} performed a similar computational analysis and obtained good agreement in comparison with Brown’s expression\textsuperscript{112} for the turbulent r.m.s velocity profile for low jet submergences.
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Hochstein et al.\textsuperscript{155} also investigated isothermal jet mixing. Instead of Neumann conditions on the turbulent kinetic energy, they prescribed it to be zero at the interface. Unfortunately, no comparisons to experiments were made. Hochstein et al.\textsuperscript{156}, again employing a k-\(\epsilon\) turbulence model, neglecting buoyancy, and allowing the free surface to deform, were not able to obtain a solution for high jet flow rates. For lower jet speeds, they were able to model the interface as a static boundary. Wendl et al.\textsuperscript{157} were able to predict the flow patterns (including geysering) Aydelott observed\textsuperscript{95} in his drop tower experiments but the results were only qualitatively in agreement. To better predict geyser height, Thornton and Hochstein\textsuperscript{158} performed a sensitivity study on how various parameters affect the computational solution. For all the parameters considered they found only marginal differences in the CFD solution. Critically reviewing the Aydelott experiment,\textsuperscript{95} Simmons et al.\textsuperscript{159} inferred different boundary conditions and fluid properties than had been used in previous simulations. Though, after implementing these modifications deviations between measured and predicted geyser heights persisted. Marchetta et al.\textsuperscript{160} tried to improve the geysering simulations by using a k-\(\omega\) turbulence model. However, the results indicated that the original k-\(\epsilon\) formulation yielded better agreement with the experiment. Marchetta and Bendetti\textsuperscript{161} performed 3D geysering simulations and tested a suite of two equation turbulence models. They noted that while the k-\(\epsilon\) model more accurately predicted the geyser height when geysering occurred, Menter’s SST k-\(\omega\) formulation\textsuperscript{162} was superior at predicting the different flow regimes that Aydelott had observed.

These previously mentioned deformable free surface simulations employed the vol-
Chato et al.,\textsuperscript{163} however, used Jacqmin’s phase field model\textsuperscript{164} to simulate interfacial deformation during geysering. Their simulations overpredicted the geyser height at faster jet flow rates. They attributed this discrepancy to a lack of a turbulence model. Chato\textsuperscript{165} later added a simple turbulence model which assumed a constant turbulent viscosity. This approach overcorrected the results which led to an underprediction of the geyser height. Chato\textsuperscript{166} also performed a parametric study investigating the effects of contact angle, geometry, and surface tension on the predicted geyser height. He found that by increasing the contact angle the geyser height increased.

Mukka and Rahman\textsuperscript{167} conducted a steady-state finite element analysis of a liquid jet entering a completely full tank. They evaluated the effectiveness of mixing by comparing the circulation patterns produced by different jet configurations. Ho and Rahman\textsuperscript{168} performed 3D steady-state finite element simulations of a horizontal liquid jet impinging on a heat pipe in a full cryogenic storage vessel. They primarily studied the different circulation patterns for varying jet speeds and did not include any two-phase or thermodynamic effects.

A number of investigators have built on this body of computational work involving thermal stratification and jet mixing by including the effects of self-pressurization. Lin and Hasan\textsuperscript{169} developed a simple conduction model in the liquid and coupled it to the thermodynamic pressurization model of Brown.\textsuperscript{112} They also neglected gas-phase transport but allowed the interface to expand and contract radially. In the liquid, they included a lumped compressibility term in their energy balance and found that
initially, the pressurization rate was greater for higher fill levels because of liquid expansion. After some time had elapsed however, due to the large thermal inertia of the liquid, the final pressurization rate decreased with increasing fill level. Hochstein et al.,\textsuperscript{170,171} neglecting gas-phase transport, employed an effective conductivity model to account for transport in the liquid and performed a cell-by-cell mass balance along the interface to account for evaporation. Comparisons with experiments\textsuperscript{44,76} yielded reasonable agreement for the bottom heating and uniform heating cases in 1g, but discrepancies were noted for the top heating test case in 1g and for the uniform heating case in low g. Although Hochstein\textsuperscript{172} noted that more work was required to improve the heat transport modeling in the tank, they used this model to study the effects of bulk liquid subcooling and found the self-pressurization rate decreased with increased subcooling.

Grayson et al.,\textsuperscript{173} including transport in the ullage and using the pressurization model of Hirt,\textsuperscript{174} attempted to simulate the AS-203 flight experiment.\textsuperscript{46,47} Grayson’s model resulted in a 3.5% deviation between measured and predicted pressurization rates. The reported discrepancy is however a little misleading since only the initial and final pressures were used to compute the pressurization rate. A more careful inspection of the comparison between the predicted pressure and data extrapolated from the experiment results in a larger deviation.

Merte et al.\textsuperscript{175} also developed a pressurization model which included the effects of gas-phase transport. The interface was assumed flat and the pressure for the incompressible/incompressible system was updated using a First Law energy balance.
1.1 LITERATURE SURVEY

Merte et al.\textsuperscript{176} later compared their predictions to data from the AS-203 flight but the agreement was not good. They attributed the errors to inadequately modeling the tank geometry. Val’tsiferov and Polezhaev,\textsuperscript{177} included the effects of transport in the ullage and used an integrated form of the ideal gas law to update the pressure but were not able to obtain agreement with Aydelott’s self-pressurization experiments.\textsuperscript{76} Tunc et al.\textsuperscript{178} also developed a gas-phase model to study thermal stratification and pressure behavior when a LOX tank is pressurized with GHe. While no experimental comparisons were provided, the computational results seem unreliable as the non-condensable contribution to the ullage pressure appears to be incorrectly modeled.

Given the difficulties associated with including transport effects in the ullage, it’s no surprise that several investigators continue to couple lumped thermodynamic balances in the ullage to numerical solutions in the liquid. Amirkhanyan and Cherkasov\textsuperscript{179} coupled an effective conductivity analysis in the liquid to a lumped model of the ullage. The results appear to be inconclusive. When comparing with measured experimental data, in some cases they overpredicted the pressurization rate, in other cases they underpredicted it, and in no cases did their results agree with a homogeneous thermodynamic analysis. Panzarella and Kassemi\textsuperscript{117} rigorously coupled a lumped energy and lumped mass model of the ullage to the detailed transport equations in the liquid. While experimental comparisons were not made, their simulations for a given heat load and fill level in a tank showed that the long-term self-pressurization rate is independent of the heating configuration. Additionally, the computed pressurization rates agreed with a thermodynamic analysis of the system. Extending this model to
larger LH2 tanks in microgravity, Panzarella and Kassemi\textsuperscript{180} showed that the thermal stratification in a reduced gravity field can be significant and even in a $10^{-6}$g field, ullage migration from the center to the top of the tank occurs on a much faster time scale than heat or mass transport inside the tank.

Numerical investigations have not only been limited to thermal stratification, jet mixing, and self-pressurization but have also included pressure control with a sub-cooled axial mixing jet. Albayyari\textsuperscript{181} developed a simple analytic pressure control model and seemingly validated the model. The validation claim is surprising as the nearly identical model of Bentz\textsuperscript{52} yielded better agreement with experimental data. The major difference between the two models is that different correlations were used to model the heat transfer between the impinging jet and the free surface.

In order to obtain better agreement with experimental data, more sophisticated computational models have been developed. Lin\textsuperscript{182} numerically studied the effects of jet Reynolds number (Re) and Prandtl number (Pr) on the condensation rate which he quantified in terms of an average Stanton number. His steady-state computations in a rectangular domain with a flat free surface at saturation revealed that for the range of parameters considered, the average Stanton number is independent of Re and only weakly dependent on Pr. Lin and Hasan\textsuperscript{183} continued this analysis and showed how geometry, heat load, and jet subcooling can affect the condensation rate. In the above numerical studies by Lin and colleagues, buoyancy was neglected. Hasan and Lin\textsuperscript{184} included the effects of buoyancy and showed that natural convection can reduce the condensation rate.
1.1 LITERATURE SURVEY

Panzarella et al.\textsuperscript{185} performed a numerical study of subcooled axial jet mixing in microgravity. Their lumped vapor active liquid model showed that for most jet speeds, subcooled jet mixing was effective at reducing tank pressure. For the lowest jet speed however, buoyancy, due to residual gravity, prevented the jet from reaching the interface and no pressure reduction was observed.

Van Overbeke\textsuperscript{30} developed a 1g pressure control model that neglected gas-phase transport. In this two-point vapor model, he used the temperature at the upper bulkhead of the tank and the saturation temperature at the interface to approximate the temperature gradient on the vapor-side of the interface. This approach seems questionable because in the experiments Van Overbeke was comparing against\textsuperscript{83,84} the vapor was superheated and it’s unlikely this global energy difference accurately represented the local temperature gradient on the vapor-side of the interface. Not surprisingly, the validation results were inconclusive. In some cases the pressure collapse was overpredicted while in other cases it was underpredicted.

This rather comprehensive experimental and numerical review highlights several limitations in previous research efforts. Experimentally, the degree of uncertainty and lack of more detailed measurements makes these experiments unsuitable for validating and verifying self-pressurization and pressure control models. Moreover, prior numerical-experimental validation efforts have yielded results less than satisfactory with the sources of the discrepancies often left unexplained or misunderstood.
1.2 Dissertation Objectives

The objectives of this research are to address these shortcomings by rigorously developing self-pressurization and pressure control models, discussing their strengths and weaknesses, conducting a series of ground-based experiments with well defined boundary and initial conditions, and then comparing the model’s predictions with data from the experiment. Any discrepancies between model predictions and experimental data will be honestly assessed with possible sources of the deviation discussed.

1.3 Dissertation Outline

The body of this dissertation is organized into seven chapters. In the first chapter, the relevance of this research was discussed. A literature survey was presented which highlighted the prior work in the fields of thermal stratification, self-pressurization, and pressure control. The literature review also established that several shortcomings exist in the current body of knowledge. How the current research effort addresses this knowledge gap was outlined in the objectives section. The details of the experimental apparatus and procedures are presented and both the self-pressurization and pressure control experimental results are discussed in Chapter 2. In Chapter 3, the instantaneous bulk transport equations and interfacial conditions are derived from first principles. These equations are implemented into various models of varying degrees of complexity. The model development is presented in Chapter 4. Numerical
implementation of the models is described in Chapter 5. Model predictions are compared to the experimental data in Chapter 6 and results are discussed. Finally in Chapter 7, the major conclusions of this dissertation are discussed and possible areas of future work are outlined.
Chapter 2

Experimental Investigation

A series of small-scale model fluid experiments were conducted at the NASA Glenn Research Center as part of the ground-based portion of the Zero Boil-Off Tank (ZBOT) experiment. The objective of this series of experiments was to investigate the effects of various parameters on self-pressurization. Additionally, the effectiveness of using an axial jet mixer as a means of controlling tank pressure was studied. In what follows, the experimental apparatus will be described in detail, the procedures outlined, and the results discussed.

2.1 Apparatus

2.1.1 Test Cell

A schematic of the test tank is shown in Fig. 2.1. The tank, made of R-Cast acrylic, had an internal diameter of 8” and an outer diameter of 10.125”. The cylindrical midsection of the test cell was 16” long. The tank was capped on both ends with acrylic plates 16” x 16” x 2”. A section of a sphere (R = 8.5”) was machined
Figure 2.1: Schematic of test tank (a), Relevant dimensions in inches (b).
1” into each plate. The top and bottom end caps were bolted to the cylindrical mid-
section with a single O-ring seal at the joining faces. Additionally, the bottom plate
was bolted to a vibration isolation table. For the heat loads imposed and pressures
observed, the tank was assumed rigid with negligible expansion. The density of the
acrylic was given by the manufacturer as 1190 kg/m$^3$. The thermal conductivity and
specific heat, as reported in the literature,$^{186}$ are:

$$k \left[ \frac{W}{m \cdot K} \right] = 0.18987 \sum a_i \left( \frac{T}{298.15} \right)^i$$

$$a_0 = -0.02222$$

$$a_1 = 1.67196$$

$$a_2 = -0.64984$$

$$a_3 = 0$$

$$\rho c_p \left[ \frac{kJ}{m^3 \cdot K} \right] = 1614.1 \sum b_i \left( \frac{T}{298.15} \right)^i$$

$$b_0 = -0.05640$$

$$b_1 = 1.05638$$

To insulate the tank and associated plumbing from the environment, all external sur-
faces were blanketed with Volara low density cross-linked polyethylene foam. The
thickness of the insulation was 0.5”. The density of the foam was determined to be
32 kg/m$^3$. In the literature,$^{187}$ there is some uncertainty regarding the thermal prop-
erties of the insulation. At room temperature,
2.1 APPARATUS

Prior to beginning the experimental tests, the test tank was leak checked by filling the tank with air, pumping it down to the nominal operating pressure (500 Torr), sealing it, and observing how fast the pressure rose in the system over a 24 hour period. Leak paths include gas diffusion through the acrylic, which is generally negligible, and leakage through the multitude of O-ring seals. When the thermistors entering the tank through the side wall were not present, and their respective ports were capped with O-ring sealed plugs, the leak rate was 0.22 Torr/hour, which over a two hour pressurization period amounts to less than 0.5 Torr overpressure. When all of the thermistors were present, the leak rate was higher at approximately 0.69 Torr/hour. Consequently, for most of the tests performed as part of this experimental effort, the test tank was not fully populated with thermistors. Only in the last test were all the thermistors present so that a qualitative map of the temperature field could be obtained.

2.1.2 Test Fluid

The fluid used in the experiment was HFE-7000, a transparent low boiling point refrigerant manufactured by 3M. Thermophysical properties of the test fluid are provided in Appendix A.
2.1.3 Heating

To simulate heat leaking into the tank, two etched foil Kapton heaters were affixed to the inside surface of the test tank. The 1” wide heating bands were positioned approximately 2” from either end cap. The relative positions are indicated in Fig. 2.1. The bands were 24.4” long which resulted in a slight gap in the circumference to allow for the silver-plated copper leads to exit the test cell. The leads were teflon coated Type E 24 AWG. Adhesive was initially used to affix the heating bands to the inside surface of the test cell. However, after preliminary testing revealed parts of the band separating from the wall, a flat copper spring (1” wide, 0.06” thick) was placed over the Kapton foil to keep the bands in place. The copper spring had a 0.5” gap in the circumference to allow the heater leads to exit the test cell. Power to the heaters was supplied by Keithley 2425 source meters. Prior to data acquisition, the resistances of the heaters were measured by the source meter (± 0.07% rdg + 0.3 Ω) and the voltage source (± 0.02% rdg + 12 mV) was programmed to produce the desired power output from the heaters. During the experiment, the heater’s power output was monitored by the source meter. Power output was determined by monitoring the current (0.055% rdg + 6μA) and then applying the power relationship:

\[ P = V_{\text{source}} I_{\text{meas}} \]  \hspace{1cm} (2.1)
For a typical test, the uncertainty in the measured power was approximately 1.7 mW. During the experiment, the resistance of the heaters changed due to changing temperatures within the tank. To account for this changing resistance, the applied voltage was modified periodically to keep the measured heater power to within 0.2 mW of the set point.

### 2.1.4 Subcooled Mixing

Subcooled axial jet mixing was used to control tank pressure. Fluid entered the tank from an AISI 304 stainless steel nozzle aligned along the longitudinal axis of the tank. The nozzle projected 1" into the tank and converged to a 0.25" ID 0.2" from
the nozzle exit plane as indicated in Fig. 2.2. Fluid was withdrawn from the tank through 12 ports (0.125" ID) circumferentially located about the nozzle. The outlet ports, depicted in Figs. 2.2 and 2.3, were tapped through the bottom plate at an angle 50° from the horizontal. The fluid from the outlet ports collected in a common manifold before being pumped through a heat exchanger and re-entering the tank through the nozzle. The recirculation pump was a Series 120 magnetically driven gear pump from MicroPump.

The heat exchanger was a single pass counter flow shell and tube heat exchanger from Exergy (model 00256-2). The specifications of the heat exchanger are listed in Table 2.1. In the heat exchanger, the test fluid exchanged heat with distilled water. The water was contained in a Haake F8-C25 temperature-controlled recirculation
2.1 APPARATUS

EXPERIMENTAL INVESTIGATION

Table 2.1: Heat exchanger specifications

<table>
<thead>
<tr>
<th>Specification</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of baffles</td>
<td>7</td>
</tr>
<tr>
<td>Number of tubes</td>
<td>55</td>
</tr>
<tr>
<td>Tube length</td>
<td>10”</td>
</tr>
<tr>
<td>Tube OD</td>
<td>0.125”</td>
</tr>
<tr>
<td>Tube wall</td>
<td>0.0125”</td>
</tr>
<tr>
<td>Tube Clearance</td>
<td>0.162”</td>
</tr>
<tr>
<td>Shell ID</td>
<td>1.37”</td>
</tr>
<tr>
<td>Shell OD</td>
<td>1.5”</td>
</tr>
<tr>
<td>Baffle spacing</td>
<td>1.44”</td>
</tr>
<tr>
<td>Heat Transfer Area</td>
<td>1.43 ft²</td>
</tr>
<tr>
<td>Pitch</td>
<td>Triangular</td>
</tr>
</tbody>
</table>

bath. The water was pumped through the shell-side of the heat exchanger at approximately 12 lpm. The temperature of the bath was an independent variable of the experiment and was controlled to within ± 0.01 °C.

2.1.5 Instrumentation

Ullage pressure was measured using an MKS model 120AA-01000 RCJ transducer. The transducer had a resolution of 0.1 Torr and an accuracy of 0.05% rdg. Calibration was performed independently at the calibration lab on-site at NASA Glenn. The transducer was mounted to the vibration isolation table and was piped through the upper acrylic plate of the tank using approximately 54” of 1/4” OD insulated stainless steel tubing.

Mounted axially along the cylindrical midsection of the tank were nine 4-wire 100 Ω Platinum RTD elements (Omega model SRTD-2). The RTDs were mounted to a foil
### Table 2.2: Variation of ambient temperature during the experiment

<table>
<thead>
<tr>
<th>Case No.</th>
<th>$T_{\text{min}}$ ($^\circ\text{C}$)</th>
<th>$T_{\text{max}}$ ($^\circ\text{C}$)</th>
<th>$T_{\text{avr}}$ ($^\circ\text{C}$)</th>
</tr>
</thead>
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<td>22.8</td>
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<td>22.5</td>
</tr>
<tr>
<td>2</td>
<td>23.0</td>
<td>22.0</td>
<td>22.6</td>
</tr>
<tr>
<td>3</td>
<td>23.1</td>
<td>22.1</td>
<td>22.6</td>
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<td>22.1</td>
<td>22.6</td>
</tr>
<tr>
<td>6</td>
<td>23.2</td>
<td>22.0</td>
<td>22.6</td>
</tr>
<tr>
<td>7</td>
<td>23.1</td>
<td>22.0</td>
<td>22.5</td>
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</tr>
<tr>
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</tr>
<tr>
<td>14</td>
<td>23.5</td>
<td>22.1</td>
<td>22.6</td>
</tr>
</tbody>
</table>

element 1" x 0.62" and were cemented to the outer acrylic wall using OMEGABOND 101 epoxy adhesive. RTD resistances were recorded and temperatures were determined using temperature-resistance calibration curves. For a typical test case, the self-heating for a single RTD element was 0.11 mW.

The ambient temperature of the lab near the tank was measured using a 2.2 kΩ YSI thermistor ($\pm 0.1 ^\circ\text{C}$). Room temperature was kept relatively constant throughout the duration of the experiment. The average room temperature for each test case, along with the minimum and maximum fluctuation is listed in Table 2.2. A typical time history of the ambient lab temperature is shown in Fig. 2.4. The oscillations in the response are due to the lab’s on-off air conditioning cycle.

Temperature inside the tank was measured with custom-made thermistors from YSI. The thermistors were bead-in-glass types potted in a PEEK tube. The diameter
of the glass bead was 0.06”. The outer diameter of the PEEK tube was 0.125” and the wall thickness was approximately 0.03”. PEEK was chosen to house the thermistor because of its stiffness and low thermal conductivity ($k \approx 0.25 \text{ W/m k}$). The self-heating for a single thermistor was approximately $1 \mu\text{W}$. The thermistors’ power supply and signal conditioning unit were custom built and the entire system was calibrated independently at NASA Glenn’s calibration lab at 25 °C, 30 °C, and 35 °C. The reported uncertainty was ± 0.04 °C. The thermistors internal to the tank were all positioned in the longitudinal midplane of the test cell. Fourteen thermistors entered the tank through the side wall and a single thermistor entered the tank through the center of the upper end cap. The thermistors were positioned at various depths inside the tanks as shown in Fig 2.5.

Figure 2.4: Typical time history of the ambient lab temperature.
Figure 2.5: Thermistor and RTD locations in the test tank. (Coordinates are in inches. Blue dashed lines denote approximate locations of the 26.5%, 50%, and 73.5% fill levels.)
To minimize the interference of the thermistors on the flow field (and consequently the temperature field and pressurization behavior) for most of the test cases, only the thermistor entering from the top plate (T1 in Fig. 2.5) was present. For these cases, the thermistor ports tapped through the side wall were capped with O-ring sealed plugs. For the final case of the experimental test program, the tank was fully populated with thermistors. Though interfering with the flow field somewhat, this fully populated case provides a qualitative map of the temperature field inside the tank.

The flow rate of the mixing jet was measured using a McMillan G112-7 flow meter. The flow meter had a range of 60-1000 mL/min and an accuracy of ± 0.5% FS.

Flow measurements, pressure measurements, and temperature measurements (from the RTD elements and thermistors) were recorded using an Agilent 34970A data acquisition unit with three 20 channel multiplexers. Uncertainty from the DAQ unit, which includes measurement and switching errors, were reported by the manufacturer as ±0.005% rdg + 0.4 mV for voltages and ± 0.01% rdg + 0.04Ω for resistances. During the first 13 tests, measurements were made at 1 Hz and subsequently stored on a laptop. For the last test, where the tank was fully populated with thermistors, measurements were recorded once every ten seconds to accommodate the larger amount of data generated during these runs. In all cases, the DAQ unit visited channels sequentially. The time stamp between successive channels was 50 - 60 ms.
2.2 Procedures

A schematic of the entire apparatus is shown in Fig. 2.6. Throughout the experimental program, the test fluid was stored in a 5 gal reservoir tank. The test fluid was preconditioned in the reservoir tank and then transferred to the test tank using a no-vent fill technique described below. Once filled to the desired fill fraction, the fluid was again conditioned to initialize each test case, the experiment was performed, and at the end of the test, the fluid was pumped back into the reservoir tank. Each experimental test case took approximately two days to complete with the preconditioning in the reservoir tank occurring one day prior to the actual test.
2.2 PROCEDURES

2.2.1 Preconditioning

Preconditioning of the test fluid in the reservoir was necessary to degas any non-condensable species dissolved in the fluid. To degas the fluid, a vacuum pump was used to rapidly collapse the pressure in the reservoir. As the partial pressure of the non-condensables in the ullage decayed, the dissolved species came out of solution and were subsequently vented outside. As the ullage was pumped down, the vapor pressure of the test fluid was also reduced. Consequently, bulk boiling of the test fluid occurred. Bulk liquid boiling was beneficial to the degassing process as it served to mix the fluid and carry the dissolved species to the liquid-vapor interface. Before being vented outside, the evacuated gases and vapor passed through a liquid nitrogen cold trap and the test fluid that condensed out was collected and saved for future use. Degassing was performed multiple times prior to a test case. Each degassing process only lasted several minutes and was limited by the amount of LN2 in the cold trap. After a degassing process, the reservoir tank was undisturbed for several hours in order to equilibrate to a new thermodynamic state. Subsequently, the pressure and temperature in the ullage were measured and compared with the test fluid’s saturation curve. If the measured temperature and pressure deviated significantly from the saturation curve the degassing procedure would be repeated. For all the test cases, one-to-one agreement with the saturation curve was never attained. The measured pressure was typically 20 Torr higher than the saturation pressure corresponding to the measured ullage temperature. The deviation is attributed to the presence of
2.2 PROCEDURES

EXPERIMENTAL INVESTIGATION

a non-condensable gas. As will be described shortly, this resulted in a worst-case non-condensable mole fraction of 3.6%. This non-condensable mole fraction is worst-case because the saturation condition only applies on the two-phase boundary for an inhomogeneous system. Both the temperature and pressure were recorded a distance away from the interface. Hence, these measurements do not account for any thermal stratification or hydrostatic head that may have been present in the system.

2.2.2 Filling

Once the fluid was sufficiently degassed, the test tank was filled by pumping the fluid from the reservoir to the test cell using a two-way transfer pump. Prior to fluid transfer, the test tank was pumped down using the same vacuum pump that was employed during the degassing process. During the tank pump down, pressure was monitored using both the MKS pressure transducer and an analog Varian 801 thermocouple vacuum gage. Once the pressure in the tank reached 10 mTorr, the valve between the tank and the vacuum pump was closed and the valve between the tank and the reservoir was opened. Since the reservoir was now open to an evacuated tank, some fluid in the transfer line flashed and the tank pressure rapidly rose to near the fluid’s saturation pressure. The transfer pump was activated and fluid continued to enter the ventless test tank until the desired fill fraction was reached. The liquid fill level was determined using a ruler (± 1/16”) mounted along the outer wall of the acrylic midsection. Once the fill level was recorded, the foam insulation was pulled taut around the tank and then secured.
2.2.3 Initialization

As fluid was pumped into the tank during the no-vent fill, the ullage was compressed, the tank pressure had risen above its saturation value, and consequently condensation was occurring at the liquid-vapor interface. Thus, once the fluid transfer ceased, the liquid-vapor system was not in a global equilibrium state. To accelerate the equilibration between the two phases, the fluid in the test tank was conditioned. Conditioning proceeded by running the axial jet mixing loop (with a throughput of approximately 460 mL/min) and setting the recirculation bath temperature to the desired initial temperature. Conditioning occurred for 4 hours prior to the start of a test. Approximately 10 minutes before beginning a test, the mixer was turned off and the valves between the test tank and the recirculation loop were closed. The 10 minute delay was included to allow for the jet-induced velocities to sufficiently decay. During this 10 minute mixer-off period, the tank pressure was monitored. If the tank pressure changed ± 0.1 Torr the conditioning process was repeated for an additional hour after which another check of the pressure was made. Fluid conditioning continued until this pressure criterion was met.

2.2.4 Testing

During the 10 minute mixer-off period, the source meters for the heaters were programmed and the measurement channels and recording frequency were set on the DAQ unit. At time=0, power was supplied to the heaters and the tank was allowed
2.3 TEST MATRIX

EXPERIMENTAL INVESTIGATION

to self-pressurize for 2 hours. During these 2 hours, the recirculation bath remained
active with the temperature set point now programmed to the desired subcooled jet
temperature. Approximately 30 s prior to activating the jet mixer, the jet speed was
set and the valves separating the test tank from the recirculation loop were opened.
Subcooled axial jet mixing began at time = 2 hours and continued for an additional
1.5 hours. The heaters remained active during this time.

After mixing for 1.5 hours, both the heaters and the mixing pump were deacti-
vated. The test fluid was then drained back into the reservoir using the reversible
transfer pump. All valves were then closed and the experiment was shut down.

One day after each test, the vacuum pump/LN2 cold trap system was used to purge
the test tank and fluid lines (up to the recirculation loop valves) of any remaining
HFE-7000 liquid or vapor. Once again, any test fluid that condensed in the cold trap
was reclaimed for later use.

2.3 Test Matrix

Fourteen test runs will be discussed in this dissertation. First, self-pressurization
will be examined. Here, the effects of liquid fill level and applied heat load on the
pressurization behavior of the test fluid will be discussed. Next the effectiveness
of using an axial liquid jet to control tank pressure will be analyzed. The effects
of average jet speed and degree of subcooling on the depressurization rate will be studied.
### Table 2.3: Test matrix

<table>
<thead>
<tr>
<th>Case No.</th>
<th>Liquid height</th>
<th>Heat Load</th>
<th>Heating Configuration</th>
<th>$T_{\text{sub}}$ °C</th>
<th>Pump voltage</th>
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</thead>
<tbody>
<tr>
<td>1</td>
<td>4&quot;</td>
<td>2 W</td>
<td>B</td>
<td>22.5</td>
<td>3 V</td>
</tr>
<tr>
<td>2</td>
<td>4&quot;</td>
<td>2 W</td>
<td>B</td>
<td>-</td>
<td>3 V</td>
</tr>
<tr>
<td>3</td>
<td>4&quot;</td>
<td>2 W</td>
<td>B</td>
<td>17.5</td>
<td>3 V</td>
</tr>
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<td>20.0</td>
<td>3 V</td>
</tr>
<tr>
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<td>B</td>
<td>20.0</td>
<td>2 V</td>
</tr>
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<td>9</td>
<td>4&quot;</td>
<td>2 W</td>
<td>B</td>
<td>20.0</td>
<td>1 V</td>
</tr>
<tr>
<td>10</td>
<td>4&quot;</td>
<td>1 W</td>
<td>B</td>
<td>20.0</td>
<td>3 V</td>
</tr>
<tr>
<td>11</td>
<td>4&quot;</td>
<td>3 W</td>
<td>B</td>
<td>20.0</td>
<td>3 V</td>
</tr>
<tr>
<td>12</td>
<td>8&quot;</td>
<td>2 W</td>
<td>B</td>
<td>20.0</td>
<td>3 V</td>
</tr>
<tr>
<td>13</td>
<td>12&quot;</td>
<td>2 W</td>
<td>B</td>
<td>20.0</td>
<td>3 V</td>
</tr>
<tr>
<td>14</td>
<td>4&quot;</td>
<td>2 W</td>
<td>B</td>
<td>20.0</td>
<td>3 V</td>
</tr>
</tbody>
</table>

### Table 2.4: Jet speed calibration

<table>
<thead>
<tr>
<th>Pump voltage</th>
<th>Flow rate (mL/min)</th>
<th>Jet speed (cm/s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 V</td>
<td>136.7</td>
<td>7.2</td>
</tr>
<tr>
<td>1.25 V</td>
<td>176.9</td>
<td>9.3</td>
</tr>
<tr>
<td>1.5 V</td>
<td>217.2</td>
<td>11.4</td>
</tr>
<tr>
<td>1.75 V</td>
<td>257.5</td>
<td>13.5</td>
</tr>
<tr>
<td>2 V</td>
<td>297.7</td>
<td>15.7</td>
</tr>
<tr>
<td>3 V</td>
<td>458.8</td>
<td>24.1</td>
</tr>
</tbody>
</table>

### Table 2.5: Liquid fill level

<table>
<thead>
<tr>
<th>Height of Liquid in Tank</th>
<th>Percentage of nominal interior tank volume</th>
</tr>
</thead>
<tbody>
<tr>
<td>4&quot;</td>
<td>26.5%</td>
</tr>
<tr>
<td>8&quot;</td>
<td>50.0%</td>
</tr>
<tr>
<td>12&quot;</td>
<td>73.5%</td>
</tr>
</tbody>
</table>
Table 2.6: Volume of various components in the tank

<table>
<thead>
<tr>
<th>Region</th>
<th>Volume</th>
</tr>
</thead>
<tbody>
<tr>
<td>Interior test tank (nominal)</td>
<td>855.56 in³</td>
</tr>
<tr>
<td>Copper ring(s)</td>
<td>1.44 in³</td>
</tr>
<tr>
<td>Thermistor T1</td>
<td>0.0674 in³</td>
</tr>
<tr>
<td>Outlet ports</td>
<td>0.25 in³</td>
</tr>
<tr>
<td>Nozzle inside tank</td>
<td>0.09755 in³</td>
</tr>
<tr>
<td>Nozzle inside wall</td>
<td>0.069 in³</td>
</tr>
<tr>
<td>Ports in top plate</td>
<td>0.4 in³</td>
</tr>
<tr>
<td>Ports in side wall</td>
<td>0.09 in³</td>
</tr>
<tr>
<td>Tubing (ullage to pressure transducer)</td>
<td>1.374 in³</td>
</tr>
<tr>
<td>Tubing (ullage to relief valve)</td>
<td>2.655 in³</td>
</tr>
<tr>
<td>Acrylic side (nominal)</td>
<td>484.00 in³</td>
</tr>
<tr>
<td>Acrylic top (nominal)</td>
<td>486.34 in³</td>
</tr>
<tr>
<td>Acrylic bot (nominal)</td>
<td>486.34 in³</td>
</tr>
</tbody>
</table>

The test matrix is given in Table 2.3. A malfunction in the flow meter required re-calibration after the test program was complete. The relationship between applied voltage to the pump and the resulting flow rate is provided in Table 2.4 along with the corresponding average velocity of the fluid exiting the nozzle. In the test matrix, $T_{\text{sub}}$, refers to the set point of the fluid circulating through the heat exchanger. Analysis in subsequent chapters will show how this is related to the temperature of the jet entering the test tank. Under “heat location” in Table 2.3, B indicates that only the bottom heater was active during the experiment. The liquid fill level, given in inches, is the distance between the liquid-vapor interface and the bottom of the cylindrical side wall of the test tank. The liquid fill level expressed as a percentage of the nominal interior tank volume is given in Table 2.5. The nominal interior tank volume is the region enclosed by the acrylic side, top, and bottom walls. It neglects the contribution of any ports tapped through the acrylic side wall, as well as the volume of the nozzle.
and thermistor inside the tank. To get a sense of the off-nominal value, the volumes of some of these neglected components are listed in Table 2.6. Since these off-nominal contributions are small, in subsequent calculations, only the nominal interior tank volume is used.

When processing the experimental data, in order to filter out small variations in the initial conditions, the initial pressure and temperature ($P_o$ and $T_o$, respectively) are subtracted from later measurements. In this manner, the pressure and temperature responses in subsequent plots begin at zero and may be positive or negative depending on their value relative to the initial state. The initial pressure and temperature for the different test cases are given in Table 2.7. All tests began within $492 \pm 1.99$ Torr and $22.27 \pm 0.33 \degree C$. The largest variation occurred when the tank was fully populated with thermistors which is again why this case was only used to obtain qualitative temperature maps rather than to infer any quantitative trends.

Also included in Table 2.7 is an estimate of the mole fraction, $X_g$, of the non-condensable gas present in the system during testing. In the present experiment, both the temperature and pressure were measured away from the interface. Due to a lack of more detailed spatial measurements, these measurements were used to infer a deviation from saturation. Here, the non-condensable (assumed to be air) and the vapor are assumed to be ideal gases. The mole fraction of non-condensable is then:

$$X_g \% = \frac{P_{\text{meas}} - P_{\text{sat}(22.5 \degree C)}}{P_{\text{meas}}}$$
Table 2.7: Initial conditions

<table>
<thead>
<tr>
<th>Case No.</th>
<th>( P_0 ) (Torr)</th>
<th>( T_o ) (°C)</th>
<th>( X_g )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>492.04</td>
<td>22.20</td>
<td>3.2%</td>
</tr>
<tr>
<td>2</td>
<td>492.02</td>
<td>22.20</td>
<td>3.2%</td>
</tr>
<tr>
<td>3</td>
<td>491.62</td>
<td>22.18</td>
<td>3.1%</td>
</tr>
<tr>
<td>4</td>
<td>492.44</td>
<td>22.23</td>
<td>3.3%</td>
</tr>
<tr>
<td>5</td>
<td>491.95</td>
<td>22.23</td>
<td>3.2%</td>
</tr>
<tr>
<td>6</td>
<td>491.97</td>
<td>22.37</td>
<td>3.2%</td>
</tr>
<tr>
<td>7</td>
<td>491.89</td>
<td>22.28</td>
<td>3.2%</td>
</tr>
<tr>
<td>8</td>
<td>492.31</td>
<td>22.32</td>
<td>3.3%</td>
</tr>
<tr>
<td>9</td>
<td>491.95</td>
<td>22.31</td>
<td>3.2%</td>
</tr>
<tr>
<td>10</td>
<td>491.85</td>
<td>22.29</td>
<td>3.2%</td>
</tr>
<tr>
<td>11</td>
<td>492.02</td>
<td>22.26</td>
<td>3.2%</td>
</tr>
<tr>
<td>12</td>
<td>492.41</td>
<td>22.23</td>
<td>3.3%</td>
</tr>
<tr>
<td>13</td>
<td>493.00</td>
<td>22.10</td>
<td>3.4%</td>
</tr>
<tr>
<td>14</td>
<td>491.78</td>
<td>22.33</td>
<td>3.2%</td>
</tr>
</tbody>
</table>

where \( P_{\text{meas}} \) is the measured total ullage pressure. The saturation pressure was evaluated at 22.5 °C, the set-point of the fluid initially circulating through the heat exchanger. It was felt this temperature was more representative of the interfacial temperature rather than the temperatures listed in Table 2.7, which were measured in the vapor phase away from the interface. While the contaminant gas is non-condensable, it may dissolve into the liquid phase. The dissolution of the non-condensable has been neglected in the preceding analysis.

Future experimental tests should employ a more robust degassing scheme to further reduce the amount of non-condensables in the system. Moreover, post-test characterization of the different species inside the test tank would yield a more quantitative measure of the amount of non-condensables present.
### Table 2.8: Relevant Dimensional Parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
<th>Definition</th>
<th>Range</th>
</tr>
</thead>
<tbody>
<tr>
<td>Re</td>
<td>Reynolds Number</td>
<td>$\frac{\rho V_{jet} D_{jet}}{\mu}$</td>
<td>1343 - 4646</td>
</tr>
<tr>
<td>Bo</td>
<td>Bond Number</td>
<td>$\frac{g\rho D_{jet}^2}{4\sigma}$</td>
<td>10.07 - 10.34</td>
</tr>
<tr>
<td>We</td>
<td>Weber Number</td>
<td>$\frac{\rho V_{jet}^2 D_{jet}^2}{8\sigma R_t}$</td>
<td>0.0267 - 0.296</td>
</tr>
<tr>
<td>Gr</td>
<td>Grashof Number</td>
<td>$\frac{g\beta q'' R_t^4}{k_i \nu_t^2}$</td>
<td>$1.6 \cdot 10^{10} - 5.2 \cdot 10^{10}$</td>
</tr>
<tr>
<td>Ra</td>
<td>Rayleigh Number</td>
<td>$\text{Gr} \cdot \text{Pr}$</td>
<td>$1.3 \cdot 10^{11} - 4.3 \cdot 10^{11}$</td>
</tr>
<tr>
<td>Ri</td>
<td>Richardson Number</td>
<td>$\frac{g\beta (T_s - T_{jet}) H_{jet}}{V_{jet}^2}$</td>
<td>0.02 - 1.39</td>
</tr>
</tbody>
</table>

#### 2.4 Dimensional Analysis

The approach of performing small scale experimental testing is to better understand the underlying transport phenomena occurring in the tank and to gather data that can be used to validate models. While the approach was not meant to achieve complete static and dynamic similitude with a flight-weight cryogenic system, it is nevertheless instructive to identify and evaluate the relevant dimensionless parameters (Table 2.8). The Reynolds number of the jet suggests that the liquid stream entering the tank is turbulent. The magnitude of the Bond number indicates that the static shape of the interface should be flat in this ground-based apparatus. The magnitude of the Weber number suggests the jet’s momentum is small enough that jet geysering into the ullage will not occur. The Rayleigh number range indicates that natural convection in the liquid is not quite fully turbulent but not quite laminar...
either. The flow is best characterized as being transitionary. The nearly two orders of magnitude variation in the Richardson number suggests that for some cases, the interaction between forced jet mixing and buoyancy will be weak but in other cases the interaction will be stronger.

2.5 Results

First the effects of heat load and fill level on the self-pressurization behavior will be studied. Next the effectiveness of using an axial liquid jet to control tank pressure will be examined. Finally, in the last case, the tank was fully populated with thermistors. This was done in order to obtain qualitative temperature maps to help explain the behavior of the local temperature and pressure histories. In the pressure and temperature histories, the points on the curves are instants in time from the raw data and were not averaged in any way. All the data points obtained during each run are not plotted. Sufficient points are included in order to identify the different curves on the graphs.

2.5.1 Self-Pressurization

Before examining the different case studies, it is useful to gauge the reproducibility of the data. In Fig. 2.7, the pressure and temperature time histories are shown for the first nine cases. In these first nine cases, 2 W was applied to the bottom heater and the liquid fill level was 26.5%. After self-pressurizing for 2 hours, the variation in pressure and temperature are nearly within the error bars of the measurement. For
Figure 2.7: Reproducibility of the experimental data. Pressure (a), Temperature (b).
Figure 2.8: Effect of heat input on pressure (a) and temperature (b) during self-pressurization. (Liquid fill level = 26.5%, Bottom heating configuration)
these first 9 cases, at time = 7000 s, $\Delta P = 15.93 \pm 0.29$ Torr and $\Delta T = 0.77 \pm 0.03$ K. The data reproducibility is thus deemed excellent.

The effect of applied heat load on the pressure and temperature rise inside the tank will now be examined. As shown in Fig. 2.8, as the applied heat load is reduced both the pressure rise and temperature rise decrease. This trend should be quite intuitive given that less energy is available to raise the sensible energy of the system and vaporize the liquid. The trend is not quite linear – a doubling of the heat load does not double the pressure or temperature rise. At 7000 s, the pressure rise after applying 1 W, 2 W, and 3 W is 9.1 Torr, 16.0 Torr, and 23.3 Torr respectively. The corresponding temperature rise is 0.46 K, 0.79 K, and 1.16 K. The non-linearity is due to the fact that at constant ambient temperature the heat loss to the surrounding varies among the tests. As the applied heat load increases and the sensible energy of the system rises, the driving potential for heat loss between the test tank and the ambient surroundings increases as well. Hence at higher applied heat loads, the test tank is losing more heat than at lower heater powers.

Next the effect of liquid fill level on the pressurization behavior is investigated. As indicated in Fig. 2.9a, when the bottom heater is activated, the pressure rise is largest for the lowest fill level. This result can be best understood in terms of how the applied energy is partitioned in the system. Some of the incident energy is used to raise the sensible energy of the wall, liquid, and vapor, while some is used for liquid vaporization. The energy partitions are coupled together; if the sensible energy of the wall rises faster than that of the liquid or vapor phases, the two phases would
Figure 2.9: Effect of liquid fill level on pressure (a) during self-pressurization. Inset of the pressure response (b). (Heat load = 2 W, Bottom heating configuration)
Figure 2.10: Effect of liquid fill level on temperature (a) during self-pressurization. Inset of the temperature response (b). (Heat load = 2 W, Bottom heating configuration)
tend to gain energy at the expense of the wall. At lower fill levels, there is less liquid in the tank to absorb the incident heat load. Consequently, more energy is available for vaporization and for raising the sensible energy of the vapor as suggested in Fig. 2.10.

It is also apparent from Fig. 2.9b and 2.10b that there is a lag in both the temperature and pressure response of the system. The lag is due to the finite amount of time it takes for heat to reach the vapor phase. For a fixed heater location, as the liquid fill level increases, the distance between the phase boundary and the applied heat source increases as well. For the 26.5%, 50% and 73.5% fill levels the distance between the interface and the top of lower heater is 1.625”, 5.625”, and 9.625” respectively. Based on these distances, the conduction time scales through the acrylic wall are much larger than the response lag noted in Fig. 2.9b and 2.10b, which suggests that the incident energy is being transported to the vapor phase through the bulk liquid. When the warmer fluid adjacent to the heater rises due to buoyancy, it flows along a cooler acrylic wall since heat is only being applied locally to a band 1” wide. When the warmer low-conductivity fluid comes into contact with the higher-conductivity tank wall, the fluid will give up some of its energy to the acrylic and slow down due to the reduced buoyancy force. This reduction in the buoyancy force as the fluid flows up along the wall will generally result in the thermal response being slower than a buoyant time scale.

Additional insight can be gained by observing how the temperature of the outer tank wall evolves in time during the 2 hour period of self-pressurization. In Fig.
2.5 RESULTS

Figure 2.11: Temperature profiles along the outer tank wall for the bottom heating configuration. (Liquid fill level = 50.0%, Heat load = 2 W)

2.11, the time history of wall temperature is presented. The tank is 50% full and 2 W is applied to the heater. For the temperature profiles presented in Fig. 2.11, only the bottom heater is active. After 2 hours of heat addition, the temperature of the outer acrylic wall near the heater band has risen by approximately 1 K. Farther away from the heater, after 2 hours, the wall temperature has risen by 0.5 K. The wall temperature in regions far from the heater is increasing because of both axial conduction through the acrylic and heat transfer into the acrylic from the liquid and vapor phases. Since the acrylic has a higher conductivity than both of the two bulk phases, warm liquid or vapor adjacent to the wall would tend to lose heat to the acrylic.
2.5 RESULTS

2.5.2 Pressure Control

In addition to studying how various factors effect the self-pressurization behavior of the liquid-vapor system, the effectiveness of using a mixing jet to control tank pressure was also investigated. In these pressure control tests, after the tank has self-pressurized for 2 hours, fluid is withdrawn from the bottom of the tank and pumped through a heat exchanger before re-entering the tank through an axially-aligned nozzle. During these 90 minute pressure control tests, the band heaters remain active supplying heat at the same rate as the preceding 2 hour self-pressurization test. The mixing loop is a closed system and thus the rate of mass leaving the tank through the bottom outlet ports is equal to the rate of mass re-entering the tank through the jet nozzle. The pump, heat exchanger, and flow meter were located on the floor of the lab beneath the table on which the test tank sat. This provided for a sufficient hydrostatic head that prevented any cavitation in the fluid line. The temperature of the secondary fluid in the heat exchanger was a controlled parameter that was used to vary the degree of subcooling of the liquid re-entering the tank.

Before discussing the subcooled mixing results, we first consider the case when only the pump is activated. In this quasi mixing-only case, the temperature of the jet is not being controlled by the heat exchanger. Prior to turning on the jet, both the fluid in the lines and the fluids in the heat exchanger are stationary and assumed to be in thermal equilibrium with the mean lab temperature. Once the jet is activated, both the pressure and temperature inside the tank initially decrease as shown in Fig. 2.12.
2.5 RESULTS

Figure 2.12: Effect of axial jet mixing on pressure (a) and temperature (b). (Liquid fill level = 26.5%, Heat load = 2 W, Bottom heating configuration, Jet speed = 24.2 cm/s)
2.5 RESULTS

EXPERIMENTAL INVESTIGATION

The temporary reduction is due to the passive subcooling of the fluid re-entering the test tank. During the 2 hour self-pressurization experiment immediately preceding this quasi mixing-only test, heat is being added to the band heater adjacent to the liquid phase. Because of buoyant convection, the temperature in the liquid phase stably stratifies with the cooler fluid settling to the bottom of the tank. When the pump is first turned on, this cooler fluid is drawn into the fluid lines which are subcooled themselves because they have been sitting close to the initial temperature of the tank for the previous 2 hours. When this subcooled fluid re-enters the tank and impinges on the liquid-vapor interface, condensation is promoted and heat is transferred from the vapor into the bulk liquid – both of which can lead to a pressure collapse in the ullage. Fig. 2.12a indicates that the pressure collapse is only temporary and that after the initial reduction in pressure, when the liquid becomes fully mixed, the ullage pressure continues to rise as before.

This should be expected given that the liquid subcooling was not sustained during the test. After the initially subcooled liquid re-enters the tank, it mixes with the warmer bulk liquid. This warmer liquid is eventually drawn into the fluid line before being pumped back into the tank. While passive subcooling can certainly occur – the fluid circulating in the line can lose heat to the ambient environment – these heat losses are expected to be smaller and not comparable in magnitude to the energy supplied to the band heater. Hence the pressure continues to rise even though mixing is being performed. Moreover, the power supplied to the pump is an energy source into the system which if unmitigated can further cause the tank pressure to increase.
So while axial jet mixing is able to thermally destratify the bulk liquid, it is not particularly effective at reducing tank pressure over the long term. To sustain the initial pressure collapse, energy must be removed from the liquid-vapor system.

Next, a sustained pressure reduction is investigated by making use of a subcooled liquid jet. Here, subcooling the liquid is not passively performed as in the previous case, but is actively maintained by circulating a cold thermally-conditioned fluid through the heat exchanger. As the test liquid is pumped through the heat exchanger, it continuously loses heat to the colder fluid and thus the subcooling is maintained.

First the effect of jet speed on the pressure reduction is considered. As expected, the pressure decays faster for faster jet speeds. As indicated in Fig. 2.13a, after 90 minutes of subcooled jet mixing, the pressure has barely decreased for the slowest jet speed. There are two factors that reduce the effectiveness of a subcooled jet mixer. First, the colder jet is trying to penetrate into a warmer bulk liquid. In order to reach the liquid-vapor interface, the jet’s momentum must overcome the retarding buoyancy forces which inhibit the jet’s upward flow by forcing the colder incoming liquid stream to the bottom of the tank. This phenomena would be present even if the warmer bulk liquid were quiescent. The retarding effect of buoyancy is further compounded by natural convection in the liquid. In the present experiment, a toroidal natural convection vortex is established in the bulk liquid which causes warm fluid near the heater to rise along the tank wall, flow radially inward along the free surface, and then get pulled downward near the centerline of the tank before resupplying the upwardly traveling fluid near the heater. The downward natural convection flow...
Figure 2.13: Effect of jet speed on pressure (a) and temperature (b). (Liquid fill level = 26.5%, Heat load = 2 W, Bottom heating configuration, Jet temperature = 20 °C)
near the central axis of the tank suppresses the upwardly traveling cold jet flow. Once again, the jet’s momentum must be large enough to overcome the suppressive natural convection flow in order for the jet to reach the interface. Once the colder jet finally reaches the phase boundary, the liquid removes heat from the vapor phase, condensation begins, and the tank pressure decays.

The pressure histories shown in Fig. 2.13 indicate that for moderate jet speeds, the ullage pressure decays slowly at first and then is followed by a rapid collapse. During the period of slow decay, the forced jet flow is interacting with and competing with the strong natural convection in the bulk liquid. Even though the subcooled jet has not yet reached the interface, an energy exchange is taking place between the toroidal natural convection vortex and the colder jet fluid that is mainly isolated at the bottom of the tank. The natural convection vortex pulls some of the colder fluid up towards the interface which leads to a heat transfer out of the ullage and thus a pressure reduction. As the natural convection vortex continues to exchange energy with the incoming subcooled liquid, it shrinks in size which allows the cold jet flow to penetrate deeper into the bulk. When the jet penetrates far enough so that the cold fluid directly impinges the free surface, the ullage pressure rapidly decreases.

For the fastest flow rate shown in Fig. 2.13, we see that there is no slow decay. The jet’s momentum is large enough to overcome the retarding effects of buoyancy and natural convection. As the jet speed decreases, the duration of slow pressure decay increases as expected. For the slowest jet speed, the jet’s momentum is not sufficient to overcome buoyancy and natural convection. In this case, it is unlikely
that the jet impinges the free surface. As a result, a rapid pressure collapse is not observed.

For the cases were a rapid pressure collapse followed a slow period of pressure decay, the onset of the rapid depressurization can be characterized in terms of Richardson number. The Richardson number is a dimensionless measure of the strength of the interaction between forced jet mixing and buoyancy. For small Richardson numbers, the jet’s momentum is stronger than the retarding buoyancy forces in the liquid. For large Richardson numbers, buoyancy can suppress the upward motion of
the mixing jet. In Fig. 2.14, the time lag between turning on the jet and observing
a rapid depressurization is characterized as a function of Richardson number. The
correlation does an excellent job of fitting the data and suggests that the time lag is
a quadratic function of Ri.

The corresponding temperature histories for the pressure collapse cases described
above are shown in Fig. 2.13b. For the slowest jet speed, the temperature in the
ullage decreases almost monotonically. As the jet speed increases, there is initially
only a slight decrease in ullage temperature. When the cold jet fluid finally reaches the
liquid-vapor interface and the pressure rapidly collapses, the temperature in the ullage
decreases rapidly as well. The point where the rapid temperature decay commences
corresponds closely to when the pressure rapidly collapses. As noted previously, as
jet speed increases, the transition from slight temperature decay to rapid collapse
occurs earlier due to the greater momentum of the liquid jet. In contrast to the
depressurization behavior however, for the faster jet speeds, the temperature is not
monotonically decreasing. In all of the cases except the two slowest speeds, the rapid
temperature reduction is followed by a temperature jump which occurs later in time
as the speed decreases. It is suspected that this temperature jump is being caused by
buoyant heating of the ullage from the non-wetted wall. When the cold jet impinges
the interface, condensation occurs and the ullage pressure collapses. The resulting
heat and mass flux out of the ullage, through the interface, acts as an energy sink
causing a rapid drop in ullage temperature. As ullage pressure begins to asymptote
to its final steady state value, the condensation rate decreases and the energy sink
at the interface is reduced. As the temperature of the ullage decreases, however, the heat transfer rate between the ullage and the wall increases. Energy leaking into the tank from the wall rises to the top of the tank due to buoyancy, eventually leading to a stably stratified ullage.

Thus, the onset of the thermal jump, which occurs over a time scale of minutes, is caused by condensation. While the temperature of the ullage is dropping, the ullage is losing energy through the interface but gaining energy through the walls. As the condensation rate slows, heat leaking into the tank causes the temperature to rise locally. Since the jet is still active and flowing along the liquid side of the interface a steady state is reached where the amount of energy entering the ullage through the walls is balanced by the flux of energy leaving the ullage through the interface. Consequently, the ullage pressure does not rise.

In addition to investigating the effect of jet speed on the depressurization behavior, the effect of jet subcooling was also studied. The depressurization histories for different jet subcoolings are shown in Fig. 2.15 which shows that the pressure collapses more rapidly as the temperature of the jet decreases. This is not surprising since a colder jet removes energy more effectively from the liquid-vapor system than a warmer one. The three curves asymptote to different values. If jet mixing completely homogenizes the thermal field in the tank, the ullage pressure, neglecting the hydrostatic component, would equal the saturation pressure. Since saturation pressure is an increasing function of temperature, a warmer liquid jet causes the ullage pressure in a well-mixed tank to asymptote to a higher value. The asymptotic response is
Figure 2.15: Effect of jet subcooling on pressure (a) and temperature (b). (Liquid fill level = 26.5%, Heat load = 2 W, Bottom heating configuration, Jet speed = 24.2 cm/s)
Figure 2.16: Temperature profiles along the outer tank wall for the bottom heating configurations. (Liquid fill level = 50.0%, Heat load = 2 W, Jet speed = 24.2 cm/s, Jet temperature = 20 °C)

indicative of a steady-state whereby the heat removed by the subcooled jet and lost to or gained from the ambient environment exactly balances the applied heat load.

The effect of subcooling on ullage temperature is shown in Fig. 2.15b. For the warmest jet, the ullage temperature decreases and is quite noisy which can be attributed to convection in the vapor. For the colder jets, the temperature decreases rapidly initially and then jumps to a higher value which we attribute to thermal inversion in the vapor. Both the rate and magnitude of decay increase with jet subcooling because as the temperature difference between the jet and system increases, the liquid jet can more effectively remove energy from the system.

Additional insight can be gained by plotting the time evolution of the wall tem-
2.5 RESULTS

Experimental Investigation

Temperature profiles during subcooled jet mixing. The wall profiles shown in Figs. 2.16 correspond to when the tank is 50% full under a liquid heating configuration. The temperature of the wall is hottest near where the heat load is applied. The liquid jet, subcooled to below its initial temperature, removes energy from the wall as well as from the liquid-vapor system. Consequently, after 90 minutes of subcooled jet mixing, the temperature of the wall adjacent to the liquid phase has been reduced to below its initial temperature. Interestingly, the temperature of the wall far from the heat source and adjacent to the vapor phase has not changed appreciably after 90 minutes. This suggests that any cooling of the wall adjacent to the vapor is driven by axial conduction through the acrylic which has previously been shown to be a slow process.

Even though the entire acrylic wall is blanketed in foam insulation, realistically the insulation is not perfect and some heat is inevitably transferred between the wall and the ambient environment whose average temperature is nearly constant and equal to the initial temperature. Thus when the wall temperature is greater (less) than its initial value, the wall can locally lose (gain) heat to (from) the environment. While these heat additions and subtractions may cancel each other out, a zero heat flux condition is not enforced on the outer wall of the tank. The best the insulation can do is to suppress the thermal link between the tank and its surroundings.

In addition to studying various jet speeds and subcoolings, the focus now will be on a particular jet speed and temperature and the effects of heat addition and liquid fill level on the depressurization behavior will be investigated. For these cases, the
2.5 RESULTS

The depressurization histories for three different heat inputs are presented in Fig. 2.17. The depressurization rates are not easily discernible in Fig. 2.17a because at time = 0, the liquid-vapor system is in a different thermodynamic state prior to turning on the jet owing to the three different applied heat loads. Nonetheless, the depressurization rate can be deduced from the data by computing:

\[
\frac{[P(0s) - P_o] - [P(600s) - P_o]}{600s}
\]  

(2.2)

where time = 0 corresponds to when the jet is first activated and the 600 s time interval was chosen arbitrarily. For the 1 W, 2 W, and 3 W cases, the depressurization rate is 0.040 Torr/s, 0.046 Torr/s, and 0.053 Torr/s, respectively. The depressurization rate increases with heat load because the rate of decay is a strong function of the heat removal rate which is initially higher for the 3 W case. As indicated in Fig. 2.17b, as more heat is applied to the system, at the end of the self-pressurization phase of the experiment, the system temperature is higher. Thus, when the jet is first activated, the driving potential for heat exchange – the temperature difference between the bulk fluid and the subcooled jet – is largest for the 3 W test. If the upward motion of the jet is not restricted by buoyancy or natural convection, the large temperature differences result in a higher heat removal rate and consequently a faster pressure reduction.

Similar trends are noted for the ullage temperature. Defining the temperature
Figure 2.17: Effect of heat input on pressure (a) and temperature (b) during subcooled jet mixing. (Liquid fill level = 26.5%, Bottom heating configuration, Jet speed = 24.2 cm/s, Jet temperature = 20 °C)
reduction rate similarly to eqn. (2.2), one finds that for the 1 W, 2 W, and 3 W cases, the temperature is decaying at $1.90 \times 10^{-3}$ K/s, $2.05 \times 10^{-3}$ K/s, and $2.45 \times 10^{-3}$ K/s respectively. For reasons outlined above, the rate of reduction is again greatest for the 3 W case.

Next the effects of liquid fill level on the depressurization behavior for the liquid heating configuration will be studied. For the lowest fill level shown in Fig. 2.18, the pressure response is immediate – the ullage pressure begins to collapse as soon as the subcooled jet is activated. The response is more delayed for the higher fill levels. For the 50% case, the pressure decreases slightly for the first 500 s before rapidly collapsing. At a liquid fill level of 73.5%, the response is significantly delayed. Rapid depressurization doesn’t commence until 2800 s after turning on the jet. These delays are significantly longer than the L/U transit times of 0.84 s and 1.26 s for the 50% and 73.5% cases respectively. In order for the subcooled jet to reach the interface and initiate the rapid pressure collapse, the incoming liquid stream must first remove enough energy from the bulk liquid to weaken the natural convection vortex that’s inhibiting the jet’s upward motion. For the highest fill level, the bulk liquid has absorbed more of the incident heat load than in the lower fill level cases. Since the subcooled jet would have to remove more sensible energy from the bulk liquid before reaching the interface the pressure response would be delayed. Additionally, for the 73.5% fill level case, the centrally located T1 thermistor is submerged in the liquid phase and is directly in the path of the incident jet stream. Fluid that should otherwise reach the interface stagnates on the thermistor. This inhibits the upward
Figure 2.18: Effect of liquid fill level on pressure (a) and temperature (b) during subcooled jet mixing. (Heat load = 2 W, Bottom heating configuration, Jet speed = 24.2 cm/s, Jet temperature = 20 °C)
motion of the liquid jet and also delays the pressure collapse response.

Similar delayed responses are noted in the temperature histories shown in Fig. 2.18b. No temperature jump is observed for the highest fill level but at this level the thermistor is submerged. The noisier response for this case is due to temperature fluctuations brought about by buoyancy / forced jet interactions.

2.5.3 Visualization

In this section, the term “visualization” is used loosely to describe the temperature maps obtained by fully populating the tank with thermistors. One-to-one quantitative comparisons between this last visualization test and the previous quantitative measurements are not appropriate for several reasons. First, as noted earlier, the leak rate into the tank was slightly larger when fully populated with thermistors. Secondly, and this is particularly true during subcooled mixing, the thermistors interfered with the flow field. If a thermistor was in the path of the incoming jet, fluid would stagnate on the thermistor instead of being carried to the interface. This tended to retard the depressurization rate. Thirdly, the flow meter was changed out prior to running the visualization tests. The replacement was a higher capacity flow meter which resulted in a decreased pressure drop and thus larger throughput for the same amount of power supplied to the pump. Even with these differences from previous tests, the qualitative temperature maps are nevertheless useful and can be used to support some of the hypotheses laid out in previous sections.

To construct the temperature map, the plane containing the thermistors was tri-
Figure 2.19: Data triangulation of the plane containing the thermistors.
angulated as shown in Fig. 2.19. Every vertex in the triangulated plane corresponds to a thermistor or RTD location. Here, axisymmetry is assumed which effectively doubled the number of off-axis vertices. The triangulation and pointwise temperatures were then read into tecplot® and an internal contouring algorithm was used to construct a temperature field by interpolating the vertex values.

In this fully-populated tank, the fill level is 26.5% and 2 W is applied to the bottom heater. The ullage pressure history corresponding to this case, shown in Fig. 2.20, exhibits characteristics similar to previous bottom heating test cases. The temperature histories at two locations in the tank are shown in Fig. 2.20. Thermistor T1 is recording temperature in the ullage at the same location as previous temperature measurements. Not surprisingly then, the temperature trace is similar to previous cases whereby the rapid decay beginning when the jet is first turned on is followed by a temperature jump. The histories presented in Fig. 2.20b also indicate that the temperature in the liquid above the heating band (T13) is rising faster than temperature in the vapor. Hence during self-pressurization heat is being transferred from the liquid into the vapor. During subcooled mixing, both the liquid and vapor temperatures decay at nearly the same rate initially. After approximately 750 s of subcooled jet mixing, the vapor temperature jumps while liquid temperature continues its decay. The absence of a jump in the liquid is due to both a stable stratification prior to jet activation as a result of the bottom-heating configuration and a strong subcooled mixing jet which tends to homogenize the bulk and isolate any local hot spots to regions near the heater.
Figure 2.20: Pressure (a) and temperature (b) histories. (Fill level = 26.5%, Heat load = 2 W, Bottom heating configuration, Jet flow = 800 mL/min, Jet temperature = 20 °C)
2.5 RESULTS

EXPERIMENTAL INVESTIGATION

(A)  
Time = 3300 s

(B)  
Time = 7190 s

T

<table>
<thead>
<tr>
<th>Temperature</th>
</tr>
</thead>
<tbody>
<tr>
<td>296.60</td>
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<td>296.55</td>
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<tr>
<td>296.50</td>
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<tr>
<td>295.80</td>
</tr>
<tr>
<td>295.75</td>
</tr>
</tbody>
</table>
Figure 2.21: Temperature contours at various times during self-pressurization and subcooled jet mixing. (a) $\Delta T_{\text{max}} = 0.708$ K, $\Delta T_{\text{min}} = 0.052$ K. (b) $\Delta T_{\text{max}} = 1.126$ K, $\Delta T_{\text{min}} = 0.273$ K. (c) $\Delta T_{\text{max}} = 0.772$ K, $\Delta T_{\text{min}} = -1.502$ K. (d) $\Delta T_{\text{max}} = 0.528$ K, $\Delta T_{\text{min}} = -1.788$ K.
In order to further investigate this thermal response, the temperature field, measured at discrete points and then interpolated onto the triangulated domain, is presented in Fig. 2.21 at time stamps A, B, C, and D as labeled in Fig. 2.20. While there appears to be quite a variation in temperature along the interface, this is almost certainly an artifact of constructing a field map by linearly interpolating between discrete points in the domain. Interpolating between discrete points also produces a choppiness in the temperature field that is unphysical. Nevertheless, these maps provide a useful qualitative description of the thermal response in the system.

At 3300 s into the self-pressurization experiment and continuing until subcooled mixing is about to begin, the temperature fields shown in Figs. 2.21a and 2.21b indicate that the liquid is stably stratified with the fluid at the bottom of the tank colder than fluid above the heater. In the ullage, vapor near the phase boundary is warmer than the bulk vapor which indicates that prior to turning on the jet, the vapor was in an unstable thermal configuration. Heat penetrates into the ullage and is carried upwards by conduction, buoyancy, and the flux of molecules leaving the phase boundary. The temperature maps also indicate that the ullage is warmer than its bounding walls and hence the vapor loses energy to the acrylic during self-pressurization. Nearer to the interface the wall temperature increases due to its proximity to the warmer liquid phase. The colder walls at the top of the tank confirm that axial conduction is not dominant and suggests that an increase in the temperature of the wall adjacent to the vapor phase is due primarily to heat lost from the ullage.

During subcooled jet mixing, temperature maps are shown in Figs. 2.21c and
2.21d. During the period of rapid pressure decay, the ullage is essentially isothermal. After the temperature jump, heat entering the ullage from the wall rises to the top of the tank which leads to a stably stratified ullage as shown in Fig. 2.21d.

Further insight can be gained by plotting the time history of vapor temperature shown in Fig. 2.22b. Prior to turning on the jet, the hottest vapor temperature is near the interface. Not surprising then, the warmest part of the non-wetted wall is adjacent to the interface. At the end of the 90 minute pressure control test, the hottest vapor has risen to the top of the tank. It is also interesting to note the degree of thermal stratification during both the self-pressurization and pressure control phases of the experiment. After self-pressurizing for two hours the difference between the minimum and maximum ullage temperatures is only 0.2 K. After the jump, the stratification is much more pronounced with the difference between minimum and maximum vapor temperatures now 2.25 K. This pronounced, and now stable, stratification during the pressure control test is indicative of the ability of the subcooled jet to remove heat from the ullage. It is interesting to note that temperatures jump to higher values at different times. For thermistors away from the cold interface, the times at which thermistor temperatures jump to a higher value is a strong function of how close they are to the hottest parts of the non-wetted wall. This suggests that these temperature jumps are local in nature and are being driven by wall heating.

Stratification is also present in the liquid during self-pressurization as indicated in the temperature histories shown in Fig. 2.22a. The temperature of liquid below the heater (T14 and T15) rises much more slowly that fluid above the heater due
Figure 2.22: Temperature histories in the liquid (a) and vapor (b). (Fill level = 26.5%, Heat load = 2 W, Bottom heating configuration, Jet flow = 800 mL/min, Jet temperature = 20 °C)
to the buoyant rise of warm fluid. One of the thermistor measurements above the heater (T12) is located in the bulk 3.875" away from the wall. This indicates that the temperature rise in the liquid is not confined to a thin thermal boundary layer near the wall. The natural convection vortex is pulling warmer fluid up from the heater and recirculating it along the interface and then downward near the tank centerline.
3.1 What is an Interface?

Microscopically, an interface is a thin ($\varepsilon = \frac{l}{L} << 1$) 3D transition region separating two bulk phases. The diffuse 3D interface, over which properties are continuous but undergo rapid changes, becomes a 2D singular surface as $\varepsilon \to 0$. In this limiting macroscopic viewpoint, the interface is treated as a Gibbsian dividing surface over which interfacial properties can be assigned.

In Fig. 3.1, a cylindrical vessel contains two homogeneous bulk phases separated by an interface. The density variation is plotted to the right. As the interface is approached from above, the density rapidly changes from its value in the vapor phase to its value in the liquid phase over a short distance, $l$. If the interface is treated as a 2D dividing surface, the density of each homogeneous bulk phase is assumed constant.
3.1 WHAT IS AN INTERFACE?  THEORY

Figure 3.1: Sketch of a liquid-vapor system and corresponding density profile.

By neglecting the continuous variation of density across the interface, a surface excess or deficiency is created between the actual density and the bulk phase values. The surface excess, shown in Fig. 3.1 as the shaded region in the density plot, can be expressed as:

\[ \int_{\Sigma} \rho_s \, dA = \int_V \rho \, dV - \left[ \int_{V_v} \rho_v \, dV + \int_{V_l} \rho_l \, dV \right] \tag{3.3} \]

The areal surface density, \( \rho_s \), when integrated over the surface, \( \Sigma \), gives the mass excess or deficiency of the system. It should be noted that \( \rho_s \) is not the actual value...
3.2 MATHEMATICAL DESCRIPTION

of $\rho$ at the interface. Rather, it is the value that is assigned to the interface to account for the 3D continuous property variation.

3.2 Mathematical Description

Consider a spherical vapor bubble centered in a pool of liquid as sketched in Fig. 3.2. The domain, $\Omega$, is divided into a liquid region, $\Omega^+$ and a vapor region, $\Omega^-$. The vapor region is bounded by a 2D non-Euclidean surface, $\partial \Omega$. The level set method, which can be used to capture the interfacial dynamics, embeds information about the 2D surface into a function, $\phi$, defined in 3D space.

To make this clearer, the interface sketched in Fig. 3.2 can be described by the

![Figure 3.2: Geometric description of the two-phase system.](image-url)
zeroth isocontour of the following function

\[ \phi = x^2 + y^2 + z^2 - R^2. \] (3.4)

The normal to the surface can be defined in terms of this level set function:

\[ \hat{n} = \frac{\nabla \phi}{|\nabla \phi|}. \] (3.5)

where the normal vector points in the direction of increasing \( \phi \) – into the liquid for the configuration depicted in Fig. 3.2. Once the normal is defined, the mean curvature of the surface can be computed from

\[ H = \frac{1}{2} (\nabla \cdot \hat{n}) \] (3.6)

where the curvature is positive if the interface curves away from the normal as it does in Fig. 3.2.

In what follows, the surface projection operator

\[ I_s = I - \hat{n}\hat{n} \] (3.7)

will be used. The operator projects a vector defined in 3D onto the surface. The
surface gradient, for example, is given by

\[ \nabla_s = I_s \cdot \nabla. \]  
(3.8)

The interface can deform in time. Associating the zeroth isocontour with the interface for all time requires that

\[ \frac{d\phi}{dt} = 0 \]  
(3.9)

or after expanding the total derivative

\[ \frac{\partial \phi}{\partial t} + v_s \cdot \nabla \phi = 0 \]  
(3.10)

where \( v_s \) is the interfacial velocity. The advection equation for \( \phi \) can be rewritten using eqn. (3.5):

\[ \frac{\partial \phi}{\partial t} + v_s \cdot \frac{\nabla \phi}{|\nabla \phi|} |\nabla \phi| = 0 \]  
(3.11)

\[ \frac{\partial \phi}{\partial t} + (v_s \cdot \hat{n}) |\nabla \phi| = 0. \]  
(3.12)

In the derivations that follow, the Heaviside function

\[ H(\phi) = \begin{cases} 
1 & \phi > 0 \\
0 & \phi < 0 
\end{cases} \]  
(3.13)
and the Dirac function

\[ \delta(\phi) = \frac{\partial H}{\partial \phi} \quad (3.14) \]

will be used. Various operations will be carried out the Heaviside and Dirac functions.

The gradient of the Heaviside function is:

\[
\nabla H = \frac{\partial H}{\partial \phi} \nabla \phi \\
= \frac{\partial H}{\partial \phi} |\nabla \phi| \frac{\nabla \phi}{|\nabla \phi|} \\
= \frac{\partial H}{\partial \phi} |\nabla \phi| \hat{n} \\
= \delta(\phi) |\nabla \phi| \hat{n}.
\]

(3.15)

The time derivative of the Heaviside function is given by:

\[
\frac{\partial H}{\partial t} = \frac{\partial H}{\partial \phi} \frac{\partial \phi}{\partial t} \\
= -\frac{\partial H}{\partial \phi} (\mathbf{v} \cdot \hat{n}) |\nabla \phi| \\
= -\delta(\phi) |\nabla \phi| (\mathbf{v} \cdot \hat{n}).
\]

(3.16)

The 3D analog to the 1D Dirac function defined by eqn. (3.14) is

\[ \delta(\mathbf{x}) = \nabla H \cdot \hat{n}, \quad (3.17) \]
which after making use of eqn. (3.15) can be rewritten as

$$\delta(x) = \delta(\phi)|\nabla \phi|.$$  

(3.18)

The Heaviside and Dirac functions are useful when defining quantities that vary over the entire domain. The density, for example, can be expressed as:

$$\rho = \rho_v \chi^- + \rho_l \chi^+ + \rho_s \delta(x)$$

(3.19)

where

$$\chi^- = 1 - H(\phi)$$

(3.20)

$$\chi^+ = H(\phi)$$

(3.21)

Thus,

$$x \in \Omega^-, \quad \rho = \rho_v$$

(3.22)

$$x \in \Omega^+, \quad \rho = \rho_l$$

(3.23)

$$x \in \partial \Omega, \quad \rho = \rho_s.$$  

(3.24)

The following operations will be needed in subsequent sections and follow directly
from the previous discussion:

\[ \nabla \chi^- = -\nabla H = -\delta(x) \cdot \hat{n} \]  
\[ \nabla \chi^+ = \nabla H = \delta(x) \cdot \hat{n} \]  
\[ \frac{\partial \chi^-}{\partial t} = -\frac{\partial H}{\partial t} = \delta(x)(v_s \cdot \hat{n}) \]  
\[ \frac{\partial \chi^-}{\partial t} = \frac{\partial H}{\partial t} = -\delta(x)(v_s \cdot \hat{n}) \]  

3.3 Conservation Laws

Using the operators defined in Section 3.2, the balance equations for mass, momentum, and energy can now be derived. The derivation shall be explicit for the mass conservation equation but abbreviated for the other conservation laws.

3.3.1 Mass Conservation

Beginning with the following decompositions:

\[ \rho = \rho_v \chi^- + \rho_l \chi^+ + \rho_s \delta(x) \]  
\[ \rho v = \rho_v v_v \chi^- + \rho_l v_1 \chi^+ + \rho_s v_s \delta(x) \]  

the continuity equation for the entire liquid-vapor-interfacial system can be expressed as:

\[ \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho v) = 0 \]
Substituting eqns. (3.29) and (3.30) into the continuity equation yields

\[
\begin{align*}
\chi^- & \frac{\partial \rho_v}{\partial t} + \rho_v \frac{\partial \chi^-}{\partial t} + \chi^- \nabla \cdot (\rho_v v_v) + \rho_v v_v \cdot \nabla \chi^- + \\
\chi^+ & \frac{\partial \rho_l}{\partial t} + \rho_l \frac{\partial \chi^+}{\partial t} + \chi^+ \nabla \cdot (\rho_l v_l) + \rho_l v_l \cdot \nabla \chi^+ + \\
\delta(\vec{x}) \frac{\partial \rho_s}{\partial t} + \rho_s \frac{\partial \delta}{\partial t} + \delta(\vec{x}) \nabla \cdot (\rho_s v_s) + \rho_s v_s \cdot \nabla \delta &= 0
\end{align*}
\] (3.32)

Grouping terms together and making use of eqns. (3.25)-(3.28) yields

\[
\begin{align*}
\chi^- \left[ \frac{\partial \rho_v}{\partial t} + \nabla \cdot (\rho_v v_v) \right] + \\
\chi^+ \left[ \frac{\partial \rho_l}{\partial t} + \nabla \cdot (\rho_l v_l) \right] + \\
\delta(\vec{x}) \left[ \frac{\partial \rho_s}{\partial t} + \nabla \cdot (\rho_s v_s) + \rho_l (v_l - v_s) \cdot \hat{n} - \rho_v (v_v - v_s) \cdot \hat{n} \right] + \\
\rho_s \frac{d\delta}{dt} &= 0.
\end{align*}
\] (3.33)

Due to the arbitrariness of \( \Omega^\pm \), the terms post-multiplying \( \chi^\pm \) must go to zero separately. Hence in the bulk phases,

\[
\begin{align*}
\mathbf{x} \in \Omega^- : \quad & \frac{\partial \rho_v}{\partial t} + \nabla \cdot (\rho_v v_v) = 0 \quad (3.34) \\
\mathbf{x} \in \Omega^+ : \quad & \frac{\partial \rho_l}{\partial t} + \nabla \cdot (\rho_l v_l) = 0. \quad (3.35)
\end{align*}
\]

Bedeaux et al.\textsuperscript{188} rigorously show that

\[
\frac{d\delta}{dt} = 0 \quad (3.36)
\]
and so the proof will be omitted here. Furthermore, they demonstrated that equations of the form

\[ A \delta(\vec{x}) + \mathbf{B} \cdot \nabla \delta = 0 \]  

(3.37)

imply that

\[ A = \mathbf{B} \cdot \hat{n} = 0. \]  

(3.38)

Hence, from eqn. (3.33)

\[
\frac{\partial \rho_s}{\partial t} + \nabla \cdot (\rho_s \mathbf{v}_s) + \rho_l (\mathbf{v}_l - \mathbf{v}_s) \cdot \hat{n} - \rho_v (\mathbf{v}_v - \mathbf{v}_s) \cdot \hat{n} = 0
\]  

(3.39)

If the surface excess contributions are neglected, i.e.: 

\[
\frac{\partial \rho_s}{\partial t} + \nabla \cdot (\rho_s \mathbf{v}_s) = 0
\]  

(3.40)

then the mass flux on either side of the interface are equal:

\[
\rho_l (\mathbf{v}_l - \mathbf{v}_s) \cdot \hat{n} = \rho_v (\mathbf{v}_v - \mathbf{v}_s) \cdot \hat{n}
\]  

(3.41)

For convenience, let the condensation mass flux be defined as:

\[
j \equiv \rho_l (\mathbf{v}_l - \mathbf{v}_s) \cdot \hat{n} = \rho_v (\mathbf{v}_v - \mathbf{v}_s) \cdot \hat{n}
\]  

(3.42)
3.3 CONSERVATION LAWS

3.3.2 Balance of Linear Momentum

In addition to eqns. (3.29) - (3.30), the following decompositions can be made:

\[ \rho v v = \rho_v v_v v_v \chi^- + \rho_l v_1 v_1 \chi^+ + \rho_s v_s v_s \delta(x) \]  \hspace{1cm} (3.43)

\[ T = T_v \chi^- + T_l \chi^+ + T_s \delta(x) \]  \hspace{1cm} (3.44)

where \( T_l \) and \( T_v \) are the stress tensors in the bulk liquid and vapor phases and \( T_s \)
is the surface stress tensor. Substituting these decompositions into the momentum balance

\[ \frac{\partial}{\partial t} (\rho v) = -\nabla \cdot (\rho v v + T) + \rho g \]  \hspace{1cm} (3.45)

yields

\[ x \in \Omega^- : \quad \frac{\partial}{\partial t} (\rho_v v_v) + \nabla \cdot (\rho_v v_v v_v) = -\nabla \cdot T_v + \rho_v g \]  \hspace{1cm} (3.46)

\[ x \in \Omega^+ : \quad \frac{\partial}{\partial t} (\rho_l v_1) + \nabla \cdot (\rho_l v_1 v_1) = -\nabla \cdot T_l + \rho_l g \]  \hspace{1cm} (3.47)

in the bulk phases and

\[ \frac{\partial}{\partial t} (\rho_s v_s) + \nabla \cdot (\rho_s v_s v_s) - \rho_s g + \nabla \cdot T_s + (T_l - T_v) \cdot \hat{n} + j(v_1 - v_v) = 0 \]  \hspace{1cm} (3.48)

\[ T_s \cdot \hat{n} = 0 \]  \hspace{1cm} (3.49)
at the interface. Eqn. (3.49) implies that the surface stress tensor, $T_s$, only varies tangential to the interface and not normal to it. In eqn. (3.48), neglecting terms associated with the surface mass excess yields

$$-\nabla \cdot T_s = (T_l - T_v) \cdot \hat{n} + j(v_1 - v_v).$$  \hfill (3.50)

The following constitutive models are used for the stress tensors:

$$T_i = p_i I + S_i \quad i = l, v$$ \hfill (3.51)

$$T_s = -\sigma I_s$$ \hfill (3.52)

where $p$ is the pressure and $S$ is the viscous part of the stress tensor,

$$S = -\mu \left( \nabla v + \nabla v^T \right) + \left[ \left( \frac{2}{3} \mu - \kappa \right) \nabla \cdot v \right] I.$$ \hfill (3.53)

The rheological properties of the fluid are assumed to be Newtonian.\textsuperscript{189} For the surface stress tensor, $\sigma$ is the surface tension and the viscous contribution to the surface stress has been neglected. Eqn. (3.50) can be transformed into a more recognizable form.
by noting that

\[ \nabla \cdot T_s = -\nabla \cdot (\sigma I_s) \]

\[ = -\sigma \nabla \cdot I_s - I_s \cdot \nabla \sigma \]

\[ = -\sigma \nabla \cdot (I - \hat{n}\hat{n}) - \nabla_s \sigma \]

\[ = \sigma (\nabla \cdot \hat{n})\hat{n} - \nabla_s \sigma \]

\[ = 2H \sigma \hat{n} - \nabla_s \sigma \]

Hence,

\[ -2H \sigma \hat{n} + \nabla_s \sigma = (p_l - p_v)\hat{n} + (S_l \cdot \hat{n} - S_v \cdot \hat{n}) + j(v_1 - v_v). \] (3.55)

The above vector equation can be decomposed into normal and tangential components:

\[ -2H = (p_l - p_v) + [(S_l \cdot \hat{n}) \cdot \hat{n} - (S_v \cdot \hat{n}) \cdot \hat{n}] + j(v_1 - v_v) \cdot \hat{n} \] (3.56)

\[ \nabla_s \sigma = (S_l \cdot \hat{n}) \cdot \hat{t} - (S_v \cdot \hat{n})\hat{t} \] (3.57)

where no slip has been assumed at the interface,

\[ v_1 \cdot \hat{t} = v_v \cdot \hat{t} \] (3.58)
The last term in eqn. (3.56) can be rewritten as follows

\[ j(v_1 - v_v) \cdot \hat{n} = j \left[ (v_1 - v_s) \cdot \hat{n} - (v_v - v_s) \cdot \hat{n} \right] \]

\[ = j \left[ \left( \frac{\rho_l(v_1 - v_s)}{\rho_l} \right) \cdot \hat{n} - \left( \frac{\rho_v(v_v - v_s)}{\rho_v} \right) \cdot \hat{n} \right] \]

\[ = j^2 \left( \frac{1}{\rho_l} - \frac{1}{\rho_v} \right) \]  

(3.59)

For \( j \ll 1 \), terms of \( O(j^2) \) can be neglected, which results in

\[ -2H \sigma = (p_l - p_v) + [(S_l \cdot \hat{n}) \cdot \hat{n} - (S_v \cdot \hat{n}) \cdot \hat{n}] \]  

(3.60)

\[ \nabla_s \sigma = (S_l \cdot \hat{n}) \cdot \hat{t} - (S_v \cdot \hat{n}) \hat{t} \]  

(3.61)

### 3.3.3 Conservation of Energy

The energy and energy flux can be decomposed similarly

\[ \rho_e = \rho_v e_v \chi^- + \rho_l e_l \chi^+ + \rho_s e_s \delta(x) \]  

(3.62)

\[ J_e = J_{e,v} \chi^- + J_{e,l} \chi^+ + J_{e,s} \delta(x) \]  

(3.63)

where, after neglecting potential energy contributions, the total energy is given by:

\[ e = u + \frac{v^2}{2} \]  

(3.64)
and the energy flux can be expressed as:

\[ \mathbf{J}_e = \rho_e \mathbf{v} + T \cdot \mathbf{v} + \mathbf{J}_q. \] (3.65)

The first term in the energy flux corresponds to the flux of energy advected with
the fluid, the second term corresponds to the mechanical work, and the last term
corresponds to the heat flux,

\[ \mathbf{J}_q = -k \nabla T. \] (3.66)

Substituting the above decompositions into the total energy balance,

\[ \frac{\partial}{\partial t} (\rho e) = -\nabla \cdot J_e, \] (3.67)

yields

\[
\begin{align*}
\mathbf{x} \in \Omega^- : & \quad \frac{\partial}{\partial t} (\rho_e \mathbf{v}) + \nabla \cdot (\rho_e \mathbf{v} \mathbf{v}) = -\nabla \cdot (T_v \cdot \mathbf{v}) - \nabla \cdot \mathbf{J}_{q,v} \\
\mathbf{x} \in \Omega^+ : & \quad \frac{\partial}{\partial t} (\rho_l \mathbf{v}_l) + \nabla \cdot (\rho_l \mathbf{v}_l \mathbf{v}_l) = -\nabla \cdot (T_l \cdot \mathbf{v}_l) - \nabla \cdot \mathbf{J}_{q,l}
\end{align*}
\] (3.68)

in the bulk phases. At the interface,

\[
\begin{align*}
\frac{\partial}{\partial t} (\rho_s e_s) + \nabla \cdot \mathbf{J}_{e,s} + j(e_l - e_v) + (T_l \cdot \mathbf{v}_l - T_v \cdot \mathbf{v}_v) \cdot \mathbf{n} + (\mathbf{J}_{q,l} - \mathbf{J}_{q,v}) \cdot \mathbf{n} = 0 \\
\mathbf{J}_{e,s} \cdot \mathbf{n} = 0
\end{align*}
\] (3.70, 3.71)
which implies the surface energy flux does not vary normal to the surface. Neglecting terms involving the surface mass excess and surface excess heat flux yields,

$$-\nabla \cdot (T_s \cdot \mathbf{v}_s) = j(\epsilon_l - \epsilon_v) + (T_l \cdot \mathbf{v}_l - T_v \cdot \mathbf{v}_v) \cdot \hat{n} + (\mathbf{J}_{q,l} - \mathbf{J}_{q,v}) \cdot \hat{n} \quad (3.72)$$

To simply this expression, one can first take the dot product of eqn. (3.50) with \( \mathbf{v}_s \),

$$-\mathbf{v}_s \cdot (\nabla \cdot T_s) = (T_l \cdot \hat{n} - T_v \cdot \hat{n}) \cdot \mathbf{v}_s + j(\mathbf{v}_l - \mathbf{v}_v) \cdot \mathbf{v}_s \quad (3.73)$$

and then subtract the result from eqn. (3.72), resulting in:

$$\mathbf{v}_s \cdot (\nabla \cdot T_s) - \nabla \cdot (T_s \cdot \mathbf{v}_s) = j \left[ (u_l - u_v) + \frac{1}{2} (\mathbf{v}_l \cdot \mathbf{v}_l - \mathbf{v}_v \cdot \mathbf{v}_v - 2\mathbf{v}_l \cdot \mathbf{v}_s + 2\mathbf{v}_v \cdot \mathbf{v}_s) \right] + (T_l \cdot \mathbf{v}_l \cdot \hat{n} - T_l \cdot \hat{n} \cdot \mathbf{v}_s) + (T_v \cdot \mathbf{v}_v \cdot \hat{n} - T_v \cdot \hat{n} \cdot \mathbf{v}_s) + (\mathbf{J}_{q,l} - \mathbf{J}_{q,v}) \cdot \hat{n} \quad (3.74)$$

The following terms can be rewritten:

$$\mathbf{v}_s \cdot (\nabla \cdot T_s) - \nabla \cdot (T_s \cdot \mathbf{v}_s) = T_s : \nabla \mathbf{v}_s \quad (3.75)$$
\[
\frac{1}{2} (v_1 \cdot v_1 - v_\nu \cdot v_\nu - 2v_1 \cdot v_s + 2v_\nu \cdot v_s)
\]
\[
= \frac{1}{2} \left[ (v_1 \cdot v_1 - 2v_1 \cdot v_s + v_s \cdot v_s) - (v_\nu \cdot v_\nu - 2v_\nu \cdot v_s + v_s \cdot v_s) \right]
\]
\[
= \frac{1}{2} \left[ (v_1 - v_s) \cdot (v_1 - v_s) - (v_\nu - v_s) \cdot (v_\nu - v_s) \right]
\]
\[
= \frac{1}{2} \left[ \frac{j \hat{n} \cdot j \hat{n}}{\rho_l} - \frac{j \hat{n} \cdot j \hat{n}}{\rho_v} \right]
\]
\[
= \frac{j^2}{2} \left[ \frac{1}{\rho_l^2} - \frac{1}{\rho_v^2} \right]
\]

By making use of the symmetry property of the stress tensor

\[
(T_l \cdot v_1) \cdot \hat{n} - (T_l \cdot \hat{n}) \cdot v_s = (T_l \cdot \hat{n}) \cdot (v_1 - v_s)
\]
\[
= (T_l \cdot \hat{n}) \cdot \frac{j \hat{n}}{\rho_l}
\] (3.77)

and

\[
(T_v \cdot v_\nu) \cdot \hat{n} - (T_v \cdot \hat{n}) \cdot v_s = (T_v \cdot \hat{n}) \cdot (v_\nu - v_s)
\]
\[
= (T_v \cdot \hat{n}) \cdot \frac{j \hat{n}}{\rho_v}.
\] (3.78)

The energy balance at the interface becomes:

\[
T_s : \nabla v_s = j (u_l - u_v) + \frac{j^3}{2} \left( \frac{1}{\rho_l^2} - \frac{1}{\rho_v^2} \right) + j \left[ \frac{(T_l \cdot \hat{n}) \cdot \hat{n}}{\rho_l} - \frac{(T_v \cdot \hat{n}) \cdot \hat{n}}{\rho_v} \right] + (J_{q,l} - J_{q,v}) \cdot \hat{n}
\] (3.79)
Applying eqn. (3.51) results in

\[ T_s : \nabla v_s = j(h_l - h_v) + \frac{j^3}{2} \left( \frac{1}{\rho_t^2} - \frac{1}{\rho_v^2} \right) + j \left[ \frac{(S_l \cdot \hat{n}) \cdot \hat{n}}{\rho_t} - \frac{(S_v \cdot \hat{n}) \cdot \hat{n}}{\rho_v} \right] + (J_{q,l} - J_{q,v}) \cdot \hat{n}. \]  

(3.80)

For \( j \ll 1 \), terms of \( O(j^3) \) can be neglected, which leads to

\[ T_s : \nabla v_s = j(h_l - h_v) + j \left[ \frac{(S_l \cdot \hat{n}) \cdot \hat{n}}{\rho_t} - \frac{(S_v \cdot \hat{n}) \cdot \hat{n}}{\rho_v} \right] + (J_{q,l} - J_{q,v}) \cdot \hat{n}. \]  

(3.81)

### 3.4 Equation Summary

From the derivations presented in section 3.3, one finds in the bulk phases

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

(3.82)

\[ \frac{\partial}{\partial t}(\rho v v) + \nabla \cdot (\rho v v) = -\nabla p - \nabla \cdot S + \rho g \]  

(3.83)

\[ \frac{\partial}{\partial t}(\rho e) + \nabla \cdot \left( \rho \left[ e + \frac{p}{\rho} \right] v \right) = -\nabla \cdot (S \cdot v) - \nabla \cdot J_q \]  

(3.84)

and at the interface

\[ j \equiv \rho_t (v_l - v_s) \cdot \hat{n} = \rho_v (v_v - v_s) \cdot \hat{n} \]  

(3.85)

\[ -2H \sigma = (p_l - p_v) + [(S_l \cdot \hat{n}) \cdot \hat{n} - (S_v \cdot \hat{n}) \cdot \hat{n}] \]  

(3.86)

\[ \nabla_s \sigma = (S_l \cdot \hat{n}) \cdot \hat{i} - (S_v \cdot \hat{n}) \cdot \hat{i} \]  

(3.87)

\[ T_s : \nabla v_s = j(h_l - h_v) + j \left[ \frac{(S_l \cdot \hat{n}) \cdot \hat{n}}{\rho_t} - \frac{(S_v \cdot \hat{n}) \cdot \hat{n}}{\rho_v} \right] + (J_{q,l} - J_{q,v}) \cdot \hat{n}. \]  

(3.88)
In addition to the above balance equations, equations of state are also required,

\[ p = p(\rho, T) \]  (3.89)
\[ u = u(\rho, T) \]  (3.90)
\[ \sigma = \sigma(T) \]  (3.91)

### 3.5 Evaporation Condition

In addition to the transport equations and constitutive models for stress and heat flux, an evaporation condition is required for closure. In what follows, the equilibrium conditions for the liquid-vapor-interfacial system are discussed and later generalized for non-equilibrium processes.

Consider a closed tank where the bulk phases and surface can exchange mass and energy among themselves. Each bulk phase can be treated as an open system where

\[ dU_l = T_l dS_l - p_l dV_l + \mu_l dm_l \]  (3.92)
\[ dU_v = T_v dS_v - p_v dV_v + \mu_v dm_v \]  (3.93)
\[ dU_s = T_s dS_s + \sigma dA + \mu_s dm_s. \]  (3.94)

Here, it has been assumed that only a single species exists in the tank and that potential energy contributions are negligible to the first law energy balance. The
chemical potential, \( \mu \), is defined on a mass basis: i.e.

\[
\mu_l = \left( \frac{\partial u_l}{\partial m_l} \right)_{s,v}.
\]  

(3.95)

Summing eqns. (3.92)-(3.94) yields

\[
dU_l + dU_v + dU_s = T_l dS_l + T_v dS_v + T_s dS_s
\]

\[- p_l dV_l - p_v dV_v + \sigma dA
\]

\[+ \mu_l dm_l + \mu_v dm_v + \mu_s dm_s.
\]  

(3.96)

Since the tank is closed and rigid

\[dm = dm_l + dm_v + dm_s = 0 \]  

(3.97)

\[dV = dV_l + dV_v. \]  

(3.98)

At equilibrium,

\[dU = dU_l + dU_v + dU_s = 0 \]  

(3.99)

\[dS = dS_l + dS_v + dS_s = 0. \]  

(3.100)
Hence,

\[ 0 = (T_l - T_s)\,dS_l + (T_v - T_s)\,dS_v - (p_v - p_l)\,dV_v + \sigma\,dA + (\mu_l - \mu_s)\,dm_l + (\mu_v - \mu_s)\,dm_v. \]  

(3.101)

Since these variations are independent, at equilibrium,

\[ T_l = T_v = T_s \]  

(3.102)

\[ \mu_l = \mu_v = \mu_s \]  

(3.103)

\[ p_v - p_l = \sigma \frac{dA}{dV_v} \]  

(3.104)

For a spherical ullage surrounded by a pool of liquid:

\[ \frac{dA}{dV_v} = \frac{d(4\pi r^2)}{d(4/3\pi r^3)} = \frac{2}{r} = 2H \]  

(3.105)

where H is the mean curvature defined according to eqn. (3.6). Hence, the condition for mechanical equilibrium is

\[ p_v - p_l = 2\sigma H \]  

(3.106)

which is consistent with the jump momentum balance (eqn. (3.86)) when no velocity gradients are present and the interfacial mass flux is zero.

For a pure system, the chemical potential is the specific Gibbs energy:

\[ \mu = g \]  

(3.107)
and
\[ dg = -sdT + \nu dp. \] (3.108)

At equilibrium,
\[ gl = gv \] (3.109)
\[ dg_l = dg_v. \] (3.110)

Thus,
\[ -s_l dT + \nu_l dp_l = -s_v dT + \nu_v dp_v \] (3.111)

where isothermality (eqn. (3.102)) has already been invoked. For a flat interface,
\[ pl = pv = p_{flat}. \] (3.112)

Taking differentials
\[ dp_l = dp_v = dp_{flat} \] (3.113)

which allows one to rewrite eqn. (3.111) as
\[ dp_{flat} = \frac{s_v - s_l}{\nu_v - \nu_l} dT. \] (3.114)

For a curved interface
\[ pv - pl = 2H \sigma \] (3.115)


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or

\[ dp_v - dp_t = d(2H\sigma) \] (3.116)

Expanding the differential on the right side of eqn. (3.116) yields

\[ d(2H\sigma) = 2\sigma dH + 2H d\sigma \]
\[ = 2\sigma dH + 2H \frac{\partial \sigma}{\partial H} dH \] (3.117)

If one neglects the variation of surface tension with respect to curvature, and solves eqn. (3.116) for \( dp_t \), eqn. (3.111) can be rewritten

\[ -s_l dT + \nu_l dp_v - \nu_l 2\sigma dH = -s_v dT + \nu_v dp_v \] (3.118)

or

\[ dp_v - \frac{s_v - s_l}{\nu_v - \nu_l} dT = \frac{-2\nu_l \sigma}{\nu_v - \nu_l} dH \]
\[ d(p_v - p_{flat}) = \frac{-2\nu_l \sigma}{\nu_v - \nu_l} dH. \] (3.119)

Integrating from a flat interface \( (p_v - p_{flat} = 0, H = 0) \) to an arbitrarily curved one yields

\[ p_v = p_{flat} - \frac{2\nu_l \sigma H}{\nu_v - \nu_l} \] (3.121)

where it is generally understood that \( p_{flat} \) is the saturation pressure and the curvature term is a correction to that pressure. Eqn. (3.121) is more general than other
expressions with a Poynting correction factor for the curvature because liquid incompressibility and ideal gas behavior are not assumed in the above analysis. Regardless, for most practical situations the correction due to curvature is negligible. For example, a parahydrogen system at 20 K with a 1 mm spherical ullage results in a correction of only 0.07 Pa compared to the saturation pressure of 93414 Pa. Hence in the subsequent analysis, the curvature correction will be neglected and it will be assumed that at equilibrium

\[ p_v = p_{\text{sat}}(T). \]  

(3.122)

The analysis presented thus far in section 3.5 assumes equilibrium for the liquid-vapor-interfacial system. Mass transfer is inherently a non-equilibrium process and to describe this non-equilibrium behavior an additional constitutive equation involving the mass flux is needed. The form of this constitutive model has been the subject of much scholarly debate for more than a century. In what follows, a brief overview of the different constitutive models is presented.

For non equilibrium processes, continuity of temperature across a phase boundary is generally not assured. Huang and Joseph\textsuperscript{190} describe three possible temperature boundary conditions at the interface. The temperature can be continuous with the value given by the saturation temperature corresponding either the liquid or vapor temperature. Alternatively, the temperature can be discontinuous with the surface value given by the saturation temperature corresponding to the local pressure. In the stability analysis of Huang and Joseph,\textsuperscript{190} little difference was found among these
different interfacial boundary conditions.

Experimentally, conclusions regarding interfacial discontinuities have been mixed. Shankar and Deshpande\textsuperscript{191} used fixed thermocouple locations in their experimental study of liquid/vapor phase change processes. Their data suggested jumps do exist though it’s unclear whether their experimental setup was able to resolve steep thermal gradients near the interface. Ramamurthi et al.\textsuperscript{192} performed experiments with LN2 and observed no discrete change or discontinuity in temperatures at the interface. Hisatake et al.\textsuperscript{193} studied the evaporation of water in an open vessel. A thermocouple 0.127 mm in diameter measured a temperature profile across the liquid vapor interface. Steep gradients on either side of the interface were observed and the authors drew a continuous line through the data to represent the temperature profile.

The experiments by Ward and colleagues have consistently recorded temperature discontinuities across evaporating interfaces. Fang and Ward\textsuperscript{194} measured the temperature during steady state evaporation of liquid water in a hemispherical funnel. The thermocouple was only 25.4 $\mu$m in diameter and the authors claimed to have measured vapor-side temperatures within one mean free path of the interface. They found the vapor-side temperature to be larger than the liquid-side temperature by as much as 7.8 K. Again using a hemispherical funnel, Ward and Stanga\textsuperscript{195} noted the jump is greater for evaporation than for condensation and observed a uniform temperature layer (0.5 mm thick) below the interface which is indicative of some mixing process near the interface. Duan et al.\textsuperscript{196} carried out similar experiments using an elongated funnel and measured a temperature variation tangential to the interface.
which they suggested can drive Marangoni convection. Duan and Ward\textsuperscript{197} noted that the conductive flux on either side of the interface is too small to supply the necessary energy for phase change and suggest that a surface thermal capacity contribution or thermocapillary convection contribution be included in the interfacial energy balance. The preceding experiments by Ward and colleagues were carried out at relatively low pressures, on the order of a few hundred Pascals. McGaughey and Ward\textsuperscript{198} studied the temperature discontinuity at the surface of an evaporating droplet when the operating pressure was a few thousand Pascals. Their data suggests that as pressure increases, the temperature discontinuity across the interface decreases.

Ward and Fang\textsuperscript{199} used statistical rate theory (SRT) to derive a non-linear expression for the evaporative flux at an interface. SRT applies quantum mechanics and looks at the probability of a molecule transitioning from one bulk phase to the other. Fang and Ward\textsuperscript{200} tested their theory by substituting their experimentally determined mass flux and temperatures into their expression and solved for the corresponding vapor pressure. The agreement with the experimentally measured vapor pressure was acceptable.

Though agreement of the SRT expression with experimental data from Ward’s group has generally been good, Bond\textsuperscript{201} questions the completeness of the statistical rate theory equation since it doesn’t provide a corresponding energy flux relationship. Bond also notes that the SRT flux expression is essentially a non-linear version of one derived using irreversible thermodynamics (IRT). IRT applies the 2nd law of thermodynamics to the liquid-vapor-interfacial system to arrive at an entropy source at the
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interface. The form of the entropy source can be posited as in Juric and Tryggvason\textsuperscript{202} or rigorously derived using the methods of non equilibrium thermodynamics. Once the entropy source is known, it can be decomposed into force-flux pairs where the fluxes are assumed to be linear functions of the forces or driving potentials.

The fluxes are generally coupled and Kjelstrup and Bedeaux\textsuperscript{203} note that neglecting the coupling between heat and mass transfer at the interface is not justified. Bedeaux \textit{et al.}\textsuperscript{188} derived the force-flux pairs for an interfacial system assuming no singular mass density. Kovac\textsuperscript{204} extended this work by including the presence of multicomponent species. IRT is useful for identifying relevant force-flux pairs but not capable of deriving closed expressions. IRT relates the forces and fluxes through coupling coefficients which must be determined by some other means.

Bedeaux and Kjelstrup\textsuperscript{205} computed the coupling coefficients using Ward’s experimental data\textsuperscript{194} and not surprisingly obtained agreement with the experimental evaporation rate. Bornhorst and Hatsopoulos\textsuperscript{206} used kinetic theory to evaluate the coupling coefficients for a discontinuous liquid-vapor-interfacial system. Bedeaux \textit{et al.}\textsuperscript{207} found that in order for IRT to give consistent results with kinetic theory, the interfacial temperature should be taken as the temperature of the adjacent liquid.

Kinetic theory has often been used to derive expressions for the interfacial mass flux. In kinetic theory, the statistical behavior of a system of monatomic molecules is described by a distribution function, $f$, such that $f \, dc$ represents the fraction of molecules with velocity in the range $[c, c + dc]$. Neglecting the Knudsen layer in Fig.
3.3, the net condensation mass flux at the interface can be expressed as

\[ j = \int_{c_z < 0} \int \int mc_z f_v dc - \int_{c_z > 0} \int \int mc_z f_l dc \quad (3.123) \]

where \( m \) is the molecular mass and \( c_z \) is the molecular velocity in the direction of a unit vector pointing into the vapor. If the distribution function of the evaporating molecules and condensing molecules are known, eqn. (3.123) can then be used to evaluate the interfacial mass flux. Generally, one assumes that molecules leaving the liquid surface can be described with a Maxwellian distribution. Much work has been done in trying to describe the distribution function in the vapor. The often used Hertz Knudsen expression for interfacial mass flux assumes the vapor distribution function is Maxwellian as well. Schrage\textsuperscript{208} noted that during condensation, there must be a net molecular motion towards the interface and modified the Hertz Knudsen relationship.
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by assuming a translating Maxwellian distribution for the bulk vapor molecules. In his analysis, Schrage also used the concept of an evaporation or condensation coefficient. The condensation coefficient is typically defined as the fraction of vapor molecules incident to the interface that get captured by the liquid. The remainder get reflected back into the vapor phase. The evaporation coefficient is similarly defined though more complicated conceptually due to lack of a surface to reflect liquid molecules back into the bulk. At equilibrium the condensation and evaporation fluxes are equal which imply equality between the condensation and evaporation coefficients.

In the literature, measurements of the evaporation/condensation coefficient have been scattered. Maa\textsuperscript{209} experimentally determined the evaporation coefficient to be unity for several liquids. Eames \textit{et al.}\textsuperscript{210} reviewed data on the evaporation coefficient of water and noted a wide scatter between 0.01 - 1. Davis\textsuperscript{211} also noted the large variation in reported coefficients. Paul\textsuperscript{212} compiled a list of evaporation coefficients for a variety of fluids and found large differences in reported values. Marek and Straub\textsuperscript{213} noted that the condensation coefficient for water is generally higher than the evaporation coefficient and equality of the coefficients should not be assumed. Tanasawa\textsuperscript{214} reviewed the relevant kinetic theory literature with regard to interfacial mass flux expressions and commented that no theory has proved or disproved the assumption that the condensation and evaporation coefficients are equal during a net condensation or evaporation process. To complicate matters, the evaporation/condensation coefficients have often been used interchangeably with the accommodation coefficient, which Bond\textsuperscript{201} defines as being 0 or 1 depending on whether reflecting vapor molecules
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Notwithstanding the uncertainty in the values of the condensation or evaporation coefficient, equality is often assumed which results in the Schrage mass flux expression given by

\[ j = \frac{2\sigma}{2 - \sigma} \left( \frac{M_w}{2\pi R} \right)^{1/2} \left( \frac{p_v}{\sqrt{T_v}} - \frac{p_l}{\sqrt{T_l}} \right) \]  

(3.124)

where, in this context, \( \sigma \) is the evaporation or condensation coefficient. Barrett and Clement\textsuperscript{215} point out that Schrage’s simple mass flux relationship violates strict energy and momentum conservation at the interface though this lack of conservation has been disputed by Bond.\textsuperscript{201} Schrage\textsuperscript{208} later modified his original approach by assuming a perturbed distribution function for the condensing vapor molecules. The perturbed distribution function was used to describe vapor molecules in the Knudsen layer where collisions with evaporating molecules could change the bulk vapor distribution function. Panzarella\textsuperscript{216} applied Schrage’s modified mass flux expression to film boiling and noted that Schrage’s modified equation captures asymmetries between condensation and evaporative processes. Ytrehus\textsuperscript{217} also showed that basic asymmetries exist between evaporation and condensation.

Instead of assuming a form of the vapor distribution function, a number of investigators have solved for the distribution function by taking moments of the Boltzmann equation,\textsuperscript{218,219} by solving a linearized version of the Boltzmann equation,\textsuperscript{220–222} or by numerically solving the Boltzmann equation.\textsuperscript{223} Typically these analyses suggest a temperature jump across the Knudsen layer exists even in the continuum limit as
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The kinetic theory approach to interfacial mass transfer has given way in recent years to molecular dynamics (MD) simulations. In a MD analysis, a molecular potential is assumed and Newton’s laws of motion are solved for an ensemble of molecules subject to certain constraints. Because of the computational overhead associated with a MD simulation, these analyses are often restricted to small computational domains for brief periods of time. Often MD simulations have been used to either aid in the theoretical understanding of interfacial mass transfer or to examine the assumptions in the approaches described above. Meland et al.\textsuperscript{225} performed a MD simulation on a system undergoing phase change and found that the evaporation and condensation coefficients are not equal outside of equilibrium. Ishiyama et al.\textsuperscript{226} observed that at low temperatures evaporating molecules have a half Maxwellian distribution thus supporting the boundary condition in the kinetic theory analyses. Matsumoto et al.\textsuperscript{227} performed an MD simulation to show that few vapor molecules get reflected and that condensing molecules can drive liquid molecules into the bulk vapor. Xu et al.\textsuperscript{228} used MD to show that linearity of the force-flux pairs in IRT is valid even at moderate temperature gradients. Rosjorde et al.\textsuperscript{229} using MD simulations to provide closure for IRT coupling coefficients.

While MD simulations show promise at revealing the fine scale behavior near an interface, these simulations rely on a assumed potential. As computational resources improve, perhaps the approach suggested by Sandler\textsuperscript{230} will yield further insight. Sandler suggests computing the potential using quantum mechanics and then applying
this computed potential to a MD simulation.

The above discussion provides a brief overview of various approaches to determine a constitutive model for the interfacial mass flux. In this dissertation, Schrage’s model will be used, equality of the condensation and evaporation coefficients will be assumed, these coefficients will be assumed constant, and continuity of temperature across the interface will be enforced, i.e.

\[ T_l = T_v = T_s. \]  

(3.125)

Finally, it will be assumed that the mass transfer processes are close enough to equilibrium that

\[ p_l \approx p_{sat}. \]  

(3.126)

These assumptions lead to the following constitutive relationship

\[ j = \frac{2\sigma}{2 - \sigma} \left(\frac{M_w}{2\pi RT}\right)^{1/2} (p_v - p_{sat}). \]  

(3.127)
In order to solve the system of equations derived in Chapter 3, several models are developed with varying degrees of complexity. First, a homogeneous thermodynamic model will be developed whereby the state of the liquid-vapor system is confined to the saturated PVT surface during a self-pressurization or pressure control process. Next, a multizone model is formulated which relaxes the assumption of homogeneity within the tank. The results of these models will be compared against each other and against experimental data in subsequent chapters.

Consider a spherical tank partially full of liquid subjected to external heat loads, $\dot{Q}_{wv}$ and $\dot{Q}_{wl}$, as shown in Fig. 4.1. The tank is an open system. During a typical pressure control process, fluid is withdrawn from the liquid phase and pumped through a heat exchanger to subcool it before it reenters the tank as a subcooled liquid jet. The tank, with corresponding plumbing, is a closed system so the rate of mass leaving the tank equals the rate of mass entering the tank through the jet nozzle.

Integrating the continuity equation in each of the bulk phases around their re-
Figure 4.1: Sketch of a liquid-vapor system with heat and mass entering or leaving the system.

Spective control volumes yields

\[
\frac{d}{dt} \left[ \int_{V_v} \rho_v \, dV \right] + \int_I \rho_v (v_v - v_s) \cdot \hat{n} \, dS = 0 \\
\frac{d}{dt} \left[ \int_{V_l} \rho_l \, dV \right] - \int_I \rho_l (v_l - v_s) \cdot \hat{n} \, dS + \int_{\text{out}} \rho_l v_1 \cdot n \, dS - \int_{\text{in}} \rho_l v_1 \cdot n \, dS = 0.
\]

where the surface integral over \( I \) is performed over the interfacial area, the interfacial normal, \( \hat{n} \), points into the liquid, and the normals to the outlet and inlet are outwardly
and inwardly pointing respectively. With the following definitions:

\[
\overline{\rho}_v = \frac{1}{V_v} \int_{V_v} \rho_v \, dV \quad (4.3)
\]

\[
\overline{\rho}_l = \frac{1}{V_l} \int_{V_l} \rho_l \, dV \quad (4.4)
\]

\[
j \equiv \int_I \rho_l (\mathbf{v}_l - \mathbf{v}_s) \cdot \hat{n} \, dS = \int_I \rho_l (\mathbf{v}_v - \mathbf{v}_s) \cdot \hat{n} \, dS \quad (4.5)
\]

\[
\dot{m} = \int_{\text{out}} \rho_l \mathbf{v}_l \cdot \mathbf{n} \, dS = \int_{\text{in}} \rho_l \mathbf{v}_l \cdot \mathbf{n} \, dS, \quad (4.6)
\]

one has

\[
\frac{d\overline{\rho}_v}{dt} = - \int_I j \, dS \quad (4.7)
\]

\[
\frac{d\overline{\rho}_l}{dt} = \int_I j \, dS. \quad (4.8)
\]

Summing eqns. (4.7) and (4.8) yields,

\[
\frac{d}{dt} (\overline{\rho}_v V_v + \overline{\rho}_l V_l) = 0. \quad (4.9)
\]

which implies that even though mass exchange may occur between the bulk phases and mass may be entering or leaving the tank, the total mass inside the tank is constant. Integrating eqn. (4.9) in time leads to:

\[
\overline{\rho}_v V_v + \overline{\rho}_l V_l = \overline{\rho}_{v,o} V_{v,o} + \overline{\rho}_{l,o} V_{l,o} \quad (4.10)
\]
where the subscript, \( o \), denotes some initial time. Since the total tank volume, \( V_t \), is comprised of liquid and vapor volumes,

\[
V_t = V_l + V_v. \tag{4.11}
\]

Using eqn. (4.10) and assuming the tank is rigid, one can derive an explicit equation for the vapor volume,

\[
V_v(p_v, p_l) = V_l \frac{p_{l,o} - p_l}{p_v - p_l} + V_v \frac{p_{v,o} - p_{l,o}}{p_v - p_l}. \tag{4.12}
\]

It will be convenient to use the enthalpy form of the energy balance for the bulk phases. Taking the dot product of the momentum equation with the bulk phase velocity, subtracting the result from the total energy balance (eqn. (3.84)), then neglecting viscous dissipation and potential energy contributions yields

\[
\frac{\partial}{\partial t} (\rho u) + \nabla \cdot (\rho uv) = -\nabla \cdot \mathbf{J}_q - p \nabla \cdot \mathbf{v} \tag{4.13}
\]

for the balance of internal energy. Substituting

\[
\rho u = \rho h - p \tag{4.14}
\]

leads to

\[
\frac{\partial}{\partial t} (\rho h) + \nabla \cdot (\rho hv) = -\nabla \cdot \mathbf{J}_q + \frac{dp}{dt}. \tag{4.15}
\]
Integrating around each bulk phase volume as before yields

\[
\frac{d}{dt} \left[ \int_{V_i} \rho_i h_i dV \right] - \int_{I} \rho_i h_i (v_1 - v_s) \cdot \hat{n} dS + \int_{out} \rho_i h_i v_1 \cdot \mathbf{n} dS - \int_{in} \rho_i h_i v_1 \cdot \mathbf{n} dS =
\]

\[
- \int_{w} J_{q,l} \cdot \mathbf{n} dS + \int_{I} J_{q,v} \cdot \hat{n} dS - \int_{out} J_{q,l} \cdot \mathbf{n} dS + \int_{in} J_{q,v} \cdot \hat{n} dS + \int_{V_i} \frac{d}{dt} \frac{dV}{dV} \]

(4.17)

where the normals to the wall, \( w \), are outwardly pointing. One can take a mass-average of the bulk phase enthalpies,

\[
\overline{h_i} = \frac{1}{\rho_i V_i} \int_{V_i} \rho_i h_i dV \quad i = l, v.
\]

(4.18)

One can also define \( \dot{Q}_{wl} \) and \( \dot{Q}_{wv} \) as the amount of heat entering the bulk liquid and vapor phases through the wall,

\[
\dot{Q}_{wl} = - \int_{w} J_{q,l} \cdot \mathbf{n} dS
\]

(4.19)

\[
\dot{Q}_{wv} = - \int_{w} J_{q,v} \cdot \mathbf{n} dS
\]

(4.20)

and the amount of heat leaving the vapor phase and entering the liquid phase through
the interface as:

\[
\dot{Q}_{il} = \int_I \mathbf{J}_{q,l} \cdot \hat{n} \, dS
\]

(4.21)

\[
\dot{Q}_{iv} = \int_I \mathbf{J}_{q,v} \cdot \hat{n} \, dS.
\]

(4.22)

The diffusive heat flux across the tank inlet and outlet is assumed small relative to the convective contribution. Hence,

\[
\int_{\text{out}} \mathbf{J}_{q,l} \cdot \mathbf{n} \, dS \approx 0 \quad (4.23)
\]

\[
\int_{\text{in}} \mathbf{J}_{q,l} \cdot \mathbf{n} \, dS \approx 0. \quad (4.24)
\]

If the liquid enthalpy over the cross-section of the tank inlet and outlet is assumed constant, then

\[
\int_{\text{in}} \rho_l h_l (\mathbf{v}_l \cdot \mathbf{n}) \, dS = \dot{m} h_{il}^{\text{in}} \quad (4.25)
\]

\[
\int_{\text{out}} \rho_l h_l (\mathbf{v}_l \cdot \mathbf{n}) \, dS = \dot{m} h_{il}^{\text{out}}. \quad (4.26)
\]

Finally, for this flat interface configuration:

\[
p_v = p_l = p. \quad (4.27)
\]

The tank pressure can be decomposed into a mean component and a fluctuation about
the mean:

\[ p = \bar{p}(t) + p'(x, t). \]  

(4.28)

For \( p' \ll \bar{p} \),

\[ \int_V \frac{dp}{dt} dV \approx \frac{d\bar{p}}{dt} V. \]  

(4.29)

Hence,

\[ \frac{d}{dt}(\rho v h_v V_v) + \int_I j h_v dS = \dot{Q}_{lv} - \dot{Q}_{iv} + \frac{d\bar{p}}{dt} V_v \]  

(4.30)

\[ \frac{d}{dt}(\rho_l h_l V_l) - \int_I j h_l dS = \dot{Q}_{wl} + \dot{Q}_{il} + \frac{d\bar{p}}{dt} V_l - \dot{m} \left( h_{l\text{out}} - h_{l\text{in}} \right). \]  

(4.31)

4.1 Thermodynamic Model

In this model, the temperature in the tank is assumed to be uniform and li-

quid/vapor thermodynamic quantities are assumed spatially invariant and at satura-
tion within each bulk phase. This is equivalent to

\[ T = T_{\text{sat}} \]  

\[ \rho_v = \rho_{v}^{\text{sat}}(T_{\text{sat}}) \]  

\[ \rho_l = \rho_{l}^{\text{sat}}(T_{\text{sat}}) \]  

\[ h_v = h_{v}^{\text{sat}}(T_{\text{sat}}) \]  

\[ h_l = h_{l}^{\text{sat}}(T_{\text{sat}}) \]  

Defining the evaporation rate across the interface as

\[ M = -\int_I j \, dS, \]  

one has

\[ \frac{d}{dt}(\rho_{v}^{\text{sat}} V_v) = M \]  

\[ \frac{d}{dt}(\rho_{l}^{\text{sat}} V_l) = -M. \]  

Similar to before, the vapor volume can be expressed as

\[ V_v(\rho_v^{\text{sat}}, \rho_l^{\text{sat}}) = V_l \frac{\rho_{l,0}^{\text{sat}} - \rho_{l}^{\text{sat}}}{\rho_v^{\text{sat}} - \rho_l^{\text{sat}}} + V_{v,o} \frac{\rho_v^{\text{sat}} - \rho_{l,0}^{\text{sat}}}{\rho_v^{\text{sat}} - \rho_l^{\text{sat}}}. \]
4.1 THERMODYNAMIC MODEL

MODEL DEVELOPMENT

Adding eqns. (4.30) and (4.31) and substituting in the saturation quantities described above yields:

\[
\frac{d}{dt} \left( \rho_v^{sat} h_v^{sat} V_v + \rho_i^{sat} h_i^{sat} V_i \right) + \int_I j(h_v - h_i) dS = \\
\dot{Q}_w + (\dot{Q}_d - \dot{Q}_w) + \frac{d p_{sat}}{dt} V_t - \dot{m} \left( h_i^{out} - h_i^{in} \right) \tag{4.42}
\]

where the net heat entering the tank

\[
\dot{Q}_w = \dot{Q}_{wl} + \dot{Q}_{ww}. \tag{4.43}
\]

Neglecting the viscous work terms at the interface and the energy contribution due to expansion/contraction of the interface, the integral form of eqn. (3.88) reduces to

\[
\int_I j(h_v - h_i) dS = \dot{Q}_d - \dot{Q}_w. \tag{4.44}
\]

Hence,

\[
\frac{d}{dt} \left( \rho_v^{sat} h_v^{sat} V_v + \rho_i^{sat} h_i^{sat} V_i \right) = \dot{Q}_w + \frac{d p_{sat}}{dt} V_t - \dot{m} \left( h_i^{out} - h_i^{in} \right). \tag{4.45}
\]

Carrying out the differentiation and making use of eqns. (4.39) - (4.40) leads to

\[
\rho_v^{sat} V_v \frac{dh_v^{sat}}{dt} + \rho_i^{sat} V_i \frac{dh_i^{sat}}{dt} + M \left( h_i^{sat} - h_i^{sat} \right) - \frac{d p_{sat}}{dt} V_t = \dot{Q}_w - \dot{m} \left( h_i^{out} - h_i^{in} \right). \tag{4.46}
\]
4.2 Multizone Model

The difference in liquid and vapor enthalpies at the saturation temperature is the latent heat, $L$. Expanding the time derivatives using the chain rule, one has

$$\frac{dT_{sat}}{dt} \left\{ \rho_v^{sat} V_v \frac{dh_v^{sat}}{dT_{sat}} + \rho_l^{sat} V_l \frac{dh_l^{sat}}{dT_{sat}} + \frac{d(\rho_v^{sat} V_v)}{dT_{sat}} L - \frac{dp_{sat}}{dT_{sat}} V_i \right\} = \dot{Q}_w - \dot{m} (h_{l_{out}} - h_{l_{in}}).$$

Equation (4.47) represents an evolution equation for the saturation temperature $T_{sat}$.

All derivatives with respect to temperature can be evaluated explicitly using eqns. (4.33)-(4.37) and (4.41). Once the saturation temperature is known, the tank pressure can be computed from eqn. (4.33).

4.2 Multizone Model

In a multizone formulation, uniformity within each bulk phase is still assumed, but the assumption that the phases are at the same temperature, $T_{sat}$, is relaxed. The tank is partitioned into three zones: a liquid zone, a vapor zone, and a thin massless interfacial zone at temperatures $T_l$, $T_v$, and $T_i$ respectively. The liquid phase is assumed incompressible and the vapor is treated as a compressible gas whose pressure is given by:

$$p = p(\rho_v, T_v)$$

(4.48)
Assuming uniformity within each bulk phase is equivalent to:

\[
\bar{\rho}_v = \rho_v \\
\bar{\rho}_l = \rho_l \\
\bar{h}_v = h_v \\
\bar{h}_l = h_l.
\]

(4.49)  \hspace{1cm} (4.50)  \hspace{1cm} (4.51)  \hspace{1cm} (4.52)

The integrated continuity equation in the liquid is given by:

\[
\frac{d}{dt}(\rho_l V_l) = -M \\
\rho_l \frac{dV_l}{dt} = -M \\
-\frac{\rho_l}{\rho_v} \frac{dV_v}{dt} = -M
\]

(4.53)

which implies that

\[
\frac{dV_v}{dt} = \frac{M}{\rho_v}.
\]

(4.54)

Liquid incompressibility and the volume constraint were used to arrive at eqn. (4.54).

The continuity equation in the vapor is

\[
\frac{d}{dt}(\rho_v V_v) = M \\
\rho_v \frac{dV_v}{dt} + V_v \frac{d\rho_v}{dt} = M \\
\rho_v \frac{M}{\rho_v} + V_v \frac{d\rho_v}{dt} = M
\]

(4.55)  \hspace{1cm} (4.56)  \hspace{1cm} (4.57)
which leads to

\[
\frac{d\rho_v}{dt} = \frac{M}{V_v} \left( 1 - \frac{\rho_v}{\rho_l} \right). \tag{4.58}
\]

Uniformity within each bulk phases simplifies the bulk phase energy balances to

\[
\frac{d}{dt}(\rho_l h_l V_l) + M h_l^i = -\dot{m} \left( h_l^{\text{out}} - h_l^{\text{in}} \right) + \dot{Q}_{\text{w}l} + \dot{Q}_{\text{i}l} + V_l \frac{dp_v}{dt} \tag{4.59}
\]

\[
\frac{d}{dt}(\rho_v h_v V_v) - M h_v^i = \dot{Q}_{\text{w}v} - \dot{Q}_{\text{i}v} + V_v \frac{dp_v}{dt}. \tag{4.60}
\]

The enthalpy of the bulk phases is assumed to behave as

\[
h_v = h_{v,0} + c_{p,v}(T_v - T_{v,0}) \tag{4.61}
\]

\[
h_l = h_{l,0} + c_{p,l}(T_l - T_{l,0}). \tag{4.62}
\]

Substituting these expressions into the energy balances, carrying out the differentiation, and rearranging terms leads to

\[
\rho_l c_{p,l} V_l \frac{dT_l}{dt} = M c_{p,l}(T_l - T_{l,0}) - \dot{m} c_{p,l}(T_l - T_{\text{in}}) + \dot{Q}_{\text{w}l} + \dot{Q}_{\text{i}l} + V_l \frac{dp_v}{dt} \tag{4.63}
\]

\[
\rho_v c_{p,v} V_v \frac{dT_v}{dt} = M c_{p,v}(T_v^i - T_{v,0}) + \dot{Q}_{\text{w}v} - \dot{Q}_{\text{i}v} + V_v \frac{dp_v}{dt}. \tag{4.64}
\]

where once again, liquid incompressibility has been invoked. The equation of state can be used to explicitly evaluate the pressure derivative. That is,

\[
\frac{dp_v}{dt} = \frac{\partial p_v}{\partial \rho_v} \frac{d\rho_v}{dt} + \frac{\partial p_v}{\partial T_v} \frac{dT_v}{dt}. \tag{4.65}
\]
Substituting this expression into the energy balances yields:

\[ \rho c_{p,l} V_l \frac{dT_l}{dt} = M c_{p,l} (T_l - T_i) - \dot{m} c_{p,l} (T_l - T_{in}) + \dot{Q}_{wl} + \dot{Q}_{lv} + \dot{V}_l \left( \frac{\partial p_v}{\partial \rho} \frac{d\rho}{dt} + \frac{\partial p_v}{\partial T} \frac{dT_v}{dt} \right) \]

\[ \left\{ \rho_v c_{p,v} + \frac{\partial p_v}{\partial T} \right\} V_v \frac{dT_v}{dt} = M c_{p,v} (T_v - T_i) + \dot{Q}_{wv} - \dot{Q}_{iv} + \dot{V}_v \frac{\partial p_v}{\partial \rho} \frac{d\rho}{dt}. \]

(4.66)

(4.67)

In order to solve these energy equations, expressions for the interzonal energy and mass exchange terms are required. Assuming spatial uniformity across the interface, the energy jump condition reduces to

\[ M = -\frac{\dot{Q}_{vl} - \dot{Q}_{wv}}{h_v - h_i}. \]

(4.68)

where the difference in enthalpies across the interface is assumed to be equal to the latent heat, \( L \). The interfacial temperature, \( T_i \), can be found by equating the kinetic mass flux and diffusive mass transfer rate at the interface and implicitly solving for \( T_i \):

\[ \frac{2\sigma}{2 - \sigma} A_i \left( \frac{M_w}{2\pi RT_i} \right)^{1/2} (p_{sat}(T_i) - p_v) = \frac{\dot{Q}_{vl}(T_i, T_l) - \dot{Q}_{wv}(T_i, T_v)}{L}. \]

(4.69)
The interfacial heat powers are evaluated using simple correlations which are problem specific and will be described later:

\[ \dot{Q}_{il} = h_{il} A_i (T_i - T_l) \]  \hspace{1cm} (4.70)

\[ \dot{Q}_{iv} = h_{iv} A_i (T_v - T_i). \]  \hspace{1cm} (4.71)

Once \( T_i \) is known, the heat powers are updated and the mass transfer rate through the interface can be computed using the left side of eqn. (4.69). Details regarding the numerical implementation will be presented in the next chapter.
In the previous chapter, the homogeneous and zonal models were derived. For clarity, models were derived for a pure two-phase system. Extension to multicomponent two-phase systems is described further in Appendix C. Model predictions will be validated using the experimental data presented in Chapter 2. The implementation of these models and their respective solution algorithms will be described in this chapter.

5.1 Homogeneous Model

The evolution equation for saturation temperature for a two-phase multicomponent ullage is given by eqn. (C.29). In the ground experiment, the thermal capacity of the walls is not insignificant and should be accounted for in the models. To account for the wall and other solid features in the experiment (i.e. heaters, nozzles,
insulation), the following generic energy equation for a solid region is employed

$$\frac{d}{dt}(\rho hV) = \dot{Q}_{in} - \dot{Q}_{out}. \quad (5.1)$$

Since the mass of the solid regions is constant, assuming constant specific heat, yields

$$\rho V c_p \frac{dT}{dt} = \dot{Q}_{in} - \dot{Q}_{out}. \quad (5.2)$$

After invoking the homogeneous assumption \((T = T_{sat})\), the evolution equation for saturation temperature becomes

$$\frac{dT_{sat}}{dt} \left\{ \rho_{li} V_i \frac{dh_{li}^{sat}}{dT_{sat}} + \rho_{vi} V_v \frac{dh_{vi}^{sat}}{dT_{sat}} + \rho_g V_g c_{pg} + \sum_{i=\text{solid}} \rho_i V_i c_{pi} + \frac{d(\rho_v^{sat} V_v)}{dT_{sat}} L - V_t \frac{dp}{dT_{sat}} \right\} = \dot{Q}_w + \dot{m} \left( h_{li}^{in} - h_{li}^{sat} \right). \quad (5.3)$$

Since this represents a system level energy balance, all the inter-region heat transfer mechanisms, \(\dot{Q}_{in}\) and \(\dot{Q}_{out}\) sum to zero. The only energy load on the system is \(\dot{Q}_w\), the load that is externally applied.

Considering the right side of the energy balance, the applied load, \(\dot{Q}_w\), is user specified. The sub-cooled liquid enthalpy is assumed to be of the form

$$h_{li}^{in} = h_{li}^{sat} + c_p \left( T_{jet} - T_{sat} \right). \quad (5.4)$$
5.1 HOMOGENEOUS MODEL IMPLEMENTATION

Hence,

\[ \dot{m} \left( h_{in}^l - h_{sat}^l \right) = \dot{m} c_p \left( T_{jet} - T_{sat} \right). \]  

(5.5)

On the left side of the equation, the functional relationship between \( T_{sat} \) and the saturation densities and enthalpies are known and provided in Appendix A for reference.

With \( \rho_{sat}^v \) known and an expression for \( V_v \) (eqn. (4.41)), \( \frac{d(\rho_{sat}^v V_v)}{dT_{sat}} \) can be explicitly evaluated.

The pressure derivative can be expanded

\[ \frac{dp}{dT_{sat}} = \frac{dp}{dT_{sat}} + \frac{dp_g}{dT_{sat}}. \]  

(5.6)

The saturation pressure is given by the liquid-vapor saturation curve and so the above derivative can be evaluated explicitly. To evaluate \( \frac{dp_g}{dT_{sat}} \), the non-condensable gas is assumed to behave ideally at \( T_{sat} \),

\[ p_g = \frac{m_g R_g T_{sat}}{V_v}. \]  

(5.7)

Since the mass of the gas in the ullage is constant,

\[ \frac{dp_g}{dT_{sat}} = m_g R_g \frac{dV_v}{V_v} - m_g R_g T_{sat} \frac{dV_v}{V_v^2} \frac{dT_{sat}}{dT_{sat}} \]  

\[ = \frac{m_g R_g}{V_v} - \frac{m_g R_g T_{sat}}{V_v^2} \left( \frac{\partial V_v}{\partial \rho_{sat}^v} \frac{d\rho_{sat}^v}{dT_{sat}} + \frac{\partial V_v}{\partial \rho_{sat}^l} \frac{d\rho_{sat}^l}{dT_{sat}} \right). \]  

(5.8)

These derivatives can be evaluated explicitly using property functions (see Appendix 140.
Algorithmically, a forward Euler time stepping routine is employed:

\[
T_{\text{sat}}^{n+1} = T_{\text{sat}}^n + \Delta t \left( \frac{dT_{\text{sat}}}{dt} \right)^n
\]  

(5.9)

where

\[
\frac{dT_{\text{sat}}}{dt} = \frac{\dot{Q}_w + n m c_p(T_{\text{j}} - T_{\text{sat}})}{\rho_l V_{\text{sat}} \frac{dh_{\text{sat}}}{dT_{\text{sat}}} + \rho_v V_{\text{sat}} \frac{dh_{\text{sat}}}{dT_{\text{sat}}} + \rho_g V_{\text{sat}} c_p + \sum \rho_i V_i c_p + \frac{d \rho_{\text{sat}} V_{\text{sat}}}{dT_{\text{sat}}} L - V_{\text{sat}} \frac{dp}{dT_{\text{sat}}}}.
\]  

(5.10)

When the sub-cooled jet mixer is inactive, the \(n m c_p(T_{\text{j}} - T_{\text{sat}})\) term is zero. When the mixer is on, \(n\) is computed from the user specified average jet velocity and \(T_{\text{j}}\) is computed using a heat exchanger model described in Appendix B. At every time step, after evolving the saturation temperature, the ullage pressure can be updated according to:

\[
p^{n+1} = p_{\text{sat}}(T_{\text{sat}}^{n+1}) + \frac{m_g R_g T_{\text{sat}}^{n+1}}{V_{\text{v}}(\rho_{\text{v}}(T_{\text{sat}}^{n+1}), \rho(T_{\text{sat}}^{n+1}))}.
\]  

(5.11)

5.2 Zonal Model

In the multizone model, homogeneity within each phase is still assumed but the assumption that the entire liquid, vapor, wall system is at the same temperature, \(T_{\text{sat}}\), is relaxed.

In the solid phases of the tank system (i.e. the acrylic wall, the foam insulation, and the copper heater rings), a 2D-axisymmetric finite element model is developed.
5.2 ZONAL MODEL IMPLEMENTATION

to simulate the conduction heat transfer through these regions. The finite element model is coupled to the evolution equations in the bulk liquid and vapor phases through appropriate use of thermal boundary conditions, which will be described below.

The acrylic wall, foam insulation, and copper heaters are discretized into linear triangular elements using GMSH, a open-source grid generator. A typical computational grid is shown in Fig. 5.1. Following the Galerkin approach, the residual integral for an axisymmetric heat conduction problem is:

\[- \int_V \left[ \frac{k}{r} \frac{\partial}{\partial r} \left( r \frac{\partial T}{\partial r} \right) + k \frac{\partial^2 T}{\partial z^2} + \dot{Q} - \rho c_p \frac{\partial T}{\partial t} \right] dV = 0. \tag{5.12}\]

Writing the vector of shape functions, \(\mathbf{N}\), in terms of area coordinates \(L_1\) and \(L_2\) yields:

\[
\mathbf{N} = \begin{bmatrix} L_1 \\ L_2 \\ 1 - L_1 - L_2 \end{bmatrix} \tag{5.13}
\]

where the area coordinates are shown in Fig. 5.2. Carrying out the differentiation in eqn. (5.12) and rearranging terms results in:

\[- \int_V \left[ \frac{k}{r} \frac{\partial}{\partial r} \left( \mathbf{N}_r \frac{\partial T}{\partial r} \right) + k \frac{\partial}{\partial z} \left( \mathbf{N} \frac{\partial T}{\partial z} \right) \right] dV + \int_V \left[ \frac{\partial \mathbf{N}}{\partial r} \frac{\partial T}{\partial r} + \frac{\partial \mathbf{N}}{\partial z} \frac{\partial T}{\partial z} \right] dV - \int_V \dot{\mathbf{N}} \dot{Q} dV + \int_V \mathbf{N} \rho c_p \frac{\partial T}{\partial t} dV = 0. \tag{5.14}\]

In carrying out the above differentiation, the conductivity was assumed spatially
Figure 5.1: Finite element mesh of wall, heaters, and foam insulation.
constant within each element. The first integral in eqn. (5.14) is the interelement contribution and can be transformed into a surface integral using Gauss’s theorem,

\[- \int_V \left[ \frac{k}{r} \frac{\partial}{\partial r} \left( N_r \frac{\partial T}{\partial r} \right) + k \frac{\partial}{\partial z} \left( N_z \frac{\partial T}{\partial z} \right) \right] dV = - \int N k \frac{\partial T}{\partial n} dA \quad (5.15)\]

where \( n \) is the outwardly pointing normal to the element boundary. To evaluate the conduction integrals, one can transform the volume integral into a surface integral by noting that

\[\int dV = \int 2\pi r dA. \quad (5.16)\]

Hence,

\[\int_V k \left[ \frac{\partial N}{\partial r} \frac{\partial T}{\partial r} + \frac{\partial N}{\partial z} \frac{\partial T}{\partial z} \right] dV = 2\pi \int \left( \frac{\partial N}{\partial r} \frac{\partial T}{\partial r} + \frac{\partial N}{\partial z} \frac{\partial T}{\partial z} \right) r dA \quad (5.17)\]

\[= 2\pi \int_0^{1-L_2} \int_0^{1-L_2} \left( \frac{\partial N}{\partial r} \frac{\partial T}{\partial r} + \frac{\partial N}{\partial z} \frac{\partial T}{\partial z} \right) r |J| dL_1 dL_2. \quad (5.18)\]

The last equality in the above equation follows from transforming an integral over the area, \( dA \), to an integral over \( dL_1 dL_2 \) of the canonical linear triangular element.

Noting that

\[ T = NT \quad (5.19)\]
where $\mathbf{T}$ is the vector of nodal temperatures, allows one to write

$$
\int_V k \left[ \frac{\partial \mathbf{N}}{\partial r} \frac{\partial \mathbf{T}}{\partial r} + \frac{\partial \mathbf{N}}{\partial z} \frac{\partial \mathbf{T}}{\partial z} \right] dV = 2\pi \int_0^1 \int_0^{1-L_2} \left( \frac{\partial \mathbf{N}}{\partial r} \frac{\partial \mathbf{N}^T}{\partial r} + \frac{\partial \mathbf{N}}{\partial z} \frac{\partial \mathbf{N}^T}{\partial z} \right) r|J| dL_1 dL_2 \mathbf{T}.
$$

(5.20)

In the above integrand, the Jacobian of the transformation is defined as

$$
J = \begin{bmatrix}
\sum_{i=1}^3 Z_i \frac{\partial N_i}{\partial L_1} & \sum_{i=1}^3 R_i \frac{\partial N_i}{\partial L_1} \\
\sum_{i=1}^3 Z_i \frac{\partial N_i}{\partial L_2} & \sum_{i=1}^3 R_i \frac{\partial N_i}{\partial L_2}
\end{bmatrix}
$$

(5.21)

where $(Z_i, R_i)$ are the nodal coordinates and $dN/dL_1$, $dN/dL_2$ can be computed explicitly from eqn. (5.13).
Gradients of the shape functions are computed from
\[
\begin{bmatrix}
\frac{\partial N}{\partial z} \\
\frac{\partial N}{\partial r}
\end{bmatrix} = J^{-1} \begin{bmatrix}
\frac{\partial N}{\partial L_1} \\
\frac{\partial N}{\partial L_2}
\end{bmatrix},
\] (5.22)

Finally,
\[
r = \sum_{i=1}^{3} R_i N_i.
\] (5.23)

The integral is of the form
\[
\int_{0}^{1} \int_{0}^{1-L_2} g(L_1, L_2) \, dL_1 \, dL_2
\] (5.24)

where
\[
g(L_1, L_2) = 2\pi \left( \frac{\partial N}{\partial r} \frac{\partial N^T}{\partial r} + \frac{\partial N}{\partial z} \frac{\partial N^T}{\partial z} \right) r |J|.
\] (5.25)

Integration is carried out using Gaussian quadrature,
\[
\int_{0}^{1} \int_{0}^{1-L_2} g(L_1, L_2) \, dL_1 \, dL_2 = \sum_{i=1}^{\text{N pts}} g(L_{1,i}, L_{2,i}) W_i.
\] (5.26)

The integration points and weights are listed in Table 5.1. The digits in Table 5.1 and Table 5.2 are all significant and required for accurate computation of the numerical integration.
5.2 ZONAL MODEL IMPLEMENTATION

<table>
<thead>
<tr>
<th>$L_{1,i}$</th>
<th>$L_{2,i}$</th>
<th>$2 \cdot W_i$</th>
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<td>0.22500000000000</td>
</tr>
<tr>
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</tr>
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</tr>
<tr>
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<td>0.470142064105115</td>
<td>0.132394152788506</td>
</tr>
</tbody>
</table>

Table 5.1: Integration points and weights for Gaussian quadrature over a triangular element.\(^{232}\)

The volumetric heat source integral is evaluated similarly:

\[
- \int \mathbf{N} \dot{Q} \, dV = -2\pi \int_0^1 \int_0^{1-L_2} \mathbf{N} \dot{Q} r |J| dL_1 dL_2. \tag{5.27}
\]

$\dot{Q}$ is zero in all solid regions except within the active heater.

The transient term is evaluated using the consistent approximation. That is,

\[
\frac{\partial T}{\partial t} = \mathbf{N}^T \dot{T}. \tag{5.28}
\]

The integral becomes:

\[
\int \mathbf{N} \rho c_p \frac{\partial T}{\partial t} \, dV = 2\pi \rho c_p \int \mathbf{N} \frac{\partial T}{\partial t} r \, dA \tag{5.29}
\]

\[
= 2\pi \rho c_p \left[ \int_0^1 \int_0^{1-L_2} \mathbf{N}^T r |J| dL_1 dL_2 \right] \dot{T}. \tag{5.30}
\]

The density and specific heat were assumed constant over each element. Defining the
5.2 ZONAL MODEL IMPLEMENTATION

elemental capacitance matrix, $C_E$, as

$$C_E = 2\pi \rho C_p \left[ \int_0^1 \int_0^{1-L_2} N N^T r |J| dL_1 dL_2 \right], \quad (5.31)$$

the elemental stiffness matrix, $K_E$ as

$$K_E = 2\pi k \left[ \int_0^1 \int_0^{1-L_2} \left( \frac{\partial N}{\partial r} \frac{\partial N^T}{\partial r} + \frac{\partial N}{\partial z} \frac{\partial N^T}{\partial z} \right) r |J| dL_1 dL_2 \right], \quad (5.32)$$

and the elemental force vector, $F_E$, as

$$F_E = 2\pi \int_0^1 \int_0^{1-L_2} N \dot{Q} r |J| dL_1 dL_2, \quad (5.33)$$

allows one to write the residual equation as

$$- \int N k \frac{\partial T}{\partial n} dA + K_E T - F_E + C_E \dot{T} = 0 \quad (5.34)$$

Three types of boundary conditions are required in the analysis: Dirichlet, Neumann, and mixed conditions. Over the exterior boundary of the foam insulation and over the wetted and non-wetted regions of the interior wall, mixed boundary conditions of the type

$$-k \frac{\partial T}{\partial n} = h(T - T_\infty) \quad (5.35)$$
are applied. Along the symmetry axis, Neumann conditions are applied:

$$-k \frac{\partial T}{\partial n} = q'' = 0$$  \hspace{1cm} (5.36)

Finally a Dirichlet condition is applied to the node on the interior tank wall that intersects the liquid-vapor interface:

$$T = T_i$$  \hspace{1cm} (5.37)

Care is taken during mesh generation to ensure a node is located at the initial position of the interface. During the simulation, the location of the node is fixed.

For the mixed condition, integration over the boundary yields

$$-\int Nk \frac{\partial T}{\partial n} dA = \int Nh(T - T_\infty)dA$$  \hspace{1cm} (5.38)

$$= 2\pi \int Nh(T - T_\infty)r d\Gamma$$  \hspace{1cm} (5.39)

where \( \int d\Gamma \) represents integration over the boundary. The boundary is defined by two nodes and variation over the boundary is assumed linear. Along the boundary,

$$N = \begin{bmatrix}
\frac{1}{2}(1 - \xi) \\
\frac{1}{2}(1 + \xi)
\end{bmatrix}$$  \hspace{1cm} (5.40)

where the one dimensional coordinate \( \xi \) is shown in Fig. 5.3. In the coordinate, \( \xi \),
the integral over the boundary is

\[ 2\pi \int \mathbf{N} h(T - T_{\infty}) r d\Gamma = 2\pi \frac{L}{2} \int_{-1}^{1} \mathbf{N} h(T - T_{\infty}) r d\xi \]

\[ = \left[ \pi L h \int_{-1}^{1} \mathbf{N} \mathbf{N}^T r d\xi \right] \mathbf{T} - \pi L h T_{\infty} \int_{-1}^{1} \mathbf{N} r d\xi \]  

(5.42)

where \( L \) is the length of the side of the boundary element. Integration is again performed using Gaussian quadrature:

\[ \int_{-1}^{1} g(\xi) d\xi = \sum_{i=1}^{N_{pts}} g(\xi_i) W_i. \]  

(5.43)

Integration points and weights for this one dimensional integral are listed in Table 5.2.
5.2 ZONAL MODEL IMPLEMENTATION

<table>
<thead>
<tr>
<th>$\xi_i$</th>
<th>$W_i$</th>
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<td>0.0000000000000000000</td>
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<tr>
<td>-0.9491079123427585245261897</td>
<td>0.1294849661688693270611400</td>
</tr>
</tbody>
</table>

Table 5.2: Integration points and weights for Gaussian quadrature over a 1D element.

For these mixed boundary conditions, $\pi L h T_{\infty} \int N r \, d\xi$ contributes to the elemental force vector and $\pi L h \int N N^T r \, d\xi$ contributes to the elemental stiffness matrix.

Since only zero flux Neumann conditions are considered in this analysis, these boundaries do not contribute any terms to the stiffness matrix or force vector. The direct stiffness method is used to form a global set of equations of the form

$$C \dot{T} + K T = F$$  \hspace{1cm} (5.44)

A backward Euler method is used to solve the above ODE:

$$C \left( T^{n+1} - T^n \right) + \Delta t K T^{n+1} = \Delta t F^{n+1}$$  \hspace{1cm} (5.45)

or

$$(C + \Delta t K) T^{n+1} = \Delta t K T^n + \Delta t F^{n+1}$$  \hspace{1cm} (5.46)

The global set of equations is modified\textsuperscript{233} to ensure that for the node where the
5.2 ZONAL MODEL IMPLEMENTATION

Dirichlet condition is applied

\[ T^{n+1} = T^n = T_i. \]  \hspace{1cm} (5.47)

The solver proceeds by inverting \( C + \Delta t K \) and then solving

\[ T^{n+1} = \Delta t (C + \Delta t K)^{-1} K T^n + \Delta t (C + \Delta t K)^{-1} F^{n+1}. \]  \hspace{1cm} (5.48)

The finite element equations in the solid regions are coupled to the evolution equations in the bulk liquid and vapor phases through the mixed boundary conditions.

On the wetted and non-wetted interior tank wall respectively, the mixed boundary condition becomes

\[
h(T - T_\infty) = h_{wl}(T - T_i) \hspace{1cm} (5.49)
\]

\[
h(T - T_\infty) = h_{wv}(T - T_v). \hspace{1cm} (5.50)
\]

Convection coefficients are determined by first evaluating area averages of temperature along the wetted and non-wetted parts of the wall

\[
T_{wl} = \frac{1}{A_{wl}} \int_{wl} T \, dA \hspace{1cm} (5.51)
\]

\[
T_{wv} = \frac{1}{A_{wv}} \int_{wv} T \, dA. \hspace{1cm} (5.52)
\]
A Rayleigh number can be evaluated for both bulk phases

\[
Ra = \frac{\rho^2 C_p g \beta (T_{av} - T_{bulk}) L^3}{\mu k}.
\]  

(5.53)

Transport properties in the liquid are evaluated at the film temperature, \(\frac{1}{2}(T_{wl} + T_l)\). The characteristic length along the wetted part of the wall is the interface height. Along the non-wetted part of the wall, the characteristic height is the interface height subtracted from the tank height. Transport properties in the ullage are evaluated using a mass-weighted average of the vapor and non-condensable gas properties. Defining the vapor and gas mass fractions as

\[
\rho = \rho_v + \rho_g
\]  

(5.54)

\[
\omega_v = \frac{\rho_v}{\rho}
\]  

(5.55)

\[
\omega_g = 1 - \omega_v,
\]  

(5.56)

the conductivity and viscosity can be computed

\[
k = \omega_v k_v \left(\frac{T_{wv} + T_v}{2}\right) + \omega_g k_g \left(\frac{T_{wv} + T_v}{2}\right)
\]  

(5.57)

\[
\mu = \omega_v \mu_v \left(\frac{T_{wv} + T_v}{2}\right) + \omega_g \mu_g \left(\frac{T_{wv} + T_v}{2}\right).
\]  

(5.58)

Once the Rayleigh number is computed, the following Nusselt number correlation\textsuperscript{234}
is applied:

\[ \text{Nu} = 0.12 \text{Ra}^{\frac{1}{3}}. \]  

(5.59)

Heat transfer coefficients can then be evaluated

\[ h = \frac{k \text{Nu}}{L}. \]  

(5.60)

Heat transfer coefficients and bulk temperatures defined in this way are incorporated into the mixed boundary conditions of the finite element equations. The bulk phase equations for the multizone model were derived in Chapter 4. After modifying the equation set to account for the presence of a non-condensable gas (Appendix C), these equations become

\[ \frac{dV_v}{dt} = \frac{M}{\rho_l} \]  

(5.61)

\[ \frac{d\rho_v}{dt} = \frac{M}{V_v} \left( 1 - \frac{\rho_v}{\rho_l} \right) \]  

(5.62)

\[ \frac{d\rho_g}{dt} = -\frac{M \rho_g}{V_v \rho_l} \]  

(5.63)

\[ \{ \rho_l c_{p,l} V_1 \} \frac{dT_l}{dt} = \left[ M c_{p,l}(T_l - T_i) + m c_{p,l}(T_{jet} - T_l) + \dot{Q}_{w} + \dot{Q}_{d} + \right. \]

\[ \left. V_i \left\{ \frac{\partial p_v}{\partial \rho_v} \frac{dp_v}{dt} + \frac{\partial p_g}{\partial \rho_g} \frac{d\rho_g}{dt} + \left( \frac{\partial p_v}{\partial T} + \frac{\partial p_g}{\partial T} \right) \frac{dT_v}{dt} \right\} \right] \]  

(5.64)
\[ \begin{align*}
\left\{ \rho_v c_{p,v} V_v + \rho_g c_{p,g} V_v - V_v \left( \frac{\partial p_v}{\partial T} + \frac{\partial p_g}{\partial T} \right) \right\} \frac{dT_v}{dt} &= \left[ M c_{p,v}(T_v^i - T_v) + \dot{Q}_{vw} - \dot{Q}_{iv} + V_v \left( \frac{\partial p_v}{\partial \rho_v} \frac{d\rho_v}{dt} + \frac{\partial p_g}{\partial \rho_g} \frac{d\rho_g}{dt} \right) \right].
\end{align*} \]

(5.65)

\( \dot{Q}_{wl} \) and \( \dot{Q}_{wv} \) are evaluated by integrating the mixed boundary conditions over the wetted and non-wetted parts of the wall respectively:

\[ \begin{align*}
\dot{Q}_{wl} &= \int_{wl} h_{wl}(T - T_i) \, dA \\
\dot{Q}_{wv} &= \int_{wv} h_{wv}(T - T_v) \, dA.
\end{align*} \]

(5.66) (5.67)

The jet temperature, \( T_{jet} \), is computed using the heat exchanger module described in Appendix B. During the self-pressurization phase of the simulation, \( \dot{m} = 0. \) During the mixing phase of the experiment

\[ \dot{m} = \rho_l |v_{jet}| A_{nozz}. \]

(5.68)

The interfacial temperature, \( T_i \), is computed iteratively using eqn. (4.69). Once \( T_i \) is known, the evaporative mass transfer rate can be evaluated

\[ M = \frac{2\sigma}{2 - \sigma} A_i \left( \frac{1}{2\pi R_v T_i} \right)^{\frac{3}{2}} (p_{sat}(T_i) - p_v). \]

(5.69)

The interfacial heat powers, \( \dot{Q}_{il} \) and \( \dot{Q}_{iv} \) are evaluated using heat transfer correlations.
During self-pressurization, the following Nusselt number correlation is applied

\[ \text{Nu} = 0.12 \text{Ra}^{\frac{1}{3}}. \] (5.70)

The characteristic length used to evaluate these dimensionless parameters is the tank radius. Transport properties are evaluated at

\[ T_{\text{film}} = \frac{1}{2}(T_i + T_l) \] (5.71)

on the liquid side of the interface and at

\[ T_{\text{film}} = \frac{1}{2}(T_i + T_v) \] (5.72)

on the vapor side of the interface. Once the Nusselt numbers are known, the heat transfer coefficients can be determined

\[ h = \frac{k \text{Nu}}{R_t}. \] (5.73)

The interfacial heat powers are given by

\[ \dot{Q}_{ul} = h_{ul}A_i(T_i - T_l) \] (5.74)

\[ \dot{Q}_{lv} = h_{lv}A_i(T_v - T_i). \] (5.75)
5.2 ZONAL MODEL IMPLEMENTATION

Since the interface is assumed flat,

\[ A_i = \pi R_i^2. \]  \hspace{1cm} (5.76)

During jet mixing, the liquid side heat transfer coefficient is replaced by

\[ h_{il} = \rho_l c_{p,l} |v_{jet}| \cdot 0.0198 \text{Pr}^{\frac{1}{3}} \left( 1 - \frac{1}{2} \frac{C_{p,l} |T_i - T_l|}{L} \right) \]  \hspace{1cm} (5.77)

which is derived based on a vapor condensation coefficient driven by liquid side turbulence from an axisymmetric liquid jet.\(^83\) The evolution equations in the bulk phases along with the finite element equations are evolved implicitly in time. Within the time integration loop, first the finite element equations are solved and then the bulk fluid equations. The implicit integration proceeds iteratively until the L2 norm of the change in the solution falls below \(1 \times 10^{-5}\).
In this chapter, the predictive capability of both the thermodynamic and zonal models will be assessed. Model predictions will be compared with the experimental data presented in Chapter 2. Initially, comparisons will be made to the data set corresponding to when the tank is 50% full of liquid and 2 W of heat enters the system. First the results of the thermodynamic model will be analyzed. A sensitivity analysis was performed to assess the effects of various parameters on the thermodynamic solution. The thermodynamic model was initialized using the parameters outlined for Case 12 in Table 2.3. Originally, the thermodynamic model did not include the effects of the tank wall. In this formulation, the predicted self-pressurization rate was significantly larger than the experimental data as shown in Fig. 6.1. By not including the wall, all of the applied heat load enters the liquid-ullage system which results in a large pressure rise. In the experiment, during self-pressurization, the wall acts like a heat sink - absorbing some of the applied load. When the wall is included in the model, the self-pressurization rate is underpredicted. This is a consequence of the
Figure 6.1: Effect of including the tank wall in the homogeneous model.

thermal inertia of the wall and the homogeneity assumption. Homogeneity requires that the temperature of the wall changes in a lumped fashion. Homogeneity and the large thermal capacity of the acrylic enhances the thermal sink effects of the wall which results in a smaller predicted pressure rise.

During subcooled jet mixing, the same wall effects are present. By not including the wall, the liquid-ullage system is more responsive to subcooled mixing which results in a steeper depressurization rate as shown in Fig. 6.1. During subcooled mixing, the walls act as a heat source. Before the pressure decays, the walls must give up their sensible energy. Because the walls are modeled as a lumped system, it takes longer for the wall to give up its energy than if heat transfer in the wall were accounted for in a local way. Hence, the depressurization response is slower than the measured data.
In addition to considering the effects of the presence of the wall, the effect of external heat transfer is also analyzed. In the experiment, the wall is blanketed with insulation. Ideally, the insulation should act as an adiabatic boundary. Realistically, it has a non-zero thermal conductivity and heat transfer could occur through the insulation layer. The average temperature of the ambient environment is essentially constant. Whether or not the external environment acts as a heat sink or heat source depends on whether the constant ambient temperature is greater or less than the liquid-ullage-wall system temperature. In this particular liquid heating case, the average ambient temperature is 295.75 K and the initial temperature of the system is 295.38 K. Hence, the warmer ambient environment results in an additional heat load on the system driven by natural convection at the exterior boundary of the insulation layer.
This additional heat source is reflected in the results shown in Fig. 6.2. When this heat source is accounted for, the model predicts a larger pressure rise during self-pressurization and a slower depressurization rate during subcooled mixing. While the effect of external heat transfer is small, it is non-negligible and will be accounted for in subsequent analyses.
Some of the lack of agreement between the thermodynamic model and the experimental data stems from modeling the liquid-ullage-wall system in a lumped fashion. The zonal model relaxes the homogeneity assumption by treating the bulk phases as separate systems and accounting for local heat transfer in the wall.

Before analyzing the results of the zonal model, the sensitivity of the zonal solution to grid size and time step will be discussed. The zonal model for this liquid heating case was run for different mesh densities and time steps. After 300 s, the difference between the current ullage pressure and the initial ullage pressure was computed. The results are listed in Table 6.1. The solution is fairly constant over the range of mesh densities and time steps considered. The variation in the solution over all sensitivity parameters is within 3%. In the results that follow, the finite element grid consisted of 1008 elements with a denser clustering of nodes near the heaters. During the two-hour self-pressurization simulation, the timestep was set to 10 s. During subcooled mixing, for better temporal resolution, the time step was reduced to 0.5 s.

Wall temperature contours after self-pressurizing for 1800 s and 7200 s are shown in Figs. 6.3 and 6.4 respectively.

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<th>$\Delta t$ [s]</th>
<th>$\Delta p$ [torr]</th>
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</tr>
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</table>

Table 6.1: Sensitivity of the zonal solution.
Figure 6.3: Wall temperature contours during self-pressurization.  
Time = 1800 s.
After 1800 s, the hottest part of the system is the submerged heater. Heat has barely conducted into the wall, which is not surprising given the low thermal diffusivity of the acrylic. After self-pressurizing for two hours, the hottest part of the system is still the submerged heater but the tank wall adjacent to the bulk liquid has also increased in temperature as shown in Fig. 6.4. The sensible energy of the bulk liquid increases due to the heat being supplied by the submerged heater. As the temperature of the bulk liquid increases, the liquid gives up some of its energy to the wetted wall through convection resulting in a wall temperature increase.

Temperature contours are shown in Figs. 6.5 and 6.6 when the subcooled jet mixer is activated. After 2700 s of mixing, the wall adjacent to the bulk liquid has cooled as indicated in Fig. 6.5. Since the heater is still on during mixing, locally near the heater, hot spots exist. Away from the heater, convection between the subcooled liquid and the wall has resulted in a temperature decrease. As time progresses, the degree of wall cooling increases. After two hours of mixing, the temperature of the wall adjacent to the liquid has continued to cool.

For the non-wetted part of the wall, thermal equilibration occurs over a much longer timescale as heat has to conduct either into the lower conductivity vapor or through the acrylic wall. Consequently, after two hours of subcooled mixing, the temperature of the top part of the tank wall has not changed appreciably.

In Fig. 6.7, the pressurization behavior predicted by the zonal model is compared with experimental data. During self-pressurization, the agreement between the model and the data is excellent. The model is able to predict both the pressure rise and
Figure 6.4: Wall temperature contours during self-pressurization. Time = 7200 s.
Figure 6.5: Wall temperature contours during subcooled mixing. Elapsed time after activating jet = 2700 s.
Figure 6.6: Wall temperature contours during subcooled mixing. Elapsed time after activating jet = 5400 s.
Figure 6.7: Comparison of zonal pressure prediction with experimental data.

Self-pressurization rate. During subcooled mixing, the initial stage of the depressurization is well predicted. It appears that at the end of the subcooled mixing phase of the experiment, the zonal model and the data are asymptotically approaching different thermodynamic states. When a final steady state is achieved, the ullage pressure becomes constant in time and no net condensation or evaporation occurs at the interface. Moreover, the amount of energy entering and leaving each bulk phase is balanced. In the liquid, for example, the amount of energy being removed by the subcooled jet is balanced by the energy entering the bulk liquid through the wetted walls and through the interface. In the ullage, at equilibrium, the net mass transfer rate across the interface is zero. The energy entering and leaving the ullage through the interface and walls is balanced. Hence,

\[ \dot{Q}_{iv} = \dot{Q}_{uw}. \]  

(6.1)
Or, after expressing the heat powers in terms of convection coefficients,

$$h_{iv}A_i(T_v - T_i) = h_{wv}A_{wv}(T_w - T_v) \tag{6.2}$$

where $T_w$ is the average temperature over the non-wetted wall. Solving for the ullage temperature yields

$$T_v = \frac{h_{iv}A_i}{h_{iv}A_i + h_{wv}A_{wv}}T_i + \frac{h_{wv}A_{wv}}{h_{iv}A_i + h_{wv}A_{wv}}T_w \tag{6.3}$$

The final ullage temperature is an average of the interfacial temperature and non-wetted wall temperature weighted by the product of heat transfer coefficient and area. This temperature, along with density, are substituted into the equation of state to determine the steady state equilibrium pressure in the ullage.

After 5400 s of subcooled mixing, the temperature contours shown in Fig. 6.6 suggest that the interfacial temperature is lower than the temperature of the wall adjacent to the ullage. Since the predicted ullage pressure is asymptoting to a lower pressure than the experimental data, eqn. (6.3) implies that the zonal model is over-predicting the heat transfer coefficient between the ullage and the interface. The final ullage temperature is being weighted more heavily by the colder interface resulting in a lower steady state pressure.

The lack of agreement in the final ullage pressure is a consequence of not only the correlations used to derive the heat transfer coefficients but also the assumption
The breakdown of the homogeneity assumption is also apparent in Fig. 6.8 which shows a comparison between the time history of the average ullage temperature predicted by the model and a time history of the local temperature recorded by the thermistor.

During self-pressurization, the average temperature response predicted by the zonal model lags the local temperature response recorded by the thermistor. At the end of the two hour pressurization period, the predicted temperature rise is only 0.26 K compared to the 0.80 K recorded temperature rise. During subcooled mixing, the zonal model does not capture the jump in temperature at approximately 8000 s.
In Chapter 2, it was posited that this jump was caused by local wall heating as the condensation flux decreases. Since the zonal model only tracks the average energy of the ullage, it fails to capture local energy distributions within the bulk phase.

During the self-pressurization phase of this particular liquid heating case, the primary driver for pressurization is evaporation through the interface. Given the equation of state,

\[ p = p_v(\rho_v, T_v) + p_g(\rho_g, T_v), \]

the pressure rise can be approximated by

\[ \Delta p \approx \frac{\partial p_v}{\partial \rho_v} \Delta \rho_v + \frac{\partial p_g}{\partial \rho_g} \Delta \rho_g + \left( \frac{\partial p_v}{\partial T_v} + \frac{\partial p_g}{\partial T_g} \right) \Delta T_v \]  

The contributions of these different terms are listed in Table 6.2. The partial derivatives listed in Table 6.2 are evaluated at the initial state of the ullage. The change in density and temperature are evaluated using the difference between the predicted state at the end of the two hour self-pressurization period and the initial state of the ullage. As indicated in the table, the derivative of pressure with respect to density is significantly larger than the derivative with respect to temperature. Hence, only a small change in vapor or gas density is required to affect a large change in ullage pressure. The vapor density increases because during evaporation, mass is being added to the ullage. The gas density is decreasing because as the liquid is vaporizing and the interface is receding, the ullage expands. Finally, the temperature of the ullage
\[ \Delta p \approx \frac{\partial p_v}{\partial \rho_v} \Delta \rho_v + \frac{\partial p_g}{\partial \rho_g} \Delta \rho_g + \left( \frac{\partial p_v}{\partial T_v} + \frac{\partial p_g}{\partial T_g} \right) \Delta T_v \]

\[ = 11476 \frac{\text{Pa} \cdot \text{m}^3}{\text{kg}} \cdot 0.1499 \frac{\text{kg}}{\text{m}^3} + 84774 \frac{\text{Pa} \cdot \text{m}^3}{\text{kg}} \cdot -4 \cdot 10^{-6} \frac{\text{kg}}{\text{m}^3} + 235 \frac{\text{Pa}}{\text{K}} \cdot 0.26 \text{K} \]

\[ = 1720 \text{ Pa} - 0.3 \text{ Pa} + 61.1 \text{ Pa} \]

**Table 6.2: Contributions to pressure rise.**

Increases due to heat and mass transfer additions at the ullage boundary as well as ullage compression. By noting the relative magnitudes of the different contributions to the total pressure rise, one can deduce that evaporation through the interface is driving the ullage pressure rise.

An honest assessment of the zonal model requires comparing the model’s predictions to more than just a single data point. In what follows, the model is spot-checked by comparing predictions to different cases in the experimental test matrix.

In Fig. 6.9, the zonal model is compared against a case corresponding to when the tank is 26.5% full of liquid and 2 W of heat is entering the system. During mixing, the jet speed is 0.241 cm/s and the heat exchanger bath temperature is 20 °C and 17.5 °C in Figs. 6.9a and 6.9b respectively. The model does a reasonable job of predicting the self-pressurization rate and initial depressurization rate. Similar to the 50% fill level case, the model predicts a final ullage pressure lower than the experimental data. For reasons outlined above, the discrepancy is most likely attributed to overpredicting the heat transfer coefficient between the ullage and the interface.

The zonal model is compared against a lower heat load case is Fig. 6.10. In this
Figure 6.9: Comparisons when the tank is 26.5% full and a 2 W heat load is applied. The jet speed is 0.241 cm/s and the bath temperature is (a) 20 °C and (b) 17.5 °C.
Figure 6.10: Comparisons when the tank is 26.5% full and a 1 W heat load is applied. The jet speed is 0.241 cm/s and the bath temperature is 20 °C.

case, the tank is 26.5% full of liquid and only 1 W of heat is entering the tank. The self-pressurization rate and initial depressurization rate agree well with the experimental data.

Predictions are made for a higher fill level case and comparisons are shown in Fig. 6.11. Here, the tank is 73.5% full of liquid with an incident heat load of 2 W. As indicated in the figure, there is excellent agreement between the model predictions and the experimental data during self-pressurization. During subcooled mixing, the depressurization rate is overpredicted. For this high fill level case, the liquid in the tank absorbs more incident energy than in the lower fill level cases. The subcooled jet is trying to penetrate upward into a warmer medium. Adverse buoyancy is hindering the jet’s upward flow. Consequently, the jet has to remove energy from the bulk liquid before it can impinge the interface causing the pressure collapse. Since
RESULTS

Figure 6.11: Comparisons when the tank is 73.5% full and a 2 W heat load is applied. The jet speed is 0.241 cm/s and the bath temperature is 20 °C.

This adverse buoyancy interaction is an intraphase phenomena and the zonal model assumes spatial uniformity within each bulk phase, a discrepancy exists between the model’s predictions and the experimental data.

Finally, comparisons are made in Fig. 6.12 when the tank is 26.5% full and the jet speed is only 0.114 cm/s. In this case, the self-pressurization rate is reasonably predicted, but once again, the pressure collapse during subcooled mixing occurs over a shorter time scale than what the data suggests. For this lower jet flow case, the momentum of the jet is not strong enough to directly impinge the interface. The upward motion of the jet is suppressed by buoyant convection in the liquid. Prior to interface impingement, the buoyantly driven vortices interact with the forced jet flow. The colder jet exchanges energy with the vortices, weakening them until impingement can occur. Since the zonal model is unable to resolve this intraphase interaction,
discrepancy exists between the model and the data.

Generally, the agreement between the model and the data is reasonable during self-pressurization. During subcooled mixing, the model does an excellent job of predicting the initial depressurization rate when the interaction between buoyant convection and forced jet mixing is weak. When the interaction is strong, for low jet speeds, the model predicts a faster pressure collapse than the data suggests. To resolve this discrepancy at lower jet speeds, local transport phenomena within the bulk phases must be accounted for in the model.

Figure 6.12: Comparisons when the tank is 26.5% full and a 2 W heat load is applied. The jet speed is 0.114 cm/s and the bath temperature is 20 °C.
Chapter 7

Conclusions

In this dissertation, the effectiveness of using subcooled jet mixing as a means to control tank pressure was analyzed. A small-scale experiment with a refrigerant fluid was performed in a normal gravity environment. During the self-pressurization phase of the experiment, both the liquid fill fraction and heating rate were varied. For a liquid heating configuration, the data revealed that increasing the heating rate increased the self-pressurization rate. Increasing the liquid fill fraction decreased the pressurization rate as more liquid was available to absorb the applied heat load.

After self-pressurizing for two hours, a mixing jet aligned with the tank’s central axis was used to control tank pressure. Results showed that a mixing jet alone was not sufficient to control tank pressure. Over a short time scale, after the jet is first turned on, tank pressure did decrease. However, the decrease was only temporary. When the bulk liquid became well-mixed, tank pressure began to rise at a rate higher than self-pressurization alone. The mixing pump provided an additional energy source to the liquid/vapor system and resulted in the increased pressurization rate.
In order to sustain the pressure collapse, thereby increasing the effectiveness of the jet, energy must be removed from the liquid stream. In this pressure control phase of the experiment, both the jet speed and temperature were varied. For large jet speeds, the experiment demonstrated that subcooled mixing jets are an effective way to control pressure. When the jet’s momentum is strong enough to overcome both adverse buoyancy and natural convection in the liquid, a rapid reduction in tank pressure can be realized.

As a pressure control strategy, subcooled axial jet mixing will show a gravitational dependence. In this experiment, when the jet’s momentum was small, an interaction between the forced jet flow and natural convection in the liquid took place. Before the pressure collapsed in the ullage, the forced jet would have to weaken the natural convection vortices in the bulk phase. The interaction is much weaker in a low-gravity environment due to reduced buoyancy effects. To effectively control tank pressure when operating in a range of gravitational environments, it is recommended that either the jet’s momentum to be large enough to overcome buoyancy or other gravity-independent design solutions, such as a subcooled spray mixer, be considered.

In addition to performing a ground-based experiment, in this dissertation, the governing equations were used to formulate both a homogeneous thermodynamic model and a zonal model. Comparing the thermodynamic model with the experimental data highlighted some of the deficiencies of the thermodynamic modeling approach. First, it was shown that the effects of the tank wall should not be neglected in the analysis. The wall has a large thermal inertia and neglecting the wall in these instances will
result in the model significantly overpredicting both the self-pressurization and de-
pressurization rates. When the wall was included in the analysis, the thermodynamic
model underpredicted the experimental data. This discrepancy was primarily caused
by the homogeneity assumption in the thermodynamic model. The assumption forces
the liquid, ullage, and wall to be at the same temperature which changes in a lumped
fashion based on energy conservation. When thermal non-uniformities are present in
the system, the thermodynamic model fails to capture these inhomogeneous regions
and will not be able to make detailed temperature or pressure predictions. As a design
tool, the thermodynamic model is useful at uncovering trends in the pressurization
behavior but it is limited in its predictive ability.

The zonal model relaxed the restrictive homogeneity assumption by treating the
bulk liquid and ullage as separate zones. Within each zone, all thermodynamic quan-
tities were assumed to be spatially uniform. The liquid zone and ullage zone were
coupled to each other through heat and mass transfer correlations. Additionally, the
zonal model accounted for local heat transfer in the wall by making use of a finite
element model. The finite element model solved the energy equation in the wall and
was coupled to the bulk phase transport equations through heat transfer relationships
between the wetted and non-wetted parts of the interior tank wall and the liquid and
ullage.

Comparisons between the experimental pressure data and the zonal model predic-
tions are excellent for moderate to high jet flow rates. For slower jet speeds, buoyancy
in the liquid adversely affects the effectiveness of a subcooled mixing jet. Natural con-
vection vortices in the bulk liquid suppress the upward motion of the jet. If the jet is weak, buoyancy dominates and the cooling jet never reaches the interface. If the jet is strong, the jet is able to reach the interface with little hindrance from the buoyantly driven vortices. For intermediate jet flows, an interaction occurs where the subcooled jet first has to weaken the buoyant flow before the jet can impinge the interface driving a pressure collapse. Since the zonal model assumes spatial uniformity within each bulk phase, these buoyancy-forced jet flow interactions are not captured.

For faster jet flows, the interaction is weak and the zonal model does an excellent job of predicting tank pressurization behavior. In these cases, the model can be used as a design tool to determine the pressure response of a lightweight cryogenic storage tank. As a design tool, expediency in obtaining an accurate prediction is paramount, as it affords the opportunity to evaluate multiple design solutions in a quick and straightforward manner. There are situations however where a more detailed model is warranted. In particular, to capture buoyancy-forced jet flow interactions or ullage position in low-gravity applications, it is recommended that future modeling efforts include a computational fluid dynamics simulation of the bulk phases. These simulations, while sacrificing expediency, can provide designers with a more thorough picture of the complicated transport phenomena occurring inside a storage tank.

In addition to recommending future improvements to the modeling approach, recommendations to improve future small-scale experiments are threefold. First, a more robust degassing scheme should be developed. The current method for degassing the test fluid was slow, time-consuming, and not as robust as desired. Improvements...
CONCLUSIONS

in this area would lead to a more rapid turnaround time between experiments. Second, a non-intrusive way to measure temperature is desirable. In the current experimental configuration, fully populating the test tank with thermistors resulted in a test cell with a greater leak rate than if the thermistor ports were capped. Moreover, including the thermistors in the tank resulted in an interaction with the underlying flow. If the jet flow stagnated on a thermistor, the measured depressurization rate would be smaller than if the thermistors were not present. Non-intrusive measurements provide a means to record local bulk phase temperatures without interfering with the flow. Finally, the current experiment was performed in a normal gravity environment. In low gravity environments, buoyancy effects are reduced and even slow subcooled jets may be effective at reducing tank pressure. Additionally, other effects masked by buoyancy in 1g would become more prominent. The interaction between the jet and the ullage itself may not be insignificant. The jet may geyser into the ullage or push the ullage to one side of the tank. In the ground-based experiment, the liquid vapor interface was essentially flat. In microgravity, the position of the interface and location of the ullage is less certain. To fully evaluate these scenarios, it is recommended that small-scale pressurization experiments be performed in low-gravity environments.
Appendix A

Properties of HFE-7000

For the ground-based experiment, the test fluid is HFE-7000 (C₃F₇OCH₃) - a refrigerant with a relatively low normal boiling point (34 °C) which makes it well suited for performing experiments without elaborate cryogenic thermal controls. The fluid, provided by 3M, had a stated purity level of 99.5%. The molar mass is 200 g/mol. The critical properties, as reported by Geller²³⁵ are

\[
\begin{align*}
T_c &= 437.61 \text{ K} \pm 0.03 \text{ K} \\
p_c &= 2483.3 \text{ kPa} \pm 2 \text{ kPa} \\
\rho_c &= 553 \text{ kg/m}^3 \pm 0.1 \text{ kg/m}^3.
\end{align*}
\]

Saturation tables provided by the manufacturer were used to develop correlations for relevant thermodynamic variables. These correlations, along with their coefficient of determination, and their range of validity are listed below. The density is given in kg/m³, the temperature in K, and the internal energy and enthalpy in kJ/mol.
\[ \rho_{l}^{\text{sat}}(T) = \sum_{k=1}^{5} N_k \left(1 - \frac{T}{T_c}\right)^{i_k} \]
\[ \rho_{v}^{\text{sat}}(T) = \sum_{k=1}^{5} N_k \left(1 - \frac{T}{T_c}\right)^{i_k} \]

<table>
<thead>
<tr>
<th>(N_1)</th>
<th>i_1</th>
<th>(N_2)</th>
<th>i_2</th>
<th>(N_3)</th>
<th>i_3</th>
<th>(N_4)</th>
<th>i_4</th>
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<td>8.203129740 \cdot 10^3</td>
<td>3</td>
<td>-5.332926413 \cdot 10^3</td>
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<td>8.526087154 \cdot 10^2</td>
<td>0</td>
</tr>
</tbody>
</table>

\(R^2 = 0.999\)

| Table A.1: Saturation densities for HFE-7000. |

\[ u_{l}^{\text{sat}}(T) = \sum_{k=1}^{5} N_k T^{i_k} \]
\[ u_{v}^{\text{sat}}(T) = \sum_{k=1}^{5} N_k T^{i_k} \]

<table>
<thead>
<tr>
<th>(N_1)</th>
<th>i_1</th>
<th>(N_2)</th>
<th>i_2</th>
<th>(N_3)</th>
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<th>i_4</th>
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<td>0</td>
</tr>
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</table>

\(R^2 = 0.999\)

| Table A.2: Saturation internal energies for HFE-7000. |
PROPERTIES OF HFE-7000

\[
h^\text{sat}_l(T) = \sum_{k=1}^{5} N_k T^{i_k}
\]

\[
h^\text{sat}_v(T) = \sum_{k=1}^{5} N_k T^{i_k}
\]

<table>
<thead>
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<th>(N_1)</th>
<th>(i_1)</th>
<th>(N_2)</th>
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</tbody>
</table>

\[R^2 = 0.999\]

\[230 \text{ K} < T < 388 \text{ K}\]

Table A.3: Saturation enthalpies for HFE-7000.

For the above thermodynamic data, the reference point is given as the saturated liquid state at 230 K. The pressure-temperature relationship along the saturation curve is given by the manufacturer as:

\[
\ln(p \ [\text{Pa}]) = \frac{-3548.6}{T \ [\text{K}]} + 22.978
\]

\[R^2 = 0.998\]

\[243 \text{ K} < T < T_c\]

However, a refit of saturation data provided by Geller\textsuperscript{235} (accuracy ±0.05%) results in a Wagner-type equation for vapor pressure:

---

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\[ p = p_c \exp \left[ \frac{a \tau + b \tau^{1.5} + c \tau^{2.5} + d \tau^5}{1 - \tau} \right] \]

\[
a = -8.384714 \\
b = 2.815690 \\
c = -4.166609 \\
d = -7.663946
\]

\[ R^2 = 0.999 \]

241 K < T < 370 K

where \( \tau = 1 - T/T_c \). This expression results in a better fit of the data especially around the operating temperatures of the ground experiment. Geller also provided data on the ideal gas specific heat capacity of HFE-7000. The reported accuracy on this data is estimated as less than \( \pm 0.6\% \). Fitting a polynomial through his data yields:

\[
c_p(T [K]) \left[ \frac{kJ}{kg \cdot K} \right] = \sum_{k=1}^{4} N_k T^{i_k}
\]

\[
N_1 = 3.682659933 \times 10^{-9} \quad i_1 = 3 \\
N_2 = -5.441919192 \times 10^{-6} \quad i_2 = 2 \\
N_3 = 4.143476431 \times 10^{-3} \quad i_3 = 1 \\
N_4 = -1.666666656 \times 10^{-4} \quad i_4 = 0
\]

\[ R^2 = 0.999 \]

260 K < T < 420 K
Additionally, the manufacturer provided the following expressions for properties in the liquid:

\[
\beta \left[ \frac{1}{K} \right] = 0.00219 \tag{A.1}
\]

\[
k_l \left[ \frac{W}{m \cdot K} \right] = 0.0798 - 0.000196 T \, ^\circ C \tag{A.2}
\]

\[
c_p \left[ \frac{J}{kg \cdot K} \right] = 1223.2 + 3.0803 T \, ^\circ C \tag{A.3}
\]

\[
\nu \, [cSt] = (z - 0.7) - \exp[-0.7487 - 3.295(z - 0.7) + 0.6119(z - 0.7)^2 - 0.3193(z - 0.7)^3] \tag{A.4}
\]

where

\[
z = 10^{10^{10.151 - 4.6006 \log(T \, [K])}}.
\]

The range of validity for these correlations are -120 °C to 35 °C, -120 °C to 40 °C, and -120 °C to 40 °C for the conductivity, specific heat, and kinematic viscosity respectively. Curve fitting surface tension data provided by the manufacturer yields:

\[
\sigma \left[ \frac{mN}{m} \right] = 42.830 \left( 1 - \frac{T}{T_c} \right)^{1.016} \tag{A.5}
\]

Reliable property measurements in the vapor phase have not been reported in the literature. As such, relevant vapor phase properties must be estimated using a variety of techniques. To estimate the value of the expansion coefficient and the specific heat, an equation of state (EOS) is posited for the vapor phase. Then, using classical
thermodynamics, it can be shown that:

\[ p = p(\nu, T) \quad \text{(A.6)} \]

\[ \beta = -\frac{1}{\nu} \frac{(\partial p/\partial T)_\nu}{(\partial p/\partial \nu)_T} \quad \text{(A.7)} \]

\[ c_v = c_v^0 - R - \int_{\nu}^{\infty} T \left( \frac{\partial^2 p}{\partial T^2} \right) d\nu \quad \text{(A.8)} \]

\[ c_p = c_v - T \left( \frac{\partial p/\partial T}{(\partial p/\partial \nu)_T} \right)^2 \quad \text{(A.9)} \]

where \( \nu \) is the gas constant.

The EOS that best predicted the P-V-T relationship near the saturation curve was chosen to represent HFE-7000 vapor. Some of the EOS described below make use of the accentric factor,\(^{236} \) which is defined as

\[ \omega = -\log \left[ \lim_{T/T_c \to 0.7} (p_{sat}/p_c) \right] - 1.0. \quad \text{(A.10)} \]

With the vapor pressure curve defined previously, the accentric factor for HFE-7000 evaluates to 0.413. Several EOS are evaluated to determine which EOS best describes the P-V-T behavior of HFE-7000 near the saturation curve. The following EOS are evaluated:

**Ideal Gas**

\[ p(\nu, T) = \frac{RT}{\nu} \quad \text{(A.11)} \]
**Redlich-Kwong**

\[
a = 0.42748 \frac{R^2T_c^{5/2}}{p_c}
\]

\[
b = 0.08664 \frac{RT_c}{p_c}
\]

\[
p(\nu, T) = \frac{RT}{\nu - b} - \frac{a}{\nu(\nu + b)\sqrt{T}}
\]  \hspace{1cm} (A.12)

**Peng-Robinson**

\[
a = 0.45724 \frac{(RT_c)^2}{p_c}
\]

\[
b = 0.0778 \frac{RT_c}{p_c}
\]

\[
p(\nu, T) = \frac{RT}{\nu - b} \left[ 1 + \frac{a}{\nu^2 + 2b\nu - b^2} \right]
\]  \hspace{1cm} (A.13)

**Virial**

\[
p(\nu, T) = \frac{RT}{\nu} \left[ 1 + \frac{B(T)}{\nu} + \frac{C(T)}{\nu^2} \right]
\]  \hspace{1cm} (A.14)

Tsonopoulos\(^{237-239}\) provides correlations for the 2nd virial coefficient in terms of the reduced temperature, \(T/T_c\):

\[
B = \frac{RT_c}{p_c} \left( F_o(T_r) + \omega F_1(T_r) \right)
\]  \hspace{1cm} (A.15)

\[
F_o = 0.1445 - \frac{0.330}{T_r} - \frac{0.1385}{T_r^2} - \frac{0.0121}{T_r^3} - \frac{0.000607}{T_r^8}
\]  \hspace{1cm} (A.16)

\[
F_1 = 0.0637 + \frac{0.331}{T_r^2} - \frac{0.423}{T_r^3} - \frac{0.008}{T_r^8}
\]  \hspace{1cm} (A.17)
Orbey and Vera\(^\text{240}\) provide a correlation for the 3rd virial coefficient:

\[
C = \left( \frac{RT_c}{p_c} \right)^2 \left( G_o(T_r) + \omega G_1(T_r) \right) \tag{A.18}
\]

\[
G_o = 0.01407 + \frac{0.02432}{T_r^{2.8}} - \frac{0.00313}{T_r^{10.5}} \tag{A.19}
\]

\[
G_1 = -0.02676 + \frac{0.01770}{T_r^{2.8}} + \frac{0.040}{T_r^8} - \frac{0.003}{T_r^6} - \frac{0.00228}{T_r^{10.5}} \tag{A.20}
\]

<table>
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<th>(p(\nu_{v}^{\text{sat}}, 294 \text{ K}))</th>
<th>(p(\nu_{v}^{\text{sat}}, 298 \text{ K}))</th>
<th>r.m.s. error</th>
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<td>69748 Pa</td>
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<td>59805 Pa</td>
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<tr>
<td>Peng-Robinson</td>
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<td>68921 Pa</td>
<td>516 Pa</td>
</tr>
</tbody>
</table>

Table A.6: Comparison of different EOS in predicting P-V-T behavior near the saturation curve

To assess the abilities of these models to accurately capture the P-V-T behavior near the saturation curve, the predicted vapor pressures at 290 K, 294 K, and 298 K are compared with the saturation pressure given by eqn. (A.4). The r.m.s. error is computed for each EOS. For the three representative temperatures, the Peng-Robinson EOS results in the lowest error as indicated in Table A.6. Accordingly, HFE-7000 vapor is assumed to behave as Peng-Robinson gas. Carrying out the operations
PROPER TIES OF HFE-7000

described in eqns. (A.7)-(A.9) and evaluating the results at \(\nu_{v}^{sat}(298K)\) results in:

\[
\beta = 0.00372 \frac{1}{K} \tag{A.21}
\]
\[
c_v = 808 \frac{J}{kg \cdot K} \tag{A.22}
\]
\[
c_p = 856 \frac{J}{kg \cdot K}. \tag{A.23}
\]

The computed value of \(c_v\) is within 11\% of the independent estimation provided by the manufacturer (\(c_v = 730 \text{ J/kg} \cdot \text{K}\)). With the thermodynamic properties in the vapor now estimated, the vapor viscosity and vapor thermal conductivity must be determined before the transport equations can be solved. To estimate the vapor viscosity, a corresponding states method described in Lucas\textsuperscript{241} is employed:

\[
\zeta = 0.176 \left( \frac{T_c}{M_w^3 P_c^4} \right)^{1/6} \tag{A.24}
\]
\[
\mu[\mu P] = \zeta^{-1} \left[ 0.807 T_r^{0.618} - 0.357 \exp(-0.449 T_r) + 0.340 \exp(-4.058 T_r) + 0.018 \right]. \tag{A.25}
\]

In eqn. (A.25), the molar mass is in g/mol, the temperature is in Kelvin, the pressure is in bars, and the reduced temperature, \(T_r = T/T_c\). This expression is valid for a low pressure gas. Since the operating pressure is significantly less than the critical pressure (\(p/p_c \approx 0.02\)), the high pressure corrections will be neglected. The viscosity computed by eqn. (A.25) differs by approximately 7\% from the independent estimation provided by the manufacturer (\(\mu = 109 \cdot 10^{-7} \text{Pa} \cdot \text{s}\)).
The thermal conductivity for HFE-7000 vapor can be estimated from the Eucken expression for polyatomic gases:

\[
\frac{kM_w}{\mu c_v} = 1 + \frac{9/4}{c_vR}
\]  

(A.26)

where the units of conductivity, molar mass, viscosity, and specific heat are such that the above equation is dimensionless. Computing the conductivity in this way yields \(k = 0.0091 \text{ W/m·K}\).

To improve the ability of his equation to predict thermal conductivity, Eucken later modified his original expression to:

\[
\frac{kM_w}{\mu c_v} = 1.32 + \frac{1.77}{c_vR}
\]  

(A.27)

which yields a conductivity of \(0.012 \text{ W/m·K}\). Poling et al.,\textsuperscript{242} however, notes that experimental values of \(k\) typically lie between the values computed from eqns. (A.26) and (A.27). The thermal conductivity estimated independently by the manufacturer is \(0.01 \text{ W/m·K}\).
Appendix B

Heat Exchanger Model

During the pressure control phase of the experiment, the liquid withdrawn from the tank passes through a shell and tube heat exchanger before it re-enters the tank as a subcooled axial jet. The test fluid, HFE-7000, flows through the tubes in the heat exchanger while water flows through the shell. It is assumed that the temperature of the HFE-7000 entering the heat exchanger is equal to the average fluid temperature at the tank outlet. Consequently, heat transfer to the fluid between the tank and the heat exchanger is assumed negligible. Given this inlet temperature, the mass flow rates of the two fluids, and the water inlet temperature, the following analysis describes a model used to predict the temperature of the two fluids exiting the heat exchanger. Once again, it is assumed that heat transfer to the HFE-7000 between the heat exchanger exit and the tank inlet is negligible. In the analysis that follows, the hot (HFE-7000) and cold (water) fluids correspond to the tube-side, $t$, and shell-side, $s$, of the heat exchanger respectively. Various parameters describing the heat exchanger is provided in Table 2.1. The heat exchanger is shown notionally in Fig.
Using the parameters listed in Table 2.1, the pitch, $P_T$, and hydraulic diameter, $D_e$ can be computed:

$$P_T = \text{OD}_t + C$$  \hspace{1cm} (B.1)

$$D_e = \frac{4P_T^2}{\pi \text{OD}_t} - \text{OD}_t$$  \hspace{1cm} (B.2)

where $C$ is the clearance between tubes. The equivalent areas of the tubes and shell are

$$A_t = N_t \frac{\text{ID}_t^2}{4}$$  \hspace{1cm} (B.3)

$$A_s = \frac{\text{ID}_s CB}{P_T}$$  \hspace{1cm} (B.4)
where \( N_t \) is the number of tubes and \( B \) is the baffle spacing in the shell. With the flow areas known, the flow velocities can be computed according to:

\[
V_t = \frac{\dot{m}_t}{\rho_t A_t} \quad \text{(B.5)} \\
V_s = \frac{\dot{m}_s}{\rho_s A_s} \quad \text{(B.6)}
\]

Given the Prandtl number of the fluids and the Reynolds numbers:

\[
Re_t = \frac{\rho_t V_t ID_t}{\mu_t} \quad \text{(B.7)} \\
Re_s = \frac{\rho_s V_s De}{\mu_s}, \quad \text{(B.8)}
\]

the Nusselt numbers can be evaluated using heat transfer correlations

\[
Nu_t = 1.86 \left( \frac{ID_t Re_t Pr_t}{L} \right)^{1/3} \quad \text{(B.9)}
\]

\[
Nu_s = 0.36 Re_s^{0.55} Pr_s^{1/3} \quad \text{(B.10)}
\]

In the above correlation for the tube-side Nusselt number, a modified Sieder-Tate equation for laminar flow is employed. For the jet speeds of interest, the flow in the tubes is laminar. The inner and outer heat transfer coefficients are

\[
h_i = \frac{Nu_t k_t}{ID_t} \quad \text{(B.11)}
\]

\[
h_o = \frac{Nu_s k_s}{De}. \quad \text{(B.12)}
\]
HEAT EXCHANGER MODEL

The total exchange coefficient is given by

\[
\frac{1}{U} = \frac{OD_t}{ID_t} \left( \frac{1}{h_i} + \frac{1}{h_o} \right). \tag{B.13}
\]

To compute the HFE-7000 outlet temperature, the ratio of thermal capacitances is needed:

\[
R = \frac{\dot{m}_s c_p_s}{\dot{m}_t c_p_t}. \tag{B.14}
\]

Defining

\[
S = \frac{T^\text{out}_s - T^\text{in}_s}{T^\text{in}_t - T^\text{in}_s}, \tag{B.15}
\]

one can determine the outlet temperature by solving the following equation for S:

\[
U A_o \frac{\dot{m}_s c_p_s}{\dot{m}_s c_p_s} = \frac{1}{\sqrt{R^2 + 1}} \ln \left[ \frac{2 - S(R + 1 - \sqrt{R^2 + 1})}{2 - S(R + 1 + \sqrt{R^2 + 1})} \right]. \tag{B.16}
\]

where the effective heat transfer area, \(A_o\) is listed in Table 2.1. The water outlet temperature, \(T^\text{out}_s\) can then computed using eqn. (B.15). The HFE-7000 exit temperature can finally be evaluated using a simple energy balance:

\[
\dot{m}_t c_p_t (T^\text{jet}_t - T^\text{in}_t) = \dot{m}_s c_p_s (T^\text{out}_s - T^\text{in}_s). \tag{B.17}
\]

This value, \(T^\text{jet}_t\), is the jet temperature used in the homogeneous and zonal models.
Appendix C

Non-Condensable Gases

In Chapter 4, models were developed to describe mass and energy transport in a pure two-phase system. Modifications to these models due to the presence of a non-condensable gas will now be discussed.

Consider a tank containing the liquid and vapor phases of a pure species in addition to a non-condensable gas species in the ullage. Dissolution of the non-condensable gas into the bulk liquid will be neglected. Mass conservation can be described by:

\[
\frac{d}{dt} \left[ \int_{V_l} \rho_l dV \right] - \int_{I} \rho_l (v_l - v_s) \cdot \hat{n} dS + \int_{out} \rho_l v_1 \cdot n dS - \int_{in} \rho_l v_1 \cdot n dS = 0 \quad (C.1)
\]

\[
\frac{d}{dt} \left[ \int_{V_v} \rho_v dV \right] + \int_{I} \rho_v (v_v - v_s) \cdot \hat{n} dS = 0 \quad (C.2)
\]

\[
\frac{d}{dt} \left[ \int_{V_g} \rho_g dV \right] = 0. \quad (C.3)
\]
As before, one can define,

\[ j = \rho_l (v_l - v_s) \cdot \hat{n} = \rho_v (v_v - v_s) \cdot \hat{n} \]  
(C.4)

\[ M = - \int_I j \, dS \]  
(C.5)

\[ \bar{p}_l = \frac{1}{V_l} \int_{V_l} \rho_l \, dV \]  
(C.6)

\[ \bar{p}_{v,g} = \frac{1}{V_v} \int_{V_v} \rho_{v,g} \, dV \]  
(C.7)

\[ \dot{m} = \int_{in} \rho_l v_l \cdot n \, dS = \int_{out} \rho_l v_l \cdot n \, dS \]  
(C.8)

which yields,

\[ \frac{d}{dt} (\bar{p}_l V_l) = -M \]  
(C.9)

\[ \frac{d}{dt} (\bar{p}_v V_v) = M \]  
(C.10)

\[ \frac{d}{dt} (\bar{p}_{v,g} V_v) = 0. \]  
(C.11)

Similar to the pure two-phase system, the energy balance in the liquid phase is

\[ \frac{d}{dt} \left[ \int_{V_l} \rho_l h_l \, dV \right] - \int_I \rho_l h_l (v_l - v_s) \cdot \hat{n} \, dS + \int_{out} \rho_l h_l v_l \cdot n \, dS - \int_{in} \rho_l h_l v_l \cdot n \, dS = \]

\[ - \int_w J_{q,1} \cdot n \, dS + \int_I J_{q,1} \cdot \hat{n} \, dS - \int_{out} J_{q,1} \cdot n \, dS + \int_{in} J_{q,1} \cdot n \, dS + \int_{V_l} \frac{dp}{dt} \, dV. \]

(C.12)
For the gas mixture in the ullage

\[
\frac{d}{dt} \left[ \int_{V_o} \rho h dV \right] + \int_I \rho h (v - v_s) \cdot \hat{n} dS = - \int_{w} \mathbf{J}_{q,v} \cdot \mathbf{n} dS - \int_I \mathbf{J}_{q,v} \cdot \hat{n} dS + \int_{v_c} \frac{dp}{dt} \tag{C.13}
\]

The two species in the gas mixture are assumed to mix ideally,

\[
\rho h = \rho_v h_v + \rho_g h_g \tag{C.14}
\]

\[
p = p_v(\rho_v, T) + p_g(\rho_g, T). \tag{C.15}
\]

For this multicomponent ullage, the energy flux consists of a heat flux, \( \tilde{\mathbf{J}}_q \) in addition to the flux of energy due to species diffusion

\[
\mathbf{J}_q = \tilde{\mathbf{J}}_q + \sum_{i=g,v} \mathbf{j}_i h_i \tag{C.16}
\]

where the diffusive flux is defined as:

\[
\mathbf{j}_i = \rho_i (v_i - v) \tag{C.17}
\]

In the above expression, \( v \) is the mass-averaged velocity of the gas mixture.
substituting these expressions into eqn. (C.13), it is useful to note that

\[ \rho h (v - v_s) = \rho_v h_v (v - v_s) + \rho_g h_g (v - v_s) \]  

(C.18)

\[ = \rho_v h_v (v_v - v_s) - \rho_v h_v (v_v - v) + \rho_g h_g (v_g - v_s) - \rho_g h_g (v_g - v) \]  

(C.19)

\[ = \rho_v h_v (v_v - v_s) - \sum (j_i h_i). \]  

(C.20)

The \( \rho_g (v_g - v_s) \) term is zero because there is no mass transfer of the non-condensable species across the interface. Defining similar averages and terms as in the pure two-phase system (eqns. (4.18)-(4.22)), and after substituting these expressions into the ullage energy balance, the following equations for the two phase system results:

\[ \frac{d}{dt} (\rho_v h_v V_v + \rho_g h_g V_g) + \int j_k dS = \dot{Q}_{uv} - \dot{Q}_{iv} + \frac{d\bar{V}_v}{dt} \]  

(C.21)

\[ \frac{d}{dt} (\rho_l h_l V_l) - \int j_k dS = \dot{Q}_{wl} + \dot{Q}_{il} + \frac{d\bar{V}_l}{dt} - \dot{m} \left(h_{i,\text{out}} - h_{i,\text{in}}\right). \]  

(C.22)

The energy flux due to species diffusion, which appears in eqns. (C.16) and (C.20) cancel with one another. Hence, the heat powers appearing the above equations are only due to conduction.
C.1 Homogeneous Model

Invoking the homogeneity assumption; that is, the entire system is isothermal and the liquid and vapor phases are defined by their saturation states leads to:

\[
\begin{align*}
\frac{d}{dt} \left( \rho_l^{\text{sat}} h_l^{\text{sat}} V_l \right) + M h_l^{\text{sat}} - \dot{m} \left( h_l^{\text{in}} - h_l^{\text{sat}} \right) &= \dot{Q}_{\text{wl}} + \dot{Q}_d + V_l \frac{dp}{dt} \\
\frac{d}{dt} \left( \rho_v^{\text{sat}} h_v^{\text{sat}} V_v + \rho_g h_g V_v \right) - M h_v^{\text{sat}} &= \dot{Q}_{\text{sw}} - \dot{Q}_w + V_v \frac{dp}{dt}
\end{align*}
\]

(C.23) (C.24)

Adding the above equations results in

\[
\frac{d}{dt} \left( \rho_l^{\text{sat}} h_l^{\text{sat}} V_l + \rho_v^{\text{sat}} h_v^{\text{sat}} V_v + \rho_g h_g V_v \right) - M \left( h_v^{\text{sat}} - h_l^{\text{sat}} \right) - \dot{m} \left( h_l^{\text{in}} - h_l^{\text{sat}} \right) = \dot{Q}_w + (\dot{Q}_d - \dot{Q}_w) + V_v \frac{dp}{dt}.
\]

(C.25)

Or, after carrying out the differentiation, applying eqns. (C.9)-(C.11) and the energy jump condition across the interface yields

\[
\rho_l^{\text{sat}} V_l \frac{dh_l^{\text{sat}}}{dt} + \rho_v^{\text{sat}} V_v \frac{dh_v^{\text{sat}}}{dt} + \rho_g V_v \frac{dh_g}{dt} - M \left( h_v^{\text{sat}} - h_l^{\text{sat}} \right) - V_v \frac{dp^{\text{sat}}}{dt} = \dot{Q}_w + \dot{m} \left( h_l^{\text{in}} - h_l^{\text{sat}} \right).
\]

(C.26)

Treating the non-condensable gas as an ideal gas with a constant specific heat leads to

\[
\frac{dh_g}{dt} = c_{pg} \frac{dT}{dt}.
\]

(C.27)
Since homogeneity is invoked,
\[
\frac{dh_g}{dt} = c_{ps} \frac{dT_{sat}}{dt} .
\]  
(C.28)

Hence,
\[
\frac{dT_{sat}}{dt} \left\{ \rho_{l} V_{l} \frac{dh_{l}^{sat}}{dT_{sat}} + \rho_{v} V_{v} \frac{dh_{v}^{sat}}{dT_{sat}} + \rho_{g} V_{g} c_{ps} + \frac{d(p_{v}^{sat} V_{v})}{dT_{sat}} L - V_{l} \frac{dp}{dT_{sat}} \right\} = \dot{Q}_w + \dot{m} \left( h_{l}^{in} - h_{l}^{sat} \right) .
\]  
(C.29)

C.2 Zonal Model

In a multizone formulation, uniformity within each bulk phase is still assumed, but the assumption that the phases are at the same temperature, $T_{sat}$, is relaxed. The tank is again partitioned into three zones: a liquid zone, an ullage zone, and a thin massless interfacial zone at temperatures $T_{l}$, $T_{v}$, and $T_{i}$ respectively. The liquid phase is assumed incompressible. The ullage contains both vapor and a non-condensable gas. The two gases are assumed to mix ideally,
\[
p = p(\rho_{v}, T_{v}) + p_{g}(\rho_{g}, T_{v})
\]  
(C.30)
Similar to the pure liquid vapor system, the integrated continuity equation in the liquid is given by:

\[
\frac{d}{dt}(\rho_l V_l) = -M
\]

\[
\rho_l \frac{dV_l}{dt} = -M
\]  \hspace{1cm} (C.31)

\[
-\rho_l \frac{dV_v}{dt} = -M
\]

which implies that

\[
\frac{dV_v}{dt} = \frac{M}{\rho_l}.
\]  \hspace{1cm} (C.32)

Liquid incompressibility and the volume constraint were used to arrive at eqn. (C.32).

The continuity equation for the vapor in the ullage is

\[
\frac{d}{dt}(\rho_v V_v) = M
\]  \hspace{1cm} (C.33)

\[
\rho_v \frac{dV_v}{dt} + V_v \frac{d\rho_v}{dt} = M
\]  \hspace{1cm} (C.34)

\[
\rho_v \frac{M}{\rho_l} + V_v \frac{d\rho_v}{dt} = M
\]  \hspace{1cm} (C.35)

which leads to

\[
\frac{d\rho_v}{dt} = \frac{M}{V_v} \left(1 - \frac{\rho_v}{\rho_l}\right).
\]  \hspace{1cm} (C.36)
Since no dissolution of the non-condensable gas is assumed to occur, the continuity equation for the non-condensable gas in the ullage is

\begin{align}
\frac{d}{dt}(\rho_g V_v) &= 0 \quad (C.37) \\
\rho_g \frac{dV_v}{dt} + V_v \frac{d\rho_g}{dt} &= 0 \quad (C.38) \\
\rho_g M \rho_l + V_v \frac{d\rho_g}{dt} &= 0 \quad (C.39)
\end{align}

which leads to

\begin{equation}
\frac{d\rho_g}{dt} = -\frac{M \rho_g}{V_v \rho_l} \quad (C.40)
\end{equation}

Uniformity within each bulk phase simplifies the bulk phase energy balances to

\begin{align}
\frac{d}{dt}(\rho_l h_l V_l) + M h_l^i &= -\dot{m} \left( h_l^{out} - h_l^{in} \right) + \dot{Q}_{ul} + \dot{Q}_{dl} + V_l \frac{dp}{dt} \quad (C.41) \\
\frac{d}{dt}(\rho_v h_v V_v + \rho_g h_g V_v) - M h_v^i &= \dot{Q}_{wv} - \dot{Q}_{lv} + V_v \frac{dp}{dt} \quad (C.42)
\end{align}

The enthalpy of the bulk phases is assumed to behave as

\begin{align}
h_v &= h_{v,o} + c_{p,v}(T_v - T_{v,o}) \quad (C.43) \\
h_g &= h_{g,o} + c_{p,g}(T_g - T_{g,o}) \quad (C.44) \\
h_l &= h_{l,o} + c_{p,l}(T_l - T_{l,o}) \quad (C.45)
\end{align}
Substituting these expressions into the energy balances, carrying out the differentiation, and rearranging terms leads to

\[
\rho_l c_{p,l} V_l \frac{dT_l}{dt} = M c_{p,l}(T_l - T_i) + \dot{m} c_{p,l}(T_l - T_{in}) + \dot{Q}_{wl} + \dot{Q}_{it} + V_l \frac{dp}{dt} \quad \text{(C.46)}
\]

\[
(\rho_v c_{p,v} + \rho_g c_{p,g}) V_v \frac{dT_v}{dt} = M c_{p,v}(T_v - T_i) + \dot{Q}_{vw} - \dot{Q}_{iv} + V_v \frac{dp}{dt} \quad \text{(C.47)}
\]

where once again, liquid incompressibility has been invoked. The equation of state can be used to explicitly evaluate the pressure derivative. That is,

\[
\frac{dp}{dt} = \left( \frac{\partial p_v}{\partial \rho_v} \frac{d\rho_v}{dt} + \frac{\partial p_v}{\partial T_v} \frac{dT_v}{dt} \right) + \left( \frac{\partial p_g}{\partial \rho_g} \frac{d\rho_g}{dt} + \frac{\partial p_g}{\partial T_g} \frac{dT_g}{dt} \right). \quad \text{(C.48)}
\]

Substituting this expression into the energy balances yields

\[
\{\rho_l c_{p,l} V_l\} \frac{dT_l}{dt} = \left[ M c_{p,l}(T_l - T_i) + \dot{m} c_{p,l}(T_l - T_{in}) + \dot{Q}_{wl} + \dot{Q}_{it} + V_l \left\{ \frac{\partial p_v}{\partial \rho_v} \frac{d\rho_v}{dt} + \frac{\partial p_v}{\partial T_v} \frac{dT_v}{dt} \right\} \right] \quad \text{(C.49)}
\]

\[
\left\{ \rho_v c_{p,v} V_v + \rho_g c_{p,g} V_v - V_v \left( \frac{\partial p_v}{\partial T_v} + \frac{\partial p_g}{\partial T_g} \right) \right\} \frac{dT_v}{dt} = \left[ M c_{p,v}(T_v - T_i) + \dot{Q}_{vw} - \dot{Q}_{iv} + V_v \left( \frac{\partial p_v}{\partial \rho_v} \frac{d\rho_v}{dt} + \frac{\partial p_g}{\partial \rho_g} \frac{d\rho_g}{dt} \right) \right]. \quad \text{(C.50)}
\]

These equations represent the integral energy balances in the liquid and ullage when a non-condensable gas is present.


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