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Critical Point Pressure Sensitivity

By

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A THESIS SUBMITTED IN PARTIAL FULFILLMENT OF THE REQUIREMENTS FOR THE DEGREE

Doctor of Philosophy

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Abstract

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A new means of heat transfer known as the piston effect was identified in 1989. The piston effect is where the expanding thermal boundary layer acts like a piston which compresses the bulk fluid. An examination of the equations for the conservation of mass, momentum, and energy identified the significant thermophysical properties as the thermal conductivity, the volume expansivity, and the isothermal compressibility. The thermal conductivity and the volume expansivity determine the thickness of the thermal boundary layer. The isothermal compressibility of the bulk fluid determines the pressure response of the bulk fluid to a given volume change. Previous researchers used only the van der Waals equation of state at conditions within mK of the critical point. The research described herein focuses on the pressure response of a fluid near the critical point to a sudden change in the boundary temperature. The use of the van der Waals equation of state for numerical simulation of the piston effect results in underpredicting the magnitude of the pressure wave by approximately 30 percent while overpredicting the acoustic heating by approximately 15 percent compared to using all fluid properties from a real gas equation of state. When evaluating the piston effect at conditions typical of cryogenic storage systems the pressure response of the fluid was observed to be six orders of magnitude larger than had been previously reported. The extent of the acoustic heating
resulted in temperature increases in the bulk fluid that were four orders of magnitude larger. The real gas equation of state was used to compare the pressure and temperature response of oxygen and hydrogen due to a thermal disturbance at the boundary. The pressure rise in hydrogen after five acoustic time periods was only 17% of the pressure rise in oxygen. The temperature increase in hydrogen was only 30% of the temperature rise in oxygen. On the diffusion time scale the pressure rise in the oxygen is an order of magnitude larger than the pressure rise in hydrogen for the same thermal penetration depth. The temperature rise in oxygen is four times greater than the temperature rise in hydrogen.
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Chapter 1 - Introduction

This research was initiated after years of personally observing the pressure behavior in the supercritical liquid oxygen and liquid hydrogen tanks on the space shuttle. Numerous occurrences of a pressure collapse have been observed in the liquid oxygen tanks. A pressure collapse is a sudden drop in the tank pressure, usually associated with a maneuvering thruster firing. A review of all space shuttle flights from 1981 to 1997 (flights STS-1 through STS-84) revealed over 160 events where the pressure had suddenly decreased in the liquid oxygen tank. At the same time, no pressure collapses were observed in the liquid hydrogen tanks. Since a sudden pressure decrease looks just like what would be expected if a large leak had developed in a piece of plumbing NASA is interested in the ability to predict the timing and magnitude of these pressure collapses. Unfortunately, no theory was available to explain the physical mechanism that was causing these sudden pressure collapses. A detailed review of the data available from the space shuttle indicated that the heater temperatures were always near the critical temperature at the time of the pressure collapse. This was independent of the bulk fluid temperature in the tank. This initiated this investigation into the heat transfer to a fluid near the critical point.

A new means of heat transfer known as the piston effect was identified in the late 1980’s by experimenters studying the specific heat of a fluid very close to the critical point. The temperature of the bulk fluid was observed to be increasing in temperature faster than could be explained by diffusion alone. The piston effect is where an expanding thermal
boundary layer acts like a piston, which compresses the bulk fluid. The expansion of the thermal boundary layer also creates a pressure wave traveling at near the speed of sound in the fluid, which transfers energy into the bulk fluid causing a temperature rise in the bulk fluid. Previous research into the piston effect considered only the van der Waals equation of state for conditions very close to the critical point. The research described herein compares the pressure response of oxygen using the van der Waals equation of state and a real gas equation of state provided by the National Institute of Standards and Technology (NIST).\(^1\) The real gas equation of state is then used to compare the pressure response of liquid oxygen to the pressure response of liquid hydrogen. The usual approach in estimating the time for a system to reach thermal equilibrium has been to apply the thermal diffusion equation to the system geometry with some appropriate intermediate value of the thermodynamic properties. This approach works well when the system is far away from the critical point of the fluid. Near the critical point, however, the experimentally measured time for thermal equilibrium indicated an equilibrium time much shorter than predicted by the diffusion equation. The pressure wave contributes to an energy equation source term, which results in a nearly uniform heating of the bulk fluid. The bulk fluid temperature achieves 90% of the steady state value in less than 5% of the time predicted by diffusion alone. It was, therefore, determined in the late 1980's that the effect of acoustic heating on the bulk fluid needs to be accounted for.

**Literature Review**

The issue of pressure control of a cryogenic storage tank in a microgravity environment has been a problem ever since man first ventured into space. A decision was made early
in the space program to store the liquid oxygen and liquid hydrogen as supercritical fluids to avoid the problem of liquid sloshing during launch and the problem of identifying the location of the liquid/vapor interface in a microgravity environment. The lack of a significant gravity field results in the cryogenic tank becoming thermally stratified. This has resulted in a large number of occurrences where the pressure in the space shuttle liquid oxygen tank would suddenly decrease during firing of the spacecraft maneuvering thrusters. An attempt was made by the National Aeronautics and Space Administration (NASA) in 1975 to quantify the effects of thermal stratification on the proposed space shuttle orbiter liquid oxygen tanks. Utilizing data from the Apollo missions, the Boeing Aerospace Company\textsuperscript{2,4} constructed a five-node finite difference computer model in an attempt to predict the behavior of the Power Reactant Storage and Distribution (PRSD) liquid oxygen tanks on the space shuttle. The model attempted to simulate the thermal stratification based on a temperature difference between the bulk fluid and the heater surface. The potential pressure collapse was calculated by assuming that fluid mixing within the tank would result in uniform conditions being restored. The model underpredicted the magnitude of the pressure decay by greater than 50% based on data from the Apollo missions. The first space shuttle flight did not occur until April 1981. The PRSD stratification model developed by Boeing was never compared to actual data from the space shuttle flights in an effort to improve the accuracy of the model. A review of the pressure decays in the space shuttle liquid oxygen tanks revealed that the temperature and pressure were always near the critical point at the time of the pressure decay. This points to a connection between the pressure decay and the change in the fluid properties at the critical point. In 1987 Wildhaber\textsuperscript{3} performed a summary of research
efforts into the thermal stratification of sub-critical and supercritical cryogenic storage systems. The only source of microgravity data was from the Apollo and Space Shuttle programs. He concluded that there was an inadequate database to determine anything about the impact of thermal stratification on the design and operation of space based cryogenic storage systems. Since the problem being addressed is the pressure sensitivity of a fluid near its critical point a review of the previous research into heat transfer to a fluid near the critical point was needed.

There have been a considerable number of experimental and theoretical investigations into heat transfer to a fluid near the critical point. Most of these studies have been for turbulent flow since it is the most typical situation for heat transfer equipment design. A few researchers have performed numerical investigations into the problem of laminar flow in a vertical tube, with and without buoyancy force, for supercritical fluids. There is much less research in the area of laminar flow than for turbulent flow. Additional researchers have investigated heat transfer to supercritical fluids near the laminar/transitional flow region. A number of researchers have investigated the unusually fast times observed for thermal equilibration for fluids near the critical point. Dahl and Moldover studied the thermal relaxation times of normal helium, He, near the critical point. They experienced the typical slowing down of the thermal relaxation time when approaching the critical temperature from the two-phase system but experienced very fast equilibration times for the single-phase system. Equilibration times of less than six seconds were observed for the single-phase system while the diffusion equation predicted equilibration times of greater than 200 seconds.
They attributed the very fast equilibration times to the presence of convection in the fluid sample. Typical diffusion controlled equilibration times were observed for the two-phase system. In light of more recent experimental results the fast thermal equilibration observed in the single-phase system could better be interpreted as an indication of the presence of acoustic heating.

Nitsche and Straub\textsuperscript{22} studied the variation of the specific heat at constant volume, $C_v$, near the critical point of sulfur hexafluoride (SF$_6$) during the D1-Spacelab mission on the space shuttle in October 1985. They subjected the fluid to continuous heating from slightly below the critical temperature to slightly above the critical temperature. The D1-Spacelab results were compared to terrestrial results and microgravity results from a previous Technologische EXperimente Unter Schwerelosigkeit (TEXUS) 8 sounding rocket flight. They found that the bulk fluid temperature closely followed the boundary temperature regardless of the presence or absence of gravity. Boukari et.al.\textsuperscript{23} experimentally studied the thermal equilibration time for a sample of xenon at the critical density. The authors observed thermal equilibration times on the order of seconds compared to hundreds of hours predicted by pure diffusion. The equilibration times based on pure diffusion were estimated to be 180 hrs at 90 mK above the critical temperature and 900 hrs at 3 mK above the critical temperature. The fluid achieved faster thermal equilibration times when the temperature was closer to the critical temperature. Klein et.al.\textsuperscript{24} conducted phase transition experiments on a TEXUS sounding rocket. The sample of sulfur hexafluoride was quenched from 5 mK above the critical temperature to 2, 5, and 10 mK below the critical temperature. In the single-phase region the
temperature of the fluid sample was observed to closely follow the temperature of the container wall. The rate of cooling decreased significantly in the two-phase region. The predicted thermal equilibration time was on the order of a hundred hours but actual equilibration times of a few seconds were observed for the single-phase region.

Garrabos et.al.\textsuperscript{25} and Zappoli et.al.\textsuperscript{26} studied the heat transport in carbon dioxide near its critical point using a TEXUS rocket. They studied the time for thermal equilibration after suddenly changing the wall temperature. In one experiment they changed the wall temperature from 2 mK above the critical temperature to 1 mK above the critical temperature. The temperature change was performed over a period of 40 msecs. The thermal equilibration time based on thermal diffusion would have required six days but the experimental results achieved equilibration in about 30 seconds. The density and temperature gradients still relaxed diffusely but the bulk fluid achieved the majority of its temperature change very quickly. The hydrodynamic time predicted for the experiment conducted by Garrabos et.al.\textsuperscript{25} was around 160 secs. Thus, the thermal equilibration time observed is comparable to the hydrodynamic time. In two related experiments, Garrabos et.al.\textsuperscript{25} changed the temperatures from 1 mK above to 1 mK below the critical temperature and from 1 mK below to 1 mK above the critical temperature. These experiments showed that the piston effect was still present in the two-phase region near the critical point. Garrabos et.al.\textsuperscript{27} reviewed the results of a critical point carbon dioxide experiment on the TEXUS 25 sounding rocket and a sulfur hexafluoride critical point experiment on the IML-1 Spacelab mission. Both of these experiments provided evidence of the piston effect as indicated by rapid thermal equilibration of the bulk fluid and a lack of density
and thermal gradients in the bulk fluid. The TEXUS 25 critical point carbon dioxide results indicated thermal equilibration in just a few seconds compared to the 1000 seconds estimated by pure diffusion. The sulfur hexafluoride experiment on IML-1 also showed thermal equilibration times of just a few seconds.

Guenoun et al.\textsuperscript{28} conducted experiments on the TEXUS 25 sounding rocket to determine the presence of the piston effect in a sample of carbon dioxide at its critical point. They varied the temperature from 2.5 mK above the critical point to 0.8 mK below the critical point. Pure diffusion predicted a thermal equilibration time of about one week but experimental results showed equilibration times of just a few seconds. Density and temperature gradients in the thermal boundary layer were unaffected by the thermal equilibration due to the piston effect and were seen to relax diffusely. Outside of the thermal boundary layer no density or temperature gradients were present. Bonetti et al.\textsuperscript{29} experimentally studied the microgravity thermal response of carbon dioxide near its critical density to varying heat inputs. They observed density gradients only within the thermal boundary layer and uniform density throughout the bulk fluid. The characteristic time for establishing the density gradient layer was given as $t = L^2 / 4 D_n (\gamma - 1)^2$ where $L$ is a characteristic length, $D_n$ is the thermal diffusivity, and $\gamma$ is the ratio of specific heats. The lack of any density gradients and uniform heating in the bulk fluid is an indication of the piston effect.
Straub et al.\textsuperscript{30} conducted experiments during the German Spacelab mission D-2 in 1993 to gather microgravity data on the existence of the piston effect. They used a calorimeter filled with sulfur hexafluoride at the critical density. The calorimeter was subjected to stepwise temperature changes and the spatial temperature distribution was monitored. There were small temperature and density gradients in the thermal boundary layer but no gradients in the bulk fluid. With a temperature difference between the bulk fluid and the critical temperature of 0.1 K the thickness of the thermal boundary layer was calculated to be 0.2 mm. This shows that small temperature differences can cause significant changes in the thermal boundary layer when near the critical point. This sensitivity increases as the system gets closer to the critical temperature. The bulk fluid temperature was observed to closely follow the wall temperature.

Kassoy\textsuperscript{31} conducted a theoretical investigation of the response of a confined perfect gas to a small thermal disturbance. He showed that an acoustic wave is generated in any fluid within a confined volume when the boundary temperature is suddenly changed. The strength of the acoustic wave is dependent on the magnitude of the temperature change and how rapidly the fluid properties vary with temperature. Since the fluid properties show the greatest sensitivity at the critical point this means that the acoustic waves will be strongest when near the critical point of the fluid. These acoustic effects are dominant only on very short time frames and quickly dissipate when a steady boundary temperature is established. Boukari et al.\textsuperscript{32} performed a numerical simulation of the thermal response of a layer of liquid initially at the critical point of the fluid. For the time scales of interest, much larger than the acoustic time scale, the pressure can be considered to be
uniform throughout the volume. The acoustic time is given as $t_a = L/c$ where $L$ is a characteristic length and $c$ is the speed of sound in the fluid. The pressure is still a function of time but it is independent of position. In solving the usual problem of heat conduction in an incompressible fluid changes in the internal energy are due only to temperature variations. For a compressible fluid the adiabatic change of temperature and density due to the variation of pressure with time must also be considered. In a near critical fluid the compressibility is so large that the adiabatic effect dominates the process of equilibration. The authors considered both a sudden quenching of the boundaries of the one-dimensional container and a continuous increase of one of the boundary temperatures. The fluid properties of xenon near the critical point were used in the numerical simulation. The results were compared to data gathered from a sulfur hexafluoride experiment conducted aboard a TEXUS sounding rocket. When the boundary temperature was suddenly decreased from 20 mK above the critical temperature to 10 mK above the critical temperature the bulk fluid achieved 99% of the thermal response within 5 secs, significantly less time than predicted by diffusion alone.

Around the same time, Zappoli et.al. performed a numerical analysis of carbon dioxide near its critical point. They determined that an acoustic wave was generated by the expansion of the thermal boundary layer. The volume expansivity shows an extreme sensitivity to small temperature changes at the critical point. The acoustic wave contributes to a uniform heat generation in the bulk fluid and results in the bulk fluid being quickly brought to thermal equilibrium with the imposed boundary temperature.
They named this heat transfer mechanism the "piston effect" since the expanding thermal boundary layer acts like a piston, compressing the bulk fluid. Onuki et al.\textsuperscript{14} used the diffusion of entropy of an enclosed volume of fluid to explain the fast thermal equilibration of a fluid near its critical point. The resulting predicted thermal equilibration times closely matched the results of Nitsche and Straub\textsuperscript{22}. Using linear hydrodynamic theory Onuki and Ferrell\textsuperscript{14} analytically studied the adiabatic heat transfer to a fluid near the critical point. Their analysis showed that on the acoustic time scale the temperature and pressure are nearly homogeneous in the single-phase fluid outside of the thermal boundary layer. The entropy change caused by the sudden change in the boundary temperature still follows the diffusive relaxation. For a two-phase fluid the rate of thermal transport follows the diffusive relaxation until very close to the critical point of the fluid. Thus, the system experiences the typical slowing down of thermal transport when approaching the critical point from the two-phase region but a speeding up when approaching from the single-phase region. Even the two-phase system demonstrates a critical speeding up when very close to the critical point. They determined that the expansion of the thermal boundary layer acts as a piston, which compresses the remaining fluid in a fixed volume container. This adiabatic process quickly transfers heat from the heated surface to the bulk liquid in a nearly uniform manner. They determined that the time required to establish the thermal boundary layer was given as

\[ t_L = t_D^{\frac{1}{2}} \gamma^2 \propto (T - T_c)^{1.7} \]

where \( \gamma \) is the ratio of specific heats at constant pressure and volume and \( t_D \) is the diffusion time. They showed that this time is proportional to the temperature difference between the bulk fluid temperature, \( T \), and the critical point.
temperature, $T_c$. Evaluating this time estimate at conditions 1 mK above the critical
temperature of carbon dioxide gives a time of 22 μs to establish the thermal boundary
layer. This shows how quickly temperature changes can occur when near the critical
point. The time to establish the boundary layer is similar to that proposed by Bonetti
et.al. 29.

Zappoli and Bailly36 compared a numerical solution of the one-dimensional low Mach
number compressible flow equations to first and second order asymptotic analytical
solutions. The numerical solutions were solved using the Pressure Implicit with Splitting
of Operators (PISO) algorithm37, 38. The numerical solution was shown to approximate
the asymptotic solution to within the truncation error. There are no analytical solutions
for two-dimensional or three-dimensional problems so numerical methods are the only
solution techniques available. Behringer et.al.39 studied the thermal equilibration times
for pure normal helium, He$^3$, and mixtures of normal helium and superfluid helium, He$^3$-
He$^4$. Using linearized hydrodynamic theory and Laplace transforms they solved the
Navier-Stokes and energy equations to determine the transient thermal response of the
system under either constant pressure or constant volume conditions. They found that
when the fluid temperature is greater than the critical temperature the thermal
equilibration time for a fluid with a specific heat ration $\gamma = C_p/C_v >> 1$ in a constant
volume system was four times faster than for a constant pressure system. The agreement
between the constant pressure and constant volume systems becomes much better when
the fluid is closer to the critical temperature. They also found very little difference
between the equilibration times for a pure fluid and a binary fluid. The adiabatic effect is
more pronounced for larger values of the specific heat ratio $\gamma$.

Using one-dimensional hydrodynamic theory Zappoli\textsuperscript{40} and Djennaoui et.al.\textsuperscript{41} performed
an asymptotic solution of the one-dimensional Navier-Stokes equation for a van der
Waals fluid near the critical point. They predicted a thermal equilibration time of
$t_L \propto (T - T_c)^{\frac{3}{2}}$. Their predicted time agrees with the predictions of Onuki and Ferrell\textsuperscript{35}.
The difference in the exponents of Zappoli vs. Onuki and Ferrell is caused by the
difference between mean-field theory exponents and Ising theory exponents. Later,
Zappoli et.al.\textsuperscript{42} extended their previous one-dimensional hydrodynamic equations to
include two-dimensional unsteady heat transfer effects and gravity. Their efforts
demonstrated that the piston effect was still present in a normal earth gravity condition
and results in fast thermal equilibration of the bulk fluid prior to the onset of buoyancy-
driven convection. The density gradient remaining after the thermal equilibration is the
driving mechanism for the onset of convection.

Since the piston effect requires knowledge of the fluid properties near the critical point an
accurate model of the equation of state is needed. Typical analytical forms of the
equation of state predict finite values of the specific heats $C_p$ and $C_v$, the thermal
conductivity, and the speed of sound at the critical point. It is well established by
experimental results that the specific heats and the thermal conductivity diverge to
infinity as the critical point is approached. Garland and Williams\textsuperscript{43} studied the speed of
sound in xenon near its critical point. The speed of sound varies as $\frac{1}{\sqrt{C_v}}$ and therefore as $C_v$ goes to infinity near the critical point the speed of sound will go to zero. They showed that although the speed of sound approaches zero at the critical temperature it is still larger than 10 m/s for $(T - T_c)/T_c > 10^{-9}$. It is common to all fluids for the speed of sound to go to zero at the critical point. The use of an empirical equation of state is required to adequately model the change in the fluid properties near the critical point. Hendricks et al.44 developed a computer program to provide the thermophysical properties of ten different cryogenic fluids. The program did not attempt to model the anomalous behavior near the critical point and therefore could not be utilized for this research effort. Emanuel45 applied critical point theory to predict the thermodynamic properties of a real fluid near the critical point. The theory is applicable to any fluid and accurately predicts the divergence of the properties of interest at the critical point. The use of critical point theory needs further investigation and is beyond the scope of this research. Nwobi et al.46 used molecular dynamics theory to predict the thermodynamic properties of supercritical oxygen. The approach accurately predicts the divergence of certain important properties near the critical point but is much too computer time intensive to be of any practical use in numerical simulations. The thermodynamic properties utilized in this research effort were calculated using a computer program originally created by the NIST4 in 1980 for the NASA Johnson Space Center. The program reproduces the values from the NIST tables for fifteen cryogenic fluids. The program accurately reproduces the divergence of the fluid properties at the critical point. The output from the program was compared to the published tables from NIST with very
close correlation, often within 1% of the tabulated values except near the critical point where the maximum error is estimated to be about 10%.

The research described in the literature review focused on the fast thermal equilibration of a fluid near the critical point. All the previous researchers used only the van der Waals equation of state to evaluate the density of the fluid. The research contained in this dissertation focuses on the pressure and temperature changes in a fluid near the critical point and compares results from the van der Waals equation of state to the results obtained using the NIST equation of state. No previous efforts to determine the pressure sensitivity of a fluid at the critical point were identified during the literature review. The temperatures investigated in this research effort also include bulk fluid temperatures significantly below the critical temperature, which were not investigated previously. All of the previous research looked at conditions within a few mK of the critical temperature. The physics that result in large pressure changes due to changes in the thermal boundary layer thickness are described in the following section.
A theoretical basis for predicting the pressure sensitivity of a fluid near the critical point can be developed by examining the equations of motion and heat transfer. From the fundamental conservation equations the significant fluid properties can be identified and their contribution to the fast thermal equilibration and extreme pressure sensitivity of a fluid near the critical point can be explained.

**Conservation of mass**

The conservation of mass for a compressible fluid, written in Cartesian coordinates, is given by

\[
\frac{\partial p}{\partial t} + \frac{\partial}{\partial x} (\rho u) + \frac{\partial}{\partial y} (\rho v) + \frac{\partial}{\partial z} (\rho w) = 0 \tag{2-1}
\]

where \( \rho \) is the density and \( u, v, \) and \( w \) are the fluid velocities along the three coordinate axes. For the two-dimensional problem this reduces to

\[
\frac{\partial p}{\partial t} + \frac{\partial}{\partial x} (\rho u) + \frac{\partial}{\partial y} (\rho v) = 0 \tag{2-2}
\]

**Conservation of Momentum**

The Navier-Stokes equations for a compressible fluid, written in Cartesian coordinates, is given by

\[
\frac{\partial p}{\partial t} + \frac{\partial p u^2}{\partial x} + \frac{\partial p u v}{\partial y} + \frac{\partial p u w}{\partial z} = -\frac{\partial p}{\partial x} + \frac{\partial \tau_{xx}}{\partial x} + \frac{\partial \tau_{yx}}{\partial y} + \frac{\partial \tau_{zx}}{\partial z} \tag{2-3}
\]
\[
\frac{\partial \rho v}{\partial t} + \frac{\partial \rho v u}{\partial x} + \frac{\partial \rho v^2}{\partial y} + \frac{\partial \rho v w}{\partial z} = -\frac{\partial P}{\partial y} + \frac{\partial \tau_{xy}}{\partial x} + \frac{\partial \tau_{yz}}{\partial y} + \frac{\partial \tau_{xz}}{\partial z}
\]

(2-4)

\[
\frac{\partial \rho w}{\partial t} + \frac{\partial \rho u w}{\partial x} + \frac{\partial \rho v w}{\partial y} + \frac{\partial \rho w^2}{\partial z} = -\frac{\partial P}{\partial z} + \frac{\partial \tau_{xz}}{\partial x} + \frac{\partial \tau_{yz}}{\partial y} + \frac{\partial \tau_{zx}}{\partial z}
\]

(2-5)

where P is the pressure. Using Stokes hypothesis, the shear stress is defined as

\[
\tau_{ij} = \mu \left[ \left( \partial_i v_j + \partial_j v_i \right) - \frac{2}{3} \partial_k v_k \delta_{ij} \right]
\]

(2-6)

where \( \mu \) is the viscosity. Applying the definition of the shear stress to the momentum equations gives

\[
\frac{\partial \rho u}{\partial t} + \frac{\partial \rho u^2}{\partial x} + \frac{\partial \rho u v}{\partial y} + \frac{\partial \rho u w}{\partial z} = -\frac{\partial P}{\partial x} + \frac{\partial}{\partial x} \left( \frac{4}{3} \mu \frac{\partial u}{\partial x} - \frac{2}{3} \mu \frac{\partial v}{\partial y} - \frac{2}{3} \mu \frac{\partial w}{\partial z} \right)
\]

\[
+ \frac{\partial}{\partial y} \left( \mu \frac{\partial u}{\partial y} + \mu \frac{\partial v}{\partial x} \right) + \frac{\partial}{\partial z} \left( \mu \frac{\partial u}{\partial z} + \mu \frac{\partial w}{\partial x} \right)
\]

(2-7)

\[
\frac{\partial \rho v}{\partial t} + \frac{\partial \rho u v}{\partial x} + \frac{\partial \rho v^2}{\partial y} + \frac{\partial \rho v w}{\partial z} = -\frac{\partial P}{\partial y} + \frac{\partial}{\partial y} \left( \frac{4}{3} \mu \frac{\partial v}{\partial y} - \frac{2}{3} \mu \frac{\partial u}{\partial x} - \frac{2}{3} \mu \frac{\partial w}{\partial z} \right)
\]

\[
+ \frac{\partial}{\partial z} \left( \mu \frac{\partial v}{\partial z} + \mu \frac{\partial w}{\partial y} \right)
\]

(2-8)

\[
\frac{\partial \rho w}{\partial t} + \frac{\partial \rho u w}{\partial x} + \frac{\partial \rho v w}{\partial y} + \frac{\partial \rho w^2}{\partial z} = -\frac{\partial P}{\partial z} + \frac{\partial}{\partial z} \left( \mu \frac{\partial w}{\partial z} + \mu \frac{\partial w}{\partial x} \right)
\]

\[
+ \frac{\partial}{\partial x} \left( \mu \frac{\partial w}{\partial x} + \mu \frac{\partial w}{\partial y} \right) + \frac{\partial}{\partial y} \left( \frac{4}{3} \mu \frac{\partial w}{\partial y} - \frac{2}{3} \mu \frac{\partial u}{\partial x} - \frac{2}{3} \mu \frac{\partial v}{\partial y} \right)
\]

(2-9)

For the two-dimensional case this reduces to

\[
\frac{\partial \rho u}{\partial t} + \frac{\partial \rho u^2}{\partial x} + \frac{\partial \rho u v}{\partial y} = -\frac{\partial P}{\partial x} + \frac{\partial}{\partial x} \left( \frac{4}{3} \mu \frac{\partial u}{\partial x} - \frac{2}{3} \mu \frac{\partial v}{\partial y} \right) + \frac{\partial}{\partial y} \left( \mu \frac{\partial u}{\partial y} + \mu \frac{\partial v}{\partial x} \right)
\]

(2-10)
\[
\frac{\partial \rho v}{\partial t} + \frac{\partial \rho uv}{\partial x} + \frac{\partial \rho v^2}{\partial y} = -\frac{\partial P}{\partial y} + \frac{\partial}{\partial x}\left(\mu \frac{\partial u}{\partial y} + \mu \frac{\partial v}{\partial x}\right) + \frac{\partial}{\partial y}\left(\frac{4}{3} \mu \frac{\partial v}{\partial y} - \frac{2}{3} \mu \frac{\partial u}{\partial x}\right) 
\]
(2-11)

For most fluids, the pressure gradient term dominates the source term since the viscosity is very small. This is valid for cryogenic fluids regardless of the proximity to the critical point.

**Conservation of Energy**

The energy equation for a compressible fluid is given in Cartesian coordinates as

\[
\frac{\partial \rho E}{\partial t} + \frac{\partial \rho Hu}{\partial x} + \frac{\partial \rho Hv}{\partial y} + \frac{\partial \rho Hw}{\partial z} = \frac{\partial}{\partial x}\left(k \frac{\partial T}{\partial x}\right) + \frac{\partial}{\partial y}\left(k \frac{\partial T}{\partial y}\right) + \frac{\partial}{\partial z}\left(k \frac{\partial T}{\partial z}\right) + \nabla \cdot \left(\overline{\tau} \cdot \overline{v}\right) 
\]
(2-12)

where \(k\) is the thermal conductivity. Gravity effects are not included in either the momentum or energy equations to better observe the piston effect since the relative magnitude of convective heat transfer induced by gravity would mask the effects from the acoustic heating. The total enthalpy, \(H\), is defined as

\[
H = e + \frac{p}{\rho} + \frac{u^2}{2} + \frac{v^2}{2} + \frac{w^2}{2} = E + \frac{p}{\rho} 
\]
(2-13)

where \(e\) is the internal energy and \(E\) is the total internal energy. The viscous contribution to the energy equation source term is given as

\[
\nabla \cdot \left(\overline{\tau} \cdot \overline{v}\right) = \frac{\partial}{\partial x}\left[\mu u \tau_{xx} + \nu \tau_{xy} + \nu \tau_{xz}\right] + \frac{\partial}{\partial y}\left[\mu u \tau_{yx} + \nu \tau_{yy} + \nu \tau_{yz}\right] + \frac{\partial}{\partial z}\left[\mu u \tau_{zx} + \nu \tau_{zy} + \nu \tau_{zz}\right] 
\]
(2-14)

which can be written in Cartesian coordinates as

\[
\nabla \cdot \left(\overline{\tau} \cdot \overline{v}\right) = \frac{\partial}{\partial x}\left[\mu u \left(\frac{4}{3} \frac{\partial u}{\partial x} - \frac{2}{3} \frac{\partial v}{\partial y} - \frac{2}{3} \frac{\partial w}{\partial z}\right)\right] + \mu \nu \left(\frac{\partial v}{\partial x} + \frac{\partial u}{\partial y}\right) + \mu w \left(\frac{\partial w}{\partial x} + \frac{\partial u}{\partial z}\right) 
\]
\[ + \frac{\partial}{\partial y} \left[ \mu \left( \frac{\partial v}{\partial x} \frac{\partial u}{\partial y} \right) + \mu \nu \left( \frac{4}{3} \frac{\partial v}{\partial x} - \frac{2}{3} \frac{\partial u}{\partial x} - \frac{2}{3} \frac{\partial w}{\partial x} \right) + \mu \nu \left( \frac{4}{3} \frac{\partial v}{\partial z} - \frac{2}{3} \frac{\partial u}{\partial z} - \frac{2}{3} \frac{\partial w}{\partial z} \right) \right] \]

\[ + \frac{\partial}{\partial z} \left[ \mu \nu \left( \frac{\partial w}{\partial x} + \frac{\partial u}{\partial z} \right) + \mu \left( \frac{\partial v}{\partial z} + \frac{\partial w}{\partial y} \right) + \mu \nu \left( \frac{4}{3} \frac{\partial w}{\partial z} - \frac{2}{3} \frac{\partial u}{\partial x} - \frac{2}{3} \frac{\partial v}{\partial y} \right) \right] \] (2-15)

The left-hand side of (2-12) can be rewritten as

\[ \frac{\partial \rho E}{\partial t} + \frac{\partial \rho H_u}{\partial x} + \frac{\partial \rho H_v}{\partial y} + \frac{\partial \rho H_w}{\partial z} = \frac{\partial \rho E}{\partial t} + \frac{\partial \rho E_u}{\partial x} + \frac{\partial \rho E_v}{\partial y} + \frac{\partial \rho E_w}{\partial z} + \frac{\partial \rho u}{\partial x} + \frac{\partial \rho v}{\partial y} + \frac{\partial \rho w}{\partial z} \] (2-16)

Inserting (2-13) through (2-16) back into the energy equation (2-12), expanding the derivatives involving the internal energy, \( e \), and applying the continuity equation gives

\[ \rho \frac{\partial e}{\partial t} + \rho u \frac{\partial e}{\partial x} + \rho v \frac{\partial e}{\partial y} + \rho w \frac{\partial e}{\partial z} + \frac{\partial}{\partial y} \left[ \frac{\rho v}{2} \left( u^2 + v^2 + w^2 \right) \right] + \frac{\partial}{\partial z} \left[ \frac{\rho w}{2} \left( u^2 + v^2 + w^2 \right) \right] \]

\[ + \frac{\partial}{\partial y} \left[ \frac{\rho v}{2} \left( u^2 + v^2 + w^2 \right) \right] + \frac{\partial}{\partial z} \left[ \frac{\rho w}{2} \left( u^2 + v^2 + w^2 \right) \right] \]

\[ + \frac{\partial \rho u}{\partial x} + \frac{\partial \rho v}{\partial y} + \frac{\partial \rho w}{\partial z} = \frac{\partial}{\partial x} \left( k \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left( k \frac{\partial T}{\partial y} \right) + \frac{\partial}{\partial z} \left( k \frac{\partial T}{\partial z} \right) \]

\[ + \frac{\partial}{\partial x} \left[ \mu u \left( \frac{4}{3} \frac{\partial u}{\partial x} - \frac{2}{3} \frac{\partial v}{\partial x} - \frac{2}{3} \frac{\partial w}{\partial x} \right) + \mu v \left( \frac{4}{3} \frac{\partial v}{\partial x} - \frac{2}{3} \frac{\partial u}{\partial x} - \frac{2}{3} \frac{\partial w}{\partial x} \right) + \mu w \left( \frac{4}{3} \frac{\partial w}{\partial x} - \frac{2}{3} \frac{\partial u}{\partial x} - \frac{2}{3} \frac{\partial v}{\partial x} \right) \right] \]

\[ + \frac{\partial}{\partial y} \left[ \mu u \left( \frac{4}{3} \frac{\partial u}{\partial y} - \frac{2}{3} \frac{\partial v}{\partial y} - \frac{2}{3} \frac{\partial w}{\partial y} \right) + \mu v \left( \frac{4}{3} \frac{\partial v}{\partial y} - \frac{2}{3} \frac{\partial u}{\partial y} - \frac{2}{3} \frac{\partial w}{\partial y} \right) + \mu w \left( \frac{4}{3} \frac{\partial w}{\partial y} - \frac{2}{3} \frac{\partial u}{\partial y} - \frac{2}{3} \frac{\partial v}{\partial y} \right) \right] \]

\[ + \frac{\partial}{\partial z} \left[ \mu u \left( \frac{4}{3} \frac{\partial u}{\partial z} - \frac{2}{3} \frac{\partial v}{\partial z} - \frac{2}{3} \frac{\partial w}{\partial z} \right) + \mu v \left( \frac{4}{3} \frac{\partial v}{\partial z} - \frac{2}{3} \frac{\partial u}{\partial z} - \frac{2}{3} \frac{\partial w}{\partial z} \right) + \mu w \left( \frac{4}{3} \frac{\partial w}{\partial z} - \frac{2}{3} \frac{\partial u}{\partial z} - \frac{2}{3} \frac{\partial v}{\partial z} \right) \right] \] (2-17)

From thermodynamics we have the variation of internal energy for a compressible fluid given by
\[ \text{de} = C_v \text{dT} - \left[ T \left( \frac{\partial P}{\partial T} \right)_p - P \right] \frac{1}{\rho^2} \, \text{d} \rho \]  

(2-18)

Inserting (2-18) into (2-17), rearranging terms and dividing through by \( C_v \) gives

\[
\frac{\partial P T}{\partial t} + \frac{\partial \rho u T}{\partial x} + \frac{\partial \rho v T}{\partial y} + \frac{\partial \rho w T}{\partial z} - \frac{1}{C_v} \frac{\partial}{\partial x} \left( k \frac{\partial T}{\partial x} \right) - \frac{1}{C_v} \frac{\partial}{\partial y} \left( k \frac{\partial T}{\partial y} \right) - \frac{1}{C_v} \frac{\partial}{\partial z} \left( k \frac{\partial T}{\partial z} \right) =
\]

\[
- \frac{1}{C_v} \frac{\partial \rho u}{\partial x} - \frac{1}{C_v} \frac{\partial \rho v}{\partial y} - \frac{1}{C_v} \frac{\partial \rho w}{\partial z} + \frac{T}{C_v} \left( \frac{\partial P}{\partial T} \right)_p - P \left[ \frac{1}{\rho} \frac{\partial \rho}{\partial t} + \frac{u}{\rho} \frac{\partial \rho}{\partial x} + \frac{v}{\rho} \frac{\partial \rho}{\partial y} + \frac{w}{\rho} \frac{\partial \rho}{\partial z} \right] =
\]

\[
- \frac{1}{C_v} \frac{\partial}{\partial t} \left[ \frac{\rho}{2} \left( u^2 + v^2 + w^2 \right) \right] - \frac{1}{C_v} \frac{\partial}{\partial x} \left[ \frac{\rho u}{2} \left( u^2 + v^2 + w^2 \right) \right]
\]

\[
- \frac{1}{C_v} \frac{\partial}{\partial y} \left[ \frac{\rho v}{2} \left( u^2 + v^2 + w^2 \right) \right] - \frac{1}{C_v} \frac{\partial}{\partial z} \left[ \frac{\rho w}{2} \left( u^2 + v^2 + w^2 \right) \right]
\]

\[
+ \frac{1}{C_v} \frac{\partial}{\partial x} \left[ \mu \left( \frac{4}{3} \frac{\partial u}{\partial x} - \frac{2}{3} \frac{\partial v}{\partial y} - \frac{2}{3} \frac{\partial w}{\partial z} \right) + \mu \left( \frac{\partial v}{\partial x} + \frac{\partial u}{\partial y} \right) + \mu \left( \frac{\partial w}{\partial x} + \frac{\partial u}{\partial z} \right) \right]
\]

\[
+ \frac{1}{C_v} \frac{\partial}{\partial y} \left[ \mu \left( \frac{\partial v}{\partial x} + \frac{\partial u}{\partial y} \right) + \mu \left( \frac{4}{3} \frac{\partial v}{\partial y} - \frac{2}{3} \frac{\partial u}{\partial x} - \frac{2}{3} \frac{\partial w}{\partial z} \right) + \mu \left( \frac{\partial w}{\partial y} + \frac{\partial u}{\partial z} \right) \right]
\]

\[
+ \frac{1}{C_v} \frac{\partial}{\partial z} \left[ \mu \left( \frac{\partial w}{\partial x} + \frac{\partial u}{\partial z} \right) + \mu \left( \frac{\partial v}{\partial z} + \frac{\partial u}{\partial y} \right) + \mu \left( \frac{4}{3} \frac{\partial w}{\partial z} - \frac{2}{3} \frac{\partial u}{\partial x} - \frac{2}{3} \frac{\partial v}{\partial y} \right) \right]
\]  

(2-19)

We want to bring \( C_v \) inside the derivative for the terms involving the thermal conductivity. This will create some new terms in the equation to account for the variable specific heat. After collecting terms and applying the continuity equation, the final form of the energy equation is given as

\[
\frac{\partial P T}{\partial t} + \frac{\partial}{\partial x} \left( \rho u T - \frac{k}{C_v} \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left( \rho u T - \frac{k}{C_v} \frac{\partial T}{\partial y} \right) + \frac{\partial}{\partial z} \left( \rho u T - \frac{k}{C_v} \frac{\partial T}{\partial z} \right) =
\]

\[
\frac{k}{C_v^2} \left( \frac{\partial T}{\partial x} \frac{\partial C_v}{\partial x} + \frac{\partial T}{\partial y} \frac{\partial C_v}{\partial y} + \frac{\partial T}{\partial z} \frac{\partial C_v}{\partial z} \right) - \frac{u}{C_v} \frac{\partial P}{\partial x} - \frac{v}{C_v} \frac{\partial P}{\partial y} - \frac{w}{C_v} \frac{\partial P}{\partial z}
\]

We want to bring \( C_v \) inside the derivative for the terms involving the thermal conductivity. This will create some new terms in the equation to account for the variable specific heat. After collecting terms and applying the continuity equation, the final form of the energy equation is given as

\[
\frac{\partial P T}{\partial t} + \frac{\partial}{\partial x} \left( \rho u T - \frac{k}{C_v} \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left( \rho u T - \frac{k}{C_v} \frac{\partial T}{\partial y} \right) + \frac{\partial}{\partial z} \left( \rho u T - \frac{k}{C_v} \frac{\partial T}{\partial z} \right) =
\]

\[
\frac{k}{C_v^2} \left( \frac{\partial T}{\partial x} \frac{\partial C_v}{\partial x} + \frac{\partial T}{\partial y} \frac{\partial C_v}{\partial y} + \frac{\partial T}{\partial z} \frac{\partial C_v}{\partial z} \right) - \frac{u}{C_v} \frac{\partial P}{\partial x} - \frac{v}{C_v} \frac{\partial P}{\partial y} - \frac{w}{C_v} \frac{\partial P}{\partial z}
\]
\[- \frac{T}{C_v} \left( \frac{\partial P}{\partial T} \right)_p \left( \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} \right) \]

\[- \frac{1}{C_v} \frac{\partial}{\partial t} \left[ \frac{P}{2} (u^2 + v^2 + w^2) \right] - \frac{1}{C_v} \frac{\partial}{\partial x} \left[ \frac{\rho u}{2} (u^2 + v^2 + w^2) \right] \]

\[- \frac{1}{C_v} \frac{\partial}{\partial y} \left[ \frac{\rho v}{2} (u^2 + v^2 + w^2) \right] - \frac{1}{C_v} \frac{\partial}{\partial z} \left[ \frac{\rho w}{2} (u^2 + v^2 + w^2) \right] \]

\[+ \frac{1}{C_v} \frac{\partial}{\partial x} \left[ \mu u \left( \frac{4 \partial u}{3 \partial x} - \frac{2 \partial v}{3 \partial y} - \frac{2 \partial w}{3 \partial z} \right) + \mu v \left( \frac{\partial v}{\partial x} + \frac{\partial u}{\partial y} \right) + \mu w \left( \frac{\partial w}{\partial x} + \frac{\partial u}{\partial z} \right) \right] \]

\[+ \frac{1}{C_v} \frac{\partial}{\partial y} \left[ \mu u \left( \frac{\partial v}{\partial x} + \frac{\partial u}{\partial y} \right) + \mu v \left( \frac{4 \partial v}{3 \partial y} - \frac{2 \partial u}{3 \partial x} - \frac{2 \partial w}{3 \partial z} \right) + \mu w \left( \frac{\partial w}{\partial y} + \frac{\partial u}{\partial z} \right) \right] \]

\[+ \frac{1}{C_v} \frac{\partial}{\partial z} \left[ \mu u \left( \frac{\partial w}{\partial x} + \frac{\partial u}{\partial z} \right) + \mu v \left( \frac{\partial v}{\partial z} + \frac{\partial w}{\partial y} \right) + \mu w \left( \frac{4 \partial w}{3 \partial z} - \frac{2 \partial u}{3 \partial x} - \frac{2 \partial v}{3 \partial y} \right) \right] \quad (2-20) \]

This form of the energy equation for a compressible fluid is a slight modification of the form given by Arpaci and Larsen\textsuperscript{47}. The difference is that the specific heat was brought inside of the derivative for the thermal conductivity. This results in creating a source term involving the derivative of the specific heat. A dimensional analysis was performed on the entire energy equation to determine which portions of the source term are of significance. In one-dimensional Cartesian coordinates the energy equation is given as

\[\frac{\partial \rho T}{\partial t} + \frac{\partial}{\partial x} \left( \rho u T - \frac{k}{C_v} \frac{\partial T}{\partial x} \right) = \frac{k}{C_v} \frac{\partial T}{\partial x} \frac{\partial C_v}{\partial x} - \frac{u}{C_v} \frac{\partial P}{\partial x} - \frac{T}{C_v} \left( \frac{\partial P}{\partial T} \right)_p \frac{\partial u}{\partial x} \]

\[- \frac{1}{C_v} \frac{\partial}{\partial t} \left[ \frac{\rho u^2}{2} \right] - \frac{1}{C_v} \frac{\partial}{\partial x} \left[ \frac{\rho u^3}{2} \right] + \frac{1}{C_v} \frac{\partial}{\partial x} \left[ \mu u \frac{4 \partial u}{3 \partial x} \right] \quad (2-21) \]

The non-dimensional variables are defined as

\[t' = \frac{t c}{L} \quad (2-22a)\]
\[ x' = \frac{x}{L} \]  
(2-22b)

\[ p' = \frac{p}{\rho V^2} \]  
(2-22c)

\[ u' = \frac{u}{V} \]  
(2-22d)

\[ T' = \frac{T}{T_0} \]  
(2-22e)

\[ \rho' = \frac{\rho}{\rho_0} \]  
(2-22f)

\[ k' = \frac{k}{k_0} \]  
(2-22g)

\[ C_v' = \frac{C_v}{C_{v0}} \]  
(2-22h)

\[ \mu' = \frac{\mu}{\mu_0} \]  
(2-22i)

\[ \left( \frac{\partial p}{\partial T} \right)_\rho' = \left( \frac{\partial p}{\partial T} \right)_\rho \left/ \left( \frac{\partial p}{\partial T} \right)_{\rho_0} \right. \]  
(2-22j)

The time is scaled with the acoustic time. The length is scaled with a reference length.

The pressure is scaled with the dynamic pressure. The velocity is scaled with a reference velocity. The reference velocity, \( V \), is the velocity of the fluid after passage of the pressure wave and is much smaller than the speed of sound in the fluid. The temperature and the fluid properties are scaled with the values at the bulk fluid conditions. Plugging equations 2-22 into the energy equation (2-21) gives the following dimensionless form for the energy equation.
\[ \frac{\partial \rho' T'}{\partial t'} + \frac{\partial}{\partial x'} \left( \frac{V}{c} \rho' u' T' - \frac{k_o}{\rho_o C_{v_0} cL} \frac{k'}{C_{v_1}' \frac{\partial T'}{\partial x'}} \right) = \frac{k_o}{\rho_o C_{v_0} cL} \frac{k'}{C_{v_1}'} \frac{\partial T'}{\partial x'} \frac{\partial C_{v_1}'}{\partial x'} \]

\[ - \frac{V^3}{C_{v_0} T_0 c} \frac{u' \frac{\partial P'}{\partial x'}}{C_{v_0}' \frac{\partial T'}{\partial x'}} - \frac{V}{\rho_o c C_{v_0}} \left( \frac{\partial P'}{\partial T'} \right)_{T_0} \frac{T'}{C_{v_1}' \frac{\partial T'}{\partial x'}} \frac{\partial u'}{\partial x'} - \frac{V^2}{T_0 C_{v_0} c} \frac{1}{C_{v_1}'} \frac{\partial}{\partial x'} \frac{1}{2} \frac{\partial}{\partial t'} \rho' u'^2 \]

\[ - \frac{V^3}{C_{v_0} T_0 c} \frac{1}{C_{v_0}'} \frac{\partial}{\partial x'} \frac{2}{2} + \frac{\mu_o V^2}{\rho_o T_0 c L} \frac{1}{C_{v_1}'} \frac{\partial}{\partial x'} \left[ \frac{\mu' u'^4}{3} \frac{\partial u'}{\partial x'} \right] \]

(2-23)

Each of these dimensionless groups was evaluated to determine their magnitudes.

\[ \frac{V}{c} \approx 10^{-3} V \]

(2-24)

\[ \frac{k_o}{\rho_o C_{v_0} c L} \approx 7 \times 10^{-8} \]

(2-25)

\[ \frac{V}{\rho_o c C_{v_0}} \left( \frac{\partial P'}{\partial T'} \right) \approx 2.3 \times 10^{-3} V \]

(2-26)

\[ \frac{V^3}{C_{v_0} T_0 c} \approx 1.3 \times 10^{-8} V^3 \]

(2-27)

\[ \frac{V^2}{T_0 C_{v_0}} \approx 10^{-5} V^2 \]

(2-28)

\[ \frac{\mu_o V^2}{\rho_o T_0 c L} \approx 6 \times 10^{-13} V^2 \]

(2-29)

The acoustic heating term (2-26) is the item of interest in this research so all the dimensionless groups will be compared to the acoustic term. The convection term (2-24) on the left-hand side of the equation is of the same magnitude as the acoustic term so must be included. The variable specific heat term (2-25) is significant if the velocities are less than 0.03 m/s. The variable specific heat term must be included. The diffusion term (2-27) is significant for velocities above 13 m/s so it can be neglected. The kinetic
heating term (2-27 and 2-28) needs velocities above 0.2 m/s to become significant so it can be neglected. Due to the very low viscosity of liquid oxygen the viscous heating term (2-29) needs velocities above 3x10^6 m/s to be significant. The viscous heating contribution is ten orders of magnitude smaller than the acoustic heating term and can be neglected. The only contributions to the source term result from the acoustic heating and the variable specific heat. The dimensionless form of the energy equation reduces to

$$\frac{\partial p' T'}{\partial t'} + \frac{\partial}{\partial x'} \left( \frac{V}{c_p} p' u'T' - \frac{k_0}{\rho_0 C_{v_0} c_L} \frac{k'}{C_{v_0}' \partial x'} \right) = \frac{k_0}{\rho_0 C_{v_0} c_L} \frac{k'}{C_{v_0}^2} \frac{\partial T'}{\partial x'} \frac{\partial C_{v_0}'}{\partial x'}$$

$$- \frac{V}{\rho_0 c C_{v_0}} \left( \frac{\partial P}{\partial \rho} \right) \rho_0 \frac{T'}{C_{v_0}'} \left( \frac{\partial P}{\partial T} \right) \rho \frac{\partial u'}{\partial x'}$$

(2-30)

The algorithm was developed using the dimensional form of the conservation equations since the reference velocity, V, is not known ahead of time. All of the source terms were included in the computer code. The computer code was implemented such that the user could enable or disable the individual contributions to the energy equation source term. Numerous runs were conducted to verify that neglecting the diffusion, viscous and kinetic heating terms did not impact the solution. The energy equation can therefore be reduced to

$$\frac{\partial p T}{\partial t} + \frac{\partial}{\partial x} \left( \rho u T - \frac{k}{C_v} \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left( \rho u T - \frac{k}{C_v} \frac{\partial T}{\partial y} \right) + \frac{\partial}{\partial z} \left( \rho u T - \frac{k}{C_v} \frac{\partial T}{\partial z} \right) =$$

$$- \frac{T}{C_v} \left( \frac{\partial P}{\partial \rho} \right) \left( \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} \right) + \frac{k}{C_v^2} \left( \frac{\partial T}{\partial x} \frac{\partial C_v}{\partial x} + \frac{\partial T}{\partial y} \frac{\partial C_v}{\partial y} + \frac{\partial T}{\partial z} \frac{\partial C_v}{\partial z} \right)$$

(2-31)

For the two-dimensional case this reduces to

$$\frac{\partial p T}{\partial t} + \frac{\partial}{\partial x} \left( \rho u T - \frac{k}{C_v} \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left( \rho u T - \frac{k}{C_v} \frac{\partial T}{\partial y} \right) = - \frac{T}{C_v} \left( \frac{\partial P}{\partial \rho} \right) \left( \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right)$$
\[
\frac{k}{C_v^2} \left( \frac{\partial T}{\partial x} \frac{\partial c_v}{\partial x} + \frac{\partial T}{\partial y} \frac{\partial c_v}{\partial y} \right)
\]

(2-32)

The source term can now be defined as

\[
S = -\frac{T}{C_v} \left( \frac{\partial p}{\partial T} \right)_p \left( \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right) + \frac{k}{C_v^2} \left( \frac{\partial T}{\partial x} \frac{\partial c_v}{\partial x} + \frac{\partial T}{\partial y} \frac{\partial c_v}{\partial y} \right)
\]

(2-33)

This form of the source term shows that heating in the bulk fluid results from fluid motion. The pressure derivative, \( \left( \frac{\partial P}{\partial T} \right)_p \), acts as an amplification factor and is a function of the chosen equation of state. According to the real gas equation of state, the pressure derivative is given as

\[
\left( \frac{\partial P}{\partial T} \right)_p = -\alpha \beta
\]

(2-34)

\[
\alpha = -\rho \left( \frac{\partial P}{\partial \rho} \right)_T
\]

(2-35)

\[
\beta = \frac{1}{\rho} \left( \frac{\partial P}{\partial \rho} \right)_p \left( \frac{\partial P}{\partial \rho} \right)_T
\]

(2-36)

where \( \alpha \) is the isothermal bulk modulus and \( \beta \) is the volume expansivity. For a van der Waals fluid, \( P = \frac{\rho RT}{1-\rho b} - \alpha \rho^2 \), the pressure derivative, the isothermal bulk modulus and the volume expansivity are given, respectively, as

\[
\left( \frac{\partial P}{\partial T} \right)_p = \frac{\rho R}{1-\rho b}
\]

(2-37)

\[
\alpha = -\rho \left( \frac{\partial P}{\partial \rho} \right)_T = \left\{ \frac{b \rho^2 RT}{(1-b \rho)^2} + \frac{\rho RT}{(1-b \rho)} - 2\alpha \rho^2 \right\}
\]

(2-38)
\[
\beta = \frac{1}{\rho} \left( \frac{\partial P}{\partial T} \right)_p / \left( \frac{\partial P}{\partial \rho} \right)_T = \frac{\left( \frac{\rho R}{1 - \rho b} \right) \left\{ \frac{b \rho^2 R T}{(1 - \rho b)^2} + \frac{\rho R T}{(1 - \rho b)} - 2 \alpha^2 \right\}}{\left( \frac{\rho R}{1 - \rho b} \right) - \left\{ \frac{b \rho^2 R T}{(1 - \rho b)^2} + \frac{\rho R T}{(1 - \rho b)} - 2 \alpha^2 \right\}}
\] (2-39)

Looking at the energy equation (2-32) some additional observations can be made. As the fluid approaches the critical point, \( C_v \) increases greatly and the effect of the right hand side can be neglected. Thus, the effect of acoustic heating is important only outside of the thermal boundary layer. On the left-hand side of the equation, the ratio of the thermal conductivity over the specific heat diverges to infinity and the thermal gradient term dominates the time dependence of the temperature.

The thermal diffusivity for a constant pressure process is given by \( D_{th} = k / \rho C_p \). When approaching the critical point \( C_v \) diverges approximately twice as fast as the thermal conductivity and therefore the thermal diffusivity goes to zero. As a result, extremely long thermal equilibration times are predicted, explaining the common observation of slowing thermal equilibration when approaching the critical point. This observation applies only for a constant pressure process. The thermal diffusivity for a constant volume process is given by \( D_{th} = k / \rho C_v \). In this case, the thermal conductivity diverges faster than \( C_v \) and the thermal diffusivity goes to infinity. The thermal equilibration time for a constant volume process, therefore, approaches zero, speeding up when approaching the critical point.
Two different time scales are identified in this problem: (1) the acoustic time and (2) the diffusion time. The acoustic time, \( t_a = L/c \) where \( L \) is the thickness of the fluid sample and \( c \) is the speed of sound in the fluid, is the time required for a pressure wave to travel the length of the container. The diffusion time, \( t_D = L^2 / D_\text{th} \) where \( D_\text{th} \) is the thermal diffusivity, is the time for a temperature change to be transmitted the length of the container by pure diffusion. The acoustic time is much smaller than the diffusion time.

Acoustic waves are created by the changing thermal boundary layer thickness during the heating and cooling of the heat transfer surface and dissipate shortly after a stable boundary temperature is achieved. These acoustic waves are the mechanism by which heat is transferred from the heat transfer surface to the bulk fluid. This process is referred to as the piston effect. Kassoy\(^3\) showed that the strength of the acoustic wave is dependent on the magnitude of the temperature change and how rapidly the fluid properties vary with temperature. Since the fluid properties show the greatest sensitivity at the critical point this suggests that the acoustic waves will be strongest when near the critical point of the fluid.

For the two-phase system the piston effect increases the pressure on both the liquid and vapor phases during heating. Due to differences in the fluid properties the vapor increases in temperature faster than the liquid when pressurized. This results in a superheated vapor in contact with a subcooled liquid. Evaporation mass transfer is now the mechanism by which the two phases can exchange heat. Since this is a slow process long thermal equilibration times are observed for the two-phase system as compared to
the single-phase system. During cooling from the single-phase region into the two-phase region the thermal boundary layer shrinks and the bulk fluid expands isentropically into the volume once occupied by the thermal boundary layer. The resulting liquid and vapor interface is nearly at the same temperature during the process. In both phases homogeneous nucleation occurs and simultaneously bubbles are created in the liquid phase and droplets are created in the vapor phase. Due to the latent heat transferred during the subsequent growth of these bubbles and droplets the surrounding fluid comes back to the saturation condition. Fast energy transfer takes place due to the large interfacial surface area created during this process. The energy transfer process drives the cooled two-phase system back into equilibrium whereas the heated two-phase system is driven away from equilibrium. This agrees with the observations of Straub et al.\textsuperscript{30} where the bulk fluid was seen to closely follow the wall temperatures.

Dahl and Moldover\textsuperscript{21} speculated that the slow thermal equilibration observed in the two-phase system was due to mass transfer (evaporation or condensation) at the liquid-vapor interface causing a restriction to heat transfer, which is not present in the single-phase system. This restriction results in significantly longer times for the system to come to thermal equilibrium. On the acoustic time scale the temperature and pressure are nearly homogeneous in the single-phase fluid outside of the thermal boundary layer. The entropy change caused by the sudden change in the boundary temperature still follows the diffusive relaxation. For a two-phase fluid the rate of thermal transport follows the diffusive relaxation until very close to the critical point of the fluid. Thus the system experiences a slowing down of thermal transport when approaching the critical point
from the two-phase region but a speeding up when approaching from the single-phase region. Onuki and Ferrell\textsuperscript{15} showed that even the two-phase system demonstrates a critical speeding up when very close to the critical point. This research effort will focus only on the single-phase system.

A review of the equations for the conservation of mass, momentum, and energy for a compressible fluid identified the significant thermophysical properties that play a role in predicting the temperature and pressure response of a fluid near the critical point. The most important properties were determined to be the thermal conductivity, the volume expansivity, and the isothermal compressibility. The thermal conductivity and the volume expansivity determine the thickness of the thermal boundary layer. Experimental and numerical analyses have shown that the thermal boundary layer can be considered to be a piston compressing or expanding the bulk fluid. The isothermal compressibility determines the pressure response of the bulk fluid due to the change in volume of the thermal boundary layer. A solution algorithm is needed to numerically investigate the pressure sensitivity near the critical point.
A solution algorithm was desired that could handle the extreme compressibility expected near the critical point. The Semi-Implicit Method for Pressure Linked Equations (SIMPLE) algorithm developed by Patankar\textsuperscript{48} was selected since it avoids the problems that could be encountered with most solution algorithms that employ the speed of sound as a scaling factor to normalize the fluid velocities. The fluid velocities encountered in this research are very small (Mach 10\textsuperscript{-6}) and scaling with the speed of sound would increase the stiffness of the solution matrix. An alternative means of properly scaling the compressible flow equations for the low Mach number condition\textsuperscript{49} is to use a characteristic fluid velocity instead of the speed of sound. Since this requires prior knowledge of some characteristic fluid velocity it was not practical in this problem. The SIMPLE algorithm avoids the need for scaling of the velocities. Since the SIMPLE algorithm treats most terms implicitly, with only a few terms being evaluated explicitly, it allows for a wide range of time step sizes and grid sizes while providing a stable solution.

The computational domain and some significant dimensions need to be defined before discussing the solution algorithm. For easier understanding only the derivation of the two-dimensional version of the SIMPLE algorithm will be presented. Extension to a three-dimensional algorithm will become easily understood. Figure 3-1 shows the two-dimensional grid used in the SIMPLE algorithm.
Figure 3-1 Two-dimensional staggered grid structure used in the SIMPLE algorithm
A staggered grid arrangement is employed to avoid the checkerboard effect common when both the fluid properties and velocities are co-located at the center of the control volume. A uniform grid structure is used with the fluid property nodes located at the center of each control volume. A non-uniform grid structure would require more complicated extrapolations to provide the information needed at the face of each cell. The width of each control volume is denoted by $\Delta X$ and the height by $\Delta Y$ and are the same for all control volumes. The distance from the property node to the east and west faces of the control volume is given by $\Delta X/2$ since the property node is located at the center of the control volume. Similarly, the distance from the property node to the north and south faces of the control volume is given by $\Delta Y/2$ since the property node is located at the center of the control volume. The distance from the center of the control volume to center of the control volume to the east and west are given by $\delta X_e$ and $\delta X_w$, respectively. Similarly, the distance from the center of the control volume to the center of the control volume to the north and south are given by $\delta Y_n$ and $\delta Y_s$, respectively.

Next, the $x$-direction velocity nodes, $U$, are located halfway between the property nodes at the center of the control volumes. For a uniform grid this places them on the center of the east and west faces of the control volume. The $y$-direction velocity nodes, $V$, are located halfway between the property nodes at the center of the control volumes. For a uniform grid this places them on the center of the north and south faces. To create a non-uniform grid appropriate interpolations would be required to determine the velocities on the faces of the control volumes. The final step is to surround the entire domain with a row of zero-volume control volumes. These zero-volume control volumes are
placeholders to permit easy handling of the boundary conditions. The SIMPLE algorithm solves the conservation equations for the primitive variables $u$, $v$, $P$ and $T$.

**SIMPLE Algorithm**

Start with the x-direction momentum equation, written in Cartesian coordinates.

$$
\frac{\partial pu}{\partial t} + \frac{\partial pu^2}{\partial x} + \frac{\partial puv}{\partial y} = -\frac{\partial P}{\partial x} + \frac{\partial}{\partial x}\left( \frac{4}{3} \mu \frac{\partial u}{\partial x} - \frac{2}{3} \mu \frac{\partial v}{\partial y} \right) + \frac{\partial}{\partial y}\left( \mu \frac{\partial u}{\partial y} + \mu \frac{\partial v}{\partial x} \right)
$$

(2-10)

Combine the mass flux and diffusion flux into a single term.

$$
J_x = \rho u u - \mu \frac{\partial u}{\partial x}
$$

(3-1)

$$
J_y = \rho v u - \mu \frac{\partial u}{\partial y}
$$

(3-2)

Define the source term as

$$
S = -\frac{\partial P}{\partial x} + \frac{\partial}{\partial x}\left( \mu \frac{1}{3} \frac{\partial u}{\partial x} - \mu \frac{2}{3} \frac{\partial v}{\partial y} \right) + \frac{\partial}{\partial y}\left( \mu \frac{\partial v}{\partial x} \right)
$$

(3-3)

This now allows for a much simpler form of the momentum equation.

$$
\frac{\partial pu}{\partial t} + \frac{\partial J_x}{\partial x} + \frac{\partial J_y}{\partial y} = S
$$

(3-4)

This form expresses the momentum equation as an accumulation term, two flux terms, and a source term. Integrate the momentum equation (3-4) over the control volume to get

$$
\left( \rho_p u_p - \rho_p u_p^e \right) \frac{\Delta X \Delta Y}{\Delta t} + J_e - J_w + J_n - J_s = S \Delta X \Delta Y
$$

(3-5)

where the flux terms are defined as

$$
J_e = \left( \int J_x \, dy \right)_e
$$

(3-6)
\begin{align*}
J_w &= \left( \int J_x \, dy \right)_w \\
J_n &= \left( \int J_y \, dx \right)_n \\
J_s &= \left( \int J_y \, dx \right)_s
\end{align*}

Integrate the continuity equation (2-2) over the control volume to get

\[ \left( \rho_p - \rho_p^0 \right) \frac{\Delta X \Delta Y}{\Delta t} + F_e - F_w + F_n - F_s = 0 \]  \hspace{1cm} (3-10)

where the mass flux terms are given by

\begin{align*}
F_e &= \rho_e u_e \Delta Y \\
F_w &= \rho_w u_w \Delta Y \\
F_n &= \rho_n v_n \Delta X \\
F_s &= \rho_s v_s \Delta X
\end{align*}  \hspace{1cm} (3-11) - (3-14)

Multiply the continuity equation (3-10) by the x-direction velocity, \( u_p \), and subtract from the momentum equation (3-5) to get

\[ \left( u_p - u_p^0 \right) \rho_p \frac{\Delta X \Delta Y}{\Delta t} + \left( J_e - u_p F_e \right) - \left( J_w - u_p F_w \right) + \left( J_n - u_p F_n \right) - \left( J_s - u_p F_s \right) = S \Delta X \Delta Y \]  \hspace{1cm} (3-15)

A simple velocity difference across each face of the control volume will be substituted for the flux terms.

\begin{align*}
J_e - u_p F_e &= a_E \left( u_p - u_E \right) \\
J_w - u_p F_w &= a_W \left( u_w - u_p \right) \\
J_n - u_p F_n &= a_N \left( u_p - u_N \right)
\end{align*}  \hspace{1cm} (3-16) - (3-18)
\[ J_s - u_p F_s = a_s (u_s - u_p) \]  \hspace{1cm} (3-19)

The coefficient in the velocity difference is a term that relates the relative importance of the mass flux and diffusion flux terms on that face of the control volume. The diffusion flux terms are given by

\[ D_e = \frac{\mu_e \Delta Y}{\delta X_e} \]  \hspace{1cm} (3-20)

\[ D_w = \frac{\mu_w \Delta Y}{\delta X_w} \]  \hspace{1cm} (3-21)

\[ D_n = \frac{\mu_n \Delta X}{\delta Y_n} \]  \hspace{1cm} (3-22)

\[ D_s = \frac{\mu_s \Delta X}{\delta Y_s} \]  \hspace{1cm} (3-23)

The coefficients in (3-16) through (3-19) can be expressed as a simple power law relationship of the Peclet number. This power law relationship closely approximates the exact solution for the one-dimensional problem.

\[ \text{Pe}_i = \frac{F_i}{D_i} \]  \hspace{1cm} (3-24)

\[ A(\text{Pe}) = [[0, (1 - 0.1|\text{Pe}|^3)] \]  \hspace{1cm} (3-25)

The symbol \([a, b]\) represents the maximum of the two values \(a\) or \(b\). Now the coefficients for each face of the control volume can be defined as

\[ a_e = D_e A(\text{Pe}_e) + [-F_e, 0] \]  \hspace{1cm} (3-26)

\[ a_w = D_w A(\text{Pe}_w) + [F_w, 0] \]  \hspace{1cm} (3-27)

\[ a_n = D_n A(\text{Pe}_n) + [-F_n, 0] \]  \hspace{1cm} (3-28)
\[ a_s = D_sA([P_{es}], [[F_x,0]]) \] (3-29)

This results in using an upwind scheme for the mass fluxes on the faces of the control volume. Refer to the book by Patankar\(^48\) for a complete derivation of (3-25) through (3-29). The time derivative term is evaluated using the density at the previous time step.

\[ a_p^0 = \rho_p^0 \frac{\Delta X \Delta Y}{\Delta t} \] (3-30)

The non-linearities in the source term are handled by rewriting the source term in a linear form.

\[ S = S + \left( \frac{\partial S}{\partial u} \right) (u_p^* - u_p) = S_C + S_v u_p^* \] (3-31)

The starred quantities are the values at the current iteration and the unstarred quantities are the values at the previous iteration.

\[ S = -\frac{\partial P}{\partial x} + \frac{\partial}{\partial x} \left( \mu \frac{1}{3} \frac{\partial u}{\partial x} - \mu \frac{2}{3} \frac{\partial v}{\partial y} \right) + \frac{\partial}{\partial y} \left( \mu \frac{\partial v}{\partial x} \right) \] (3-32)

Expressing in finite difference notation gives

\[ S = -\frac{P_e - P_w}{\Delta X} - \left( \frac{\mu_e}{3\Delta X \delta X_e} + \frac{\mu_w}{3 \Delta X \delta X_w} \right) u_p + \frac{\mu_e}{3 \Delta X \delta X_e} u_E + \frac{\mu_w}{3 \Delta X \delta X_w} u_w \]

\[ - \frac{2\mu_e}{3\Delta X \Delta Y} (v_{ne} - v_{se}) + \frac{2\mu_w}{3\Delta X \Delta Y} (v_{nw} - v_{sw}) + \frac{\mu_n}{\Delta X \Delta Y} (v_{ne} - v_{nw}) \]

\[ - \frac{\mu_e}{\Delta X \Delta Y} (v_{se} - v_{sw}) - \left( \frac{\mu_e}{3 \Delta X \delta X_e} + \frac{\mu_w}{3 \Delta X \delta X_w} \right) (u_p^* - u_p) \] (3-33)

which reduces to

\[ S_C = -\frac{P_e - P_w}{\Delta X} + \frac{\mu_e}{3 \Delta X \delta X_e} u_E + \frac{\mu_w}{3 \Delta X \delta X_w} u_w - \frac{2\mu_e}{3 \Delta X \Delta Y} (v_{ne} - v_{se}) \]
\[+ \frac{2\mu_v}{3\Delta X\Delta Y} (v_{sw} - v_{nw}) + \frac{\mu_s}{\Delta X\Delta Y} (v_{se} - v_{sw}) - \frac{\mu_v}{\Delta X\Delta Y} (v_{se} - v_{sw}) \]  

(3-34)

\[
S_U = \left( \frac{\mu_s}{3\Delta X\Delta X_e} + \frac{\mu_v}{3\Delta X\Delta X_w} \right) 
\]

(3-35)

\[S_U \] represents the linear dependence of the source term on the x-direction velocity and \(S_C\) represents the non-linear dependencies and all other terms not dependent on the x-direction velocity. The coefficient for the node at the center of the control volume is then defined by

\[a_p = a_E + a_w + a_N + a_s + a_p^0 - S_U \Delta X\Delta Y \]  

(3-36)

The remaining terms are collected on the right hand side.

\[b = a_p^0 u_p^0 + S_C \Delta X\Delta Y \]  

(3-37)

Substitute (3-11) through (3-14) and (3-16) through (3-37) back into the momentum equation (3-15) to get

\[a_p u_p^* = a_E u_E^* + a_w u_w^* + a_N u_N^* + a_s u_s^* + b \]  

(3-38)

Underrelaxation is employed to provide a more stable solution. Start by rewriting (3-38) by dividing through by \(a_p\) to get

\[u_p^* = \frac{a_E u_E^* + a_w u_w^* + a_N u_N^* + a_s u_s^* + b}{a_p} \]  

(3-39)

Add and subtract the x-direction velocity, \(u_p\), from the previous time step to the right hand side of (3-39).

\[u_p^* = u_p + \left( \frac{a_E u_E^* + a_w u_w^* + a_N u_N^* + a_s u_s^* + b}{a_p} - u_p \right) \]  

(3-40)
The contents of the parentheses are seen to be the change in the velocity at the current iteration. This change can be modified by the introduction of an underrelaxation factor, \( \alpha_u \), to limit the rate of change of the velocity.

\[
\dot{u}_p^* = u_p + \alpha_u \left( \frac{a_E u_E^* + a_W u_W^* + a_N u_N^* + a_S u_S^* + b}{a_p} - u_p \right)
\]  

(3-41)

Rearranging (3-41) gives the final form of the momentum equation.

\[
\frac{a_p}{\alpha_u} \dot{u}_p^* = a_E u_E^* + a_W u_W^* + a_N u_N^* + a_S u_S^* + b + (1 - \alpha_u) \frac{a_p}{\alpha_u} u_p
\]  

(3-42)

All the quantities involved are evaluated at the current time step, except for \( a_p^0 \) and \( u_p^0 \), which are evaluated at the previous time step. This is why the algorithm is called the Semi-Implicit Method for Pressure Linked Equations. No modification to the momentum equation is required to accommodate the boundary conditions since either the x-direction velocities, \( U \), are defined on the boundary or a symmetry condition is used.

A similar process is used to develop the y-momentum equation. Start with the y-direction momentum equation written in Cartesian coordinates.

\[
\frac{\partial p v}{\partial t} + \frac{\partial p v u}{\partial x} + \frac{\partial p v^2}{\partial y} = -\frac{\partial p}{\partial y} + \frac{\partial}{\partial y} \left( \mu \frac{\partial u}{\partial y} + \mu \frac{\partial v}{\partial x} \right) + \frac{\partial}{\partial y} \left( \frac{4}{3} \mu \frac{\partial v}{\partial y} - \frac{2}{3} \mu \frac{\partial u}{\partial x} \right)
\]  

(2-11)

Combine the mass flux and the diffusion flux into a single term.

\[
J_x = \rho u v - \mu \frac{\partial v}{\partial x}
\]  

(3-43)

\[
J_y = \rho v^2 - \mu \frac{\partial v}{\partial y}
\]  

(3-44)

Define the source term as...
\[ S = -\frac{\partial P}{\partial y} + \frac{\partial}{\partial x} \left( \mu \frac{\partial u}{\partial y} \right) + \frac{\partial}{\partial y} \left( \frac{1}{3} \mu \frac{\partial v}{\partial y} - \frac{2}{3} \mu \frac{\partial u}{\partial x} \right) \] (3-45)

This now allows for a much simpler form of the momentum equation.

\[ \frac{\partial \rho v}{\partial t} + \frac{\partial J_x}{\partial x} + \frac{\partial J_y}{\partial y} = S \] (3-46)

This form expresses the momentum equation as an accumulation term, two flux terms, and a source term. Integrate the momentum equation (3-46) over the control volume to get

\[ \left( \rho_r v_r - \rho_r^0 v_r^0 \right) \frac{\Delta X \Delta Y}{\Delta t} + J_e - J_w + J_n - J_s = S \Delta X \Delta Y \] (3-47)

where the flux terms are defined as

\[ J_e = \left( \int J_s \, dy \right)_e \] (3-48)

\[ J_w = \left( \int J_s \, dy \right)_w \] (3-49)

\[ J_n = \left( \int J_s \, dx \right)_n \] (3-50)

\[ J_s = \left( \int J_s \, dx \right)_s \] (3-51)

Multiply the continuity equation (3-10) by the y-direction velocity, \( v_p \), and subtract from the momentum equation (3-47) to get

\[ \left( v_p - v_p^0 \right) \rho_p \Delta X \Delta Y + \left( J_e - v_p F_e \right) - \left( J_w - v_p F_w \right) + \left( J_n - v_p F_n \right) - \left( J_s - v_p F_s \right) = S \Delta X \Delta Y \] (3-52)

where the mass flux terms are given by

\[ F_e = \rho_u u_e \Delta Y \] (3-53)

\[ F_w = \rho_w u_w \Delta Y \] (3-54)
\[ F_n = \rho_n v_n \Delta X \]  
\[ F_s = \rho_s v_s \Delta X \]  

(3-55)  
(3-56)

A simple velocity difference across each face of the control volume will be substituted for the flux terms.

\[ J_e - v_p F_e = a_E (v_p - v_E) \]  
\[ J_w - v_p F_w = a_w (v_w - v_p) \]  
\[ J_n - v_p F_n = a_N (v_p - v_N) \]  
\[ J_s - v_p F_s = a_S (v_s - v_p) \]  

(3-57)  
(3-58)  
(3-59)  
(3-60)

The coefficient in the velocity difference is a term that relates the relative importance of the mass flux and diffusion flux terms on that face of the control volume. The diffusion flux terms are given by

\[ D_e = \frac{\mu_e \Delta Y}{\delta X_e} \]  
\[ D_w = \frac{\mu_w \Delta Y}{\delta X_w} \]  
\[ D_n = \frac{\mu_n \Delta X}{\delta Y_n} \]  
\[ D_s = \frac{\mu_s \Delta X}{\delta Y_s} \]  

(3-61)  
(3-62)  
(3-63)  
(3-64)

The coefficients in (3-57) through (3-60) can be expressed as a simple power law relationship of the Peclet number. This power law relationship closely approximates the exact solution for the one-dimensional problem.
\[ \text{Pe}_i = \frac{F_i}{D_i} \quad (3-65) \]

\[ A(\text{Pe}) = [0, (1 - 0.1|\text{Pe}|)^{1.5}] \quad (3-66) \]

The symbol \([a, b])\) represents the maximum of the two values \(a\) or \(b\). Now the coefficients for each face of the control volume can be defined as

\[ a_e = D_eA(|\text{Pe}_e|) + [F_e, 0] \quad (3-67) \]

\[ a_w = D_wA(|\text{Pe}_w|) + [F_w, 0] \quad (3-68) \]

\[ a_n = D_nA(|\text{Pe}_n|) + [F_n, 0] \quad (3-69) \]

\[ a_s = D_sA(|\text{Pe}_s|) + [F_s, 0] \quad (3-70) \]

This results in using an upwind scheme for the mass fluxes on the faces of the control volume. The time derivative term is evaluated using the density at the previous time step.

\[ a_p = \rho_p^0 \frac{\Delta X \Delta Y}{\Delta t} \quad (3-71) \]

The non-linearities in the source term are handled by rewriting the source term in a linear form.

\[ S = S + \left( \frac{\partial S}{\partial v} \right) (v_p^* - v_p) = S_c + S_v v_p^* \quad (3-72) \]

The starred quantities are the values at the current iteration and the unstarred quantities are the values at the previous iteration.

\[ S = -\frac{\partial p}{\partial y} + \frac{\partial}{\partial x} \left( \mu \frac{\partial u}{\partial y} \right) + \frac{\partial}{\partial y} \left( \frac{1}{3} \mu \frac{\partial v}{\partial y} - \frac{2}{3} \mu \frac{\partial u}{\partial x} \right) \quad (3-73) \]

Expressing in finite difference notation gives
\[ S = -\frac{P_s - P_e}{\Delta Y} + \frac{\mu_e}{\Delta X \Delta Y} (u_{ne} - u_{se}) - \frac{\mu_w}{\Delta X \Delta Y} (u_{nw} - u_{sw}) - \frac{2\mu_n}{3\Delta X \Delta Y} (u_{ne} - u_{nw}) \]

\[ + \frac{2\mu_s}{3\Delta X \Delta Y} (u_{ne} - u_{sw}) + \frac{\mu_n}{3\Delta Y \delta Y_n} v_N + \frac{\mu_s}{3\Delta Y \delta Y_s} v_s \]

\[ - \left( \frac{\mu_n}{3\Delta Y \delta Y_n} + \frac{\mu_s}{3\Delta Y \delta Y_s} \right) v_p - \left( \frac{\mu_n}{3\Delta Y \delta Y_n} + \frac{\mu_s}{3\Delta Y \delta Y_s} \right) (v_p^* - v_p) \quad (3.74) \]

which reduces to

\[ S_C = -\frac{P_s - P_e}{\Delta Y} + \frac{\mu_e}{\Delta X \Delta Y} (u_{ne} - u_{se}) - \frac{\mu_w}{\Delta X \Delta Y} (u_{nw} - u_{sw}) - \frac{2\mu_n}{3\Delta X \Delta Y} (u_{ne} - u_{nw}) \]

\[ + \frac{2\mu_s}{3\Delta X \Delta Y} (u_{ne} - u_{sw}) + \frac{\mu_n}{3\Delta Y \delta Y_n} v_N + \frac{\mu_s}{3\Delta Y \delta Y_s} v_s \quad (3.75) \]

\[ S_V = -\left( \frac{\mu_n}{3\Delta Y \delta Y_n} + \frac{\mu_s}{3\Delta Y \delta Y_s} \right) \quad (3.76) \]

\( S_V \) represents the linear dependence of the source term on the y-direction velocity and \( S_C \) represents the non-linear dependencies and all other terms not dependent on the y-direction velocity. The coefficient for the node at the center of the control volume is defined by

\[ a_p = a_E + a_W + a_N + a_S + a_p^0 - S_V \Delta X \Delta Y \quad (3.77) \]

The remaining terms are collected on the right hand side.

\[ b = a_p^0 v_p^0 + S_C \Delta X \Delta Y \quad (3.78) \]

Substitute (3.53) through (3.78) back into the momentum equation (3.52) to get

\[ a_p^* v_p^* = a_E v_E^* + a_W v_W^* + a_N v_N^* + a_S v_S^* + b \quad (3.79) \]
Underrelaxation is employed to provide a more stable solution. Start by rewriting (3-79) by dividing through by \( a_p \) to get

\[
v_p^* = \frac{a_E v_E^* + a_W v_W^* + a_N v_N^* + a_S v_S^* + b}{a_p}
\]

(3-80)

Add and subtract the \( y \)-direction velocity, \( v_p \), from the previous time step to the right hand side of (3-80).

\[
v_p^* = v_p + \left( \frac{a_E v_E^* + a_W v_W^* + a_N v_N^* + a_S v_S^* + b}{a_p} - v_p \right)
\]

(3-81)

The contents of the parentheses are seen to be the change in the velocity at the current iteration. This change can be modified by the introduction of an underrelaxation factor, \( \alpha_v \), to limit the rate of change of the velocity.

\[
v_p^* = v_p + \alpha_v \left( \frac{a_E v_E^* + a_W v_W^* + a_N v_N^* + a_S v_S^* + b}{a_p} - v_p \right)
\]

(3-82)

Rearranging (3-82) gives the final form of the momentum equation.

\[
\frac{a_p}{\alpha_v} v_p^* = a_E v_E^* + a_W v_W^* + a_N v_N^* + a_S v_S^* + b + \left( 1 - \alpha_v \right) \frac{a_p}{\alpha_v} v_p
\]

(3-83)

All the quantities involved are evaluated at the current time step, except for \( a_p^0 \) and \( v_p^0 \), which are evaluated at the previous time step. No modification to the momentum equation is required to accommodate the boundary conditions since either the \( y \)-direction velocities, \( V \), are defined on the boundary or a symmetry condition is used.
Compressible Pressure Correction

A method of linking the velocity corrections and the pressure corrections is needed.

Following the approach recommended by Patankar the continuity equation is the starting point for developing a pressure correction equation. Integrate the continuity equation (2-2) over the control volume to get

\[
\left( \rho_p - \rho_p^* \right) \frac{\Delta X \Delta Y}{\Delta t} + \left[ \left( \rho u \right)_e - \left( \rho u \right)_w \right] \Delta Y + \left[ \left( \rho v \right)_n - \left( \rho v \right)_s \right] \Delta X = 0
\]  (3-84)

Define a velocity update based on the difference in the pressure updates across that face of the control volume.

\[
u_e = u_e^* + u_e = u_e^* + \frac{d}{A} \left( P_p^* - P_{p_1}^* \right)
\]  (3-85)

\[
u_w = u_w^* + u_w = u_w^* + \frac{d}{A} \left( P_w^* - P_{p_1}^* \right)
\]  (3-86)

\[
u_n = v_n^* + v_n = v_n^* + \frac{d}{A} \left( P_p^* - P_{n_1}^* \right)
\]  (3-87)

\[
u_s = v_s^* + v_s = v_s^* + \frac{d}{A} \left( P_s^* - P_{n_1}^* \right)
\]  (3-88)

The starred values represent the current values of each parameter and the primed values are the corrections to be added to each parameter at the current iteration. The pressure difference coefficients are defined as

\[
d_e = \frac{A_e}{a_{pe}}
\]  (3-89)

\[
d_w = \frac{A_w}{a_{pw}}
\]  (3-90)

\[
d_n = \frac{A_n}{a_{pe}}
\]  (3-91)
\[ d_s = \frac{A_s}{a_{ps}} \]  

(3-92)

where \( A \) is the face area of the control volume and \( a_p \) is the coefficient from the momentum equation corresponding to the velocity node located on that face of the control volume. The density update equations are a simple linear function of the pressure update.

\[ \rho_e = \rho_{e}^{*} + \rho_{e} = \rho_{e}^{*} + \left( \frac{\partial p}{\partial p} \right)_e p' \]  

(3-93)

\[ \rho_w = \rho_{w}^{*} + \rho_{w} = \rho_{w}^{*} + \left( \frac{\partial p}{\partial p} \right)_w p' \]  

(3-94)

\[ \rho_a = \rho_{a}^{*} + \rho_{a} = \rho_{a}^{*} + \left( \frac{\partial p}{\partial p} \right)_a p' \]  

(3-95)

\[ \rho_s = \rho_{s}^{*} + \rho_{s} = \rho_{s}^{*} + \left( \frac{\partial p}{\partial p} \right)_s p' \]  

(3-96)

\[ \rho_p = \rho_{p}^{*} + \rho_{p} = \rho_{p}^{*} + \left( \frac{\partial p}{\partial p} \right)_p p' \]  

(3-97)

The temperature dependence of the density update can be ignored since the SIMPLE algorithm is an iterative solver. The temperature dependence will be included when evaluating the density from the equation of state. Insert (3-85) through (3-97) into the continuity equation (3-84) to get

\[
\left( \rho_{p}^{*} + \left( \frac{\partial p}{\partial p} \right)_p p_{p} - \rho_{p}^{e} \right) \frac{\Delta X \Delta Y}{\Delta t} + \rho_{c}^{*} u_{c}^{*} \Delta Y + \rho_{c}^{*} d_{c} (p_{p} - p_{E}) \Delta Y + u_{c}^{*} \left( \frac{\partial p}{\partial p} \right)_e p_{e} \Delta Y \\
- \rho_{w}^{*} u_{w} \Delta Y - \rho_{w}^{*} d_{w} (p_{w} - p_{p}) \Delta Y - u_{w}^{*} \left( \frac{\partial p}{\partial p} \right)_w p_{w} \Delta Y
\]
\[ + \rho_a \cdot \nabla^* \Delta X + \rho_e \cdot \nabla^* \left( P_p - P_n \right) \Delta X \nabla^* \left( \frac{\partial P}{\partial p} \right) \Delta X \]

\[ - \rho_s \cdot \nabla^* \Delta X - \rho_s \cdot \nabla^* \left( P_s - P_p \right) \Delta X - \nabla^* \left( \frac{\partial P}{\partial p} \right) \Delta X = 0 \]  

(3-98)

Linear interpolations will be used to give the pressure update at the control volume face based on the pressure update values at the center of the control volumes.

\[ \left( \rho_p^* \left( \frac{\partial P}{\partial p} \right) \Delta X \Delta Y + \rho_e \cdot \nabla^* \Delta Y + \rho_e \cdot \nabla^* \left( P_p - P_e \right) \Delta Y \right. \]

\[ \left. + u_e^* \left( \frac{\partial P}{\partial p} \right) \left( P_p \left[ 1 - \frac{\Delta X}{28 X_e} \right] + P_e \left[ \frac{\Delta X}{28 X_e} \right] \right) \Delta Y - \rho_p \cdot u_e^* \Delta Y - \rho_p \cdot \nabla^* \left( P_w - P_p \right) \Delta Y \right. \]

\[ - u_w^* \left( \frac{\partial P}{\partial p} \right) \left( P_t \left[ 1 - \frac{\Delta X}{28 X_w} \right] + P_w \left[ \frac{\Delta X}{28 X_w} \right] \right) \Delta Y + \rho_w \cdot \nabla^* \Delta Y + \rho_w \cdot \nabla^* \left( P_p - P_w \right) \Delta Y \]

\[ + v_s^* \left( \frac{\partial P}{\partial p} \right) \left( P_p \left[ 1 - \frac{\Delta Y}{28 Y_s} \right] + P_s \left[ \frac{\Delta Y}{28 Y_s} \right] \right) \Delta X - \rho_s \cdot v_s^* \Delta X - \rho_s \cdot \nabla^* \left( P_s - P_p \right) \Delta X \]

\[ - v_s^* \left( \frac{\partial P}{\partial p} \right) \left( P_p \left[ 1 - \frac{\Delta Y}{28 Y_s} \right] + P_s \left[ \frac{\Delta Y}{28 Y_s} \right] \right) \Delta X = 0 \]  

(3-99)

The following terms are defined to simplify the final form of the pressure update equation.

\[ a_{E1} = \rho_e \cdot d_e \Delta Y \]  

(3-100)

\[ a_{E2} = u_e \left( \frac{\partial P}{\partial p} \right) \Delta Y \]  

(3-101)

\[ a_E = a_{E1} - a_{E2} \left[ \frac{\Delta X}{28 X_e} \right] \]  

(3-102)

\[ a_{W1} = \rho_w \cdot d_w \Delta Y \]  

(3-103)
\[ a_{w2} = u_w \left( \frac{\partial p}{\partial P} \right)_w \Delta Y \]  
(3-104)

\[ a_w = a_{w1} + a_{w2} \left[ \frac{\Delta X}{2\delta X_w} \right] \]  
(3-105)

\[ a_{N1} = \rho_s d_s \Delta X \]  
(3-106)

\[ a_{N2} = v_n \left( \frac{\partial p}{\partial P} \right)_n \Delta X \]  
(3-107)

\[ a_N = a_{N1} - a_{N2} \left[ \frac{\Delta Y}{2\delta Y_n} \right] \]  
(3-108)

\[ a_{s1} = \rho_s d_s \Delta X \]  
(3-109)

\[ a_{s2} = v_s \left( \frac{\partial p}{\partial P} \right)_s \Delta X \]  
(3-110)

\[ a_s = a_{s1} + a_{s2} \left[ \frac{\Delta Y}{2\delta Y_s} \right] \]  
(3-111)

The mass accumulation term is concentrated at the center of the control volume

\[ a_{p2} = \left( \frac{\partial p}{\partial P} \right)_p \frac{\Delta X \Delta Y}{\Delta t} \]  
(3-112)

The coefficient for the node at the center of the control volume can now be written as

\[ a_p = a_{E1} + a_{E2} \left[ 1 - \frac{\Delta X}{2\delta X_e} \right] + a_{w1} - a_{w2} \left[ 1 - \frac{\Delta X}{2\delta X_w} \right] + a_{N1} + a_{w2} \left[ 1 - \frac{\Delta Y}{2\delta Y_n} \right] \]

\[ + a_{s1} - a_{s2} \left[ 1 - \frac{\Delta Y}{2\delta Y_s} \right] + a_{p2} \]  
(3-113)

The remaining terms are collected on the right hand side

\[ b = \left( \rho_p - \rho_p^* \right) \frac{\Delta X \Delta Y}{\Delta t} + \left[ (\rho^* u^*) - (\rho^* u^*_e) \right] \Delta Y + \left[ (\rho^* v^*) - (\rho^* v^*_s) \right] \Delta X \]  
(3-114)
The right hand side of (3-114) is simply the continuity equation at the previous iteration.

The purpose of the pressure update equation is to correct the velocities coming out of the momentum equations so that they satisfy the continuity equation. The right hand side also provides a handy indicator of when to terminate the iterations and proceed to the next time step. As the iterations proceed the right hand side will approach zero as the velocities approach the correct solution. Substitute (3-100) through (3-114) back into the continuity equation (3-99) to get

\[ a_p \dot{P}_p = a_e \dot{P}_e^* + a_w \dot{P}_w^* + a_n \dot{P}_n^* + a_s \dot{P}_s^* + b \]  

(3-115)

The pressure is updated each iteration by

\[ P = P^* + \dot{P}^* \]  

(3-116)

The pressure update is limited by introducing an underrelaxation factor, \( \alpha_p \), into (3-116).

\[ P = P^* + \alpha_p \dot{P}^* \]  

(3-117)

The full pressure update is used to update the velocities according to (3-85) through (3-88). The underrelaxation on the pressure is applied only to the pressure field. All the quantities involved are evaluated at the current time step, except for \( \rho_p^0 \), which is evaluated at the previous time step. The pressure is either specified at the boundary or reflection boundary conditions are used.

Left boundary

If \( U \) is specified: \( a_{w1} = 0 \)  

(3-118)

If \( P \) is specified: \( a_{w2} = 0 \)  

(3-119)
Right boundary

If $U$ is specified: $a_{e_1} = 0$  \hspace{1cm} (3-120)

If $P$ is specified: $a_{e_2} = 0$  \hspace{1cm} (3-121)

Top boundary

If $V$ is specified: $a_{N_1} = 0$  \hspace{1cm} (3-122)

If $P$ is specified: $a_{N_2} = 0$  \hspace{1cm} (3-123)

Bottom boundary

If $V$ is specified: $a_{s_1} = 0$  \hspace{1cm} (3-124)

If $P$ is specified: $a_{s_2} = 0$  \hspace{1cm} (3-125)

For the reflection boundary condition the pressure derivative is also set to zero at the boundary.

Left boundary

$$\left( \frac{\partial P}{\partial x} \right)_w = 0$$  \hspace{1cm} (3-126)

Right boundary

$$\left( \frac{\partial P}{\partial x} \right)_e = 0$$  \hspace{1cm} (3-127)

Top boundary

$$\left( \frac{\partial P}{\partial y} \right)_s = 0$$  \hspace{1cm} (3-128)

Bottom boundary

$$\left( \frac{\partial P}{\partial y} \right)_s = 0$$  \hspace{1cm} (3-129)
The incompressible form of the pressure update equation can be recovered by setting the density derivative, \( \frac{\partial \rho}{\partial P} \), to zero. The coefficients given by (3-102), (3-105), (3-108), (3-111) and (3-113) are unstable since there is the possibility of negative coefficients. One solution to this problem is to convert the coefficients to an upwind scheme. This is the approach suggested by Patankar\(^4\). The corrected coefficients become

\[
a_E = a_{E1} + \left[ -a_{E2} \left( \frac{\Delta X}{2\delta X_e} \right), 0 \right]
\]

(3-130)

\[
a_w = a_{w1} + \left[ a_{w2} \left( \frac{\Delta X}{2\delta X_w} \right), 0 \right]
\]

(3-131)

\[
a_N = a_{N1} + \left[ -a_{N2} \left( \frac{\Delta Y}{2\delta Y_n} \right), 0 \right]
\]

(3-132)

\[
a_S = a_{S1} + \left[ a_{S2} \left( \frac{\Delta Y}{2\delta Y_s} \right), 0 \right]
\]

(3-133)

\[
a_P = a_{E1} + \left[ a_{E2} \left( 1 - \frac{\Delta X}{2\delta X_e} \right), 0 \right] + a_{w1} + \left[ -a_{w2} \left( 1 - \frac{\Delta X}{2\delta X_w} \right), 0 \right] + a_{N1} + \left[ a_{N2} \left( 1 - \frac{\Delta Y}{2\delta Y_n} \right), 0 \right] + a_{S1} + \left[ -a_{S2} \left( 1 - \frac{\Delta Y}{2\delta Y_s} \right), 0 \right] + a_{P2}
\]

(3-134)

The symbol \([a, b]\) represents the maximum of the two values \(a\) or \(b\). The upwind scheme guarantees that the coefficients are always positive in value. A much simpler pressure update is obtained when the compressibility is applied only to node \(P\) and not to
the neighboring nodes. This is accomplished by setting the density derivative, \( \frac{\partial \rho}{\partial \rho} \), equal to zero for the neighboring nodes. The nodal coefficients above then reduce to

\[
a_E = a_{Ei} \tag{3-135}
\]

\[
a_W = a_{Wi} \tag{3-136}
\]

\[
a_N = a_{Ni} \tag{3-137}
\]

\[
a_S = a_{Si} \tag{3-138}
\]

\[
a_P = a_{Ei} + a_{Wi} + a_{Ni} + a_{Si} + a_{p2} \tag{3-139}
\]

This change to the pressure update is permitted since any form of the pressure update equation will work as long as the pressure update goes to zero as the solution approaches the actual solution. The inclusion of the compressibility term to only the center node results in a system that is diagonally dominant and stable. Without the term \( a_{p2} \) the pressure update equation would become indeterminant to within a constant since pressure only shows up in the first derivatives. This term stabilizes the pressure update equation such that it gives a unique solution. The boundary conditions are the same as before.

**Energy equation**

Start with the energy equation written in Cartesian coordinates.

\[
\frac{\partial}{\partial t} (\rho T) + \frac{\partial}{\partial x} \left( \rho u T \frac{k}{C_v} \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left( \rho v T \frac{k}{C_v} \frac{\partial T}{\partial y} \right) = -\frac{T}{C_v} \left( \frac{\partial \rho}{\partial \rho} \right) \left( \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right) + \frac{k}{C_v^2} \left( \frac{\partial T}{\partial x} \frac{\partial C_v}{\partial x} + \frac{\partial T}{\partial y} \frac{\partial C_v}{\partial y} \right) \tag{2-32}
\]

Combine the mass flux and diffusion flux into a single term.
\[ J_x = p u T - \frac{k}{C_v} \frac{\partial T}{\partial x} \]  
\[ J_y = \rho v T - \frac{k}{C_v} \frac{\partial T}{\partial y} \]  

(3-140)

(3-141)

The real gas source term was defined as

\[ S = -\frac{T}{C_v} \left( \frac{\partial P}{\partial T} \right)_p \left( \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right) + \frac{k}{C_v^2} \left( \frac{\partial T}{\partial x} \frac{\partial C_v}{\partial x} + \frac{\partial T}{\partial y} \frac{\partial C_v}{\partial y} \right) \]  

(2-33)

This now allows for a much simpler form of the energy equation.

\[ \frac{\partial \rho T}{\partial t} + \frac{\partial J_x}{\partial x} + \frac{\partial J_y}{\partial y} = S \]  

(3-142)

This form expresses the energy equation as an accumulation term, two flux terms, and a source term. Integrate the energy equation (3-142) over the control volume to get

\[ \frac{(\rho_p T_p - \rho_p^0 T_p^0)}{\Delta t} \Delta X \Delta Y + J_e - J_w + J_n - J_s = S \Delta X \Delta Y \]  

(3-143)

where the flux terms are defined as

\[ J_e = \left( \int J_x \, dy \right)_e \]  

(3-144)

\[ J_w = \left( \int J_x \, dy \right)_w \]  

(3-145)

\[ J_n = \left( \int J_x \, dx \right)_n \]  

(3-146)

\[ J_s = \left( \int J_x \, dx \right)_s \]  

(3-147)

Multiply the continuity equation (3-10) by the temperature, \( T_p \), and subtract from the energy equation (3-143) to get
\[(T_p - T_p^o) \rho_p \frac{\Delta X \Delta Y}{\Delta t} + (J_e - T_p F_e) + (J_w - T_p F_w) + (J_n - T_p F_n) - (J_s - T_p F_s) = S \Delta X \Delta Y \]  

(3-148)

where the mass flux terms are given by

\[F_e = \rho_e u_e \Delta Y\]  

(3-149)

\[F_w = \rho_w u_w \Delta Y\]  

(3-150)

\[F_n = \rho_n v_n \Delta X\]  

(3-151)

\[F_s = \rho_s v_s \Delta X\]  

(3-152)

A simple temperature difference across each face of the control volume will be substituted for the flux terms.

\[J_e - T_p F_e = a_e(T_p - T_e)\]  

(3-153)

\[J_w - T_p F_w = a_w(T_w - T_p)\]  

(3-154)

\[J_n - T_p F_n = a_n(T_p - T_n)\]  

(3-155)

\[J_s - T_p F_s = a_s(T_s - T_p)\]  

(3-156)

The coefficient in the temperature difference is a term that relates the relative importance of the mass flux and diffusion flux terms on that face of the control volume. The diffusion flux terms are given by

\[D_e = \frac{k_e \Delta Y}{C_{ve} \delta X_e}\]  

(3-157)

\[D_w = \frac{k_w \Delta Y}{C_{vw} \delta X_w}\]  

(3-158)

\[D_n = \frac{k_n \Delta X}{C_{vn} \delta Y_n}\]  

(3-159)
\[ D_* = \frac{k_* \Delta X}{C_{v_*} \delta Y_*} \]  
(3-160)

The coefficient can be expressed as a simple power law relationship of the Peclet number. This power law relationship closely approximates the exact solution for the one-dimensional problem.

\[ \text{Pe}_i = \frac{F_i}{D_i} \]  
(3-161)

\[ A([\text{Pe}]) = \left[ [0, (1 - 0.1|\text{Pe}|)^5] \right] \]  
(3-162)

The symbol \([a, b]]\) represents the maximum of the two values \(a\) or \(b\). Now the coefficients for each face of the control volume can be defined as

\[ a_E = D_E A(\left|\text{Pe}_e\right|) + [-F_e, 0] \]  
(3-163)

\[ a_W = D_W A(\left|\text{Pe}_w\right|) + [F_w, 0] \]  
(3-164)

\[ a_N = D_N A(\left|\text{Pe}_n\right|) + [-F_n, 0] \]  
(3-165)

\[ a_S = D_S A(\left|\text{Pe}_s\right|) + [F_s, 0] \]  
(3-166)

This results in using an upwind scheme for the mass fluxes on the faces of the control volume. The time derivative term is evaluated using the density at the previous time step.

\[ a_p^0 = \rho_p^0 \frac{\Delta X \Delta Y}{\Delta t} \]  
(3-167)

The non-linearities in the source term are handled by rewriting the source term in a linear form.

\[ S = S + \left( \frac{\partial S}{\partial T} \right) (T_p^* - T_p) = S_c + S_T T_p^* \]  
(3-168)
The starred quantities are the values at the current iteration and the unstarred quantities are the values at the previous iteration.

\[
S = -\frac{T}{C_v}\left(\frac{\partial P}{\partial T}\right)_p \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y}\right) + \frac{k}{C_v^2} \left(\frac{\partial C_v}{\partial x} \frac{\partial \rho}{\partial x} + \frac{\partial C_v}{\partial y} \frac{\partial \rho}{\partial y}\right)
\]  

(2-23)

Expressing in finite difference notation gives

\[
S = -\frac{T^*}{C_{v,p}^*}\left(\frac{\partial P}{\partial T}\right)_{p,\Delta}\left[\frac{u_x^* - u_w^*}{\Delta x} + \frac{v_y^* - v_z^*}{\Delta y}\right] + \frac{k_p^*}{C_{v,p}^{*2}} \left[\frac{T_{e^*} - T_{w^*}}{\Delta x} \frac{C_{ve}^* - C_{vw}^*}{\Delta x} + \frac{T_{s^*} - T_{l^*}}{\Delta y} \frac{C_{vs}^* - C_{vs}^*}{\Delta y}\right]
\]

(3-169)

which reduces to

\[
S_C = \frac{k_p^*}{C_{v,p}^{*2}} \left[\frac{T_{e^*} - T_{w^*}}{\Delta x} \frac{C_{ve}^* - C_{vw}^*}{\Delta x} + \frac{T_{s^*} - T_{l^*}}{\Delta y} \frac{C_{vs}^* - C_{vs}^*}{\Delta y}\right]
\]

(3-170)

\[
S_T = -\frac{1}{C_{v,p}^*} \left(\frac{\partial P}{\partial T}\right)_{p,\Delta} \left[\frac{u_x^* - u_w^*}{\Delta x} + \frac{v_y^* - v_z^*}{\Delta y}\right]
\]

(3-171)

\(S_T\) represents the linear dependence of the source term on the temperature and \(S_C\) represents the non-linear dependencies and all other terms not dependent on the temperature. The pressure derivative term, \(\left(\frac{\partial P}{\partial T}\right)_{p}\), is evaluated based upon the particular equation of state being used. The definitions for the pressure derivative, the isothermal bulk modulus, and the isothermal volume expansivity are given by (2-24) through (2-29) in chapter 2. This form of the source term is unstable since \(S_T\) can become positive if the velocity derivatives become negative. A change is made that ensures \(S_T\) is always negative.
\[ C_1 = -\frac{1}{C'_{vp}} \left( \frac{\partial P}{\partial T} \right)_{pL} \left[ \frac{u^*_e - u^*_w}{\Delta x} + \frac{v^*_n - v^*_s}{\Delta y} \right] \]  
(3-172)

\[ S_C = T_p \left[ [C_1, 0] \right] + \frac{k_p^*}{C'_{vp}^2} \left[ \frac{T^*_e - T^*_w}{\Delta x} \frac{C'_{ve} - C'_{vw}}{\Delta x} + \frac{T^*_n - T^*_s}{\Delta y} \frac{C'_{vn} - C'_{vs}}{\Delta y} \right] \]  
(3-173)

\[ S_T = -[[ -C_1, 0]] \]  
(3-174)

The symbol \([[a, b]]\) represents the maximum of the two values a or b. The derivation of the energy equation source term including the diffusion, viscous and kinetic heating terms is included the appendix. The coefficient for the node at the center of the control volume is defined by

\[ a_p = a_E + a_w + a_N + a_s + a_p^0 - S_T \Delta X \Delta Y \]  
(3-175)

The remaining terms are collected on the right hand side.

\[ b = a_p^0 T_p^0 + S_C \Delta X \Delta Y \]  
(3-176)

Substituting (3-149) through (3-176) back into the energy equation (3-148) gives

\[ a_p T_p^* = a_E T_E^* + a_w T_w^* + a_N T_N^* + a_s T_s^* + b \]  
(3-177)

Underrelaxation is employed to provide a more stable solution. Start by rewriting (3-177) by dividing through by \(a_p\) to get

\[ T_p^* = \frac{a_E T_E^* + a_w T_w^* + a_N T_N^* + a_s T_s^* + b}{a_p} \]  
(3-178)

Add and subtract the temperature from the previous time step to the right hand side of (3-178).

\[ T_p^* = T_p + \left( \frac{a_E T_E^* + a_w T_w^* + a_N T_N^* + a_s T_s^* + b}{a_p} - T_p \right) \]  
(3-179)
The contents of the parentheses are seen to be the change in the temperature at the current iteration. This change can be modified by the introduction of an underrelaxation factor, \( \alpha_r \), to limit the rate of change of the temperature.

\[
T_p^* = T_p + \alpha_r \left( \frac{a_E T_E^* + a_W T_W^* + a_N T_N^* + a_S T_S^* + b}{a_p} - T_p \right)
\]  

(3-180)

Rearranging (3-180) gives the final form of the energy equation

\[
\frac{a_p}{\alpha_r} T_p^* = a_E T_E^* + a_W T_W^* + a_N T_N^* + a_S T_S^* + b + \left( 1 - \alpha_r \right) \frac{a_p}{\alpha_r} T_p
\]  

(3-181)

A reference temperature is introduced so that the energy equation is used to solve for a delta from the reference temperature instead of the absolute temperature. This allows for a very small temperature change to be resolved against a much higher background temperature. Start by replacing the absolute temperatures in (3-181) with a reference temperature and a delta temperature.

\[
\frac{a_p}{\alpha_r} \left( \delta T_p + T_{ref} \right) = a_E \left( \delta T_E^* + T_{ref} \right) + a_W \left( \delta T_W^* + T_{ref} \right) + a_N \left( \delta T_N^* + T_{ref} \right) + a_S \left( \delta T_S^* + T_{ref} \right)
\]

\[+ a_p \left( \delta T_p^* + T_{ref} \right) + S_c \Delta X \Delta Y + \left( 1 - \alpha_r \right) \frac{a_p}{\alpha_r} \left( \delta T_p + T_{ref} \right)
\]

(3-182)

Rearrange (3-182) to collect the reference temperatures on the right hand side of the equation.

\[
\frac{a_p}{\alpha_r} \delta T_p^* = a_E \delta T_E^* + a_W \delta T_W^* + a_N \delta T_N^* + a_S \delta T_S^* + a_p \delta T_p^* + S_c \Delta X \Delta Y
\]

\[+ \left( 1 - \alpha_r \right) \frac{a_p}{\alpha_r} \delta T_p + \left( a_p^0 + a_E + a_W + a_N + a_S - a_p \right) T_{ref}
\]

(3-183)
Apply (3-175) to the terms in brackets before the reference temperature to simplify (3-183).

\[
\frac{a_p}{\alpha_T} \delta T_p^* = a_e \delta T_E^* + a_w \delta T_E^* + a_N \delta T_N^* + a_s \delta T_S^* + a_p^0 \delta T_p^0 + S_c \Delta X \Delta Y
\]

\[+(1 - \alpha_T) \frac{a_p}{\alpha_T} \delta T_p + S_T \Delta T_{\text{ref}} \Delta X \Delta Y \]  

(3-184)

Define a new term, \( b^* \), similar to (3-176).

\[b^* = a_p^0 \delta T_p^0 + S_c \Delta X \Delta Y + S_T \Delta T_{\text{ref}} \Delta X \Delta Y = b - a_p^0 T_{\text{ref}} + S_T \Delta T_{\text{ref}} \Delta X \Delta Y \]  

(3-185)

Equation (3-185) is a modification of (3-176) to include a contribution from the reference temperature. The final form of the energy equation is now given as

\[
\frac{a_p}{\alpha_T} \delta T_p^* = a_e \delta T_E^* + a_w \delta T_E^* + a_N \delta T_N^* + a_s \delta T_S^* + b^* + (1 - \alpha_T) \frac{a_p}{\alpha_T} \delta T_p
\]  

(3-186)

This form of the energy equation will allow resolution of small temperature changes that are many orders of magnitude smaller than the average temperature. All the quantities involved are evaluated at the current time step, except for \( a_p^0, T_p^0 \) and \( \delta T_p^0 \), which are evaluated at the previous time step. The boundary conditions are either a specified temperature or a symmetry boundary condition.

**SIMPLE Algorithm**

The SIMPLE algorithm is an iterative process.

1) Start with an assumed pressure field.
2) Solve the x-direction momentum equation using a tridiagonal solver. Perform a line update in the x-direction, sweeping through the y-direction. Then perform a line update in the y-direction, sweeping through x-direction.

3) Solve the y-direction momentum equation using a tridiagonal solver. Perform a line update in the x-direction, sweeping through the y-direction. Then perform a line update in the y-direction, sweeping through the x-direction.

4) Solve the pressure update equation using a tridiagonal solver. Perform a line update in the x-direction, sweeping through the y-direction. Update the velocities and pressure using this pressure update. Then perform a line update in the y-direction, sweeping through the x-direction. Again update the velocities and pressure using the new pressure updates.

5) Solve the energy equation using a tridiagonal solver. Perform a line update in the x-direction, sweeping through the y-direction. Then perform a line update in the y-direction, sweeping through the x-direction.

6) Repeat steps 2 through 5 until the right hand side of the final pressure update in step 4 is sufficiently small, then proceed to the next time step.

Performing the line update in the x-direction followed by a line update in the y-direction each pass through the algorithm ensures that the boundary conditions at all four boundaries are brought into the interior of the calculation domain in the least number of iterations. The SIMPLE code was validated by repeating the analyses presented by Zappoli et.al.\textsuperscript{14}
Typical implementations of computational fluid dynamic (CFD) software access the equation of state whenever the fluid property is needed. This works fine if using the ideal gas law or the van der Waals equation of state. This type of implementation results in a slowly executing code when working with a real gas equation of state. A one-dimensional SIMPLE algorithm code was first implemented by evaluating the equation of state at each node when a fluid property was required. At each node the fluid property at the node under investigation, as well as the two neighboring nodes, is needed. This resulted in accessing the equation of state \(12N + 4\) times to make one pass through the SIMPLE code, where \(N\) is the number of control volumes. The time per iteration is shown in Figure 3-2 for a case employing 1000 control volumes. The three different equations of state were evaluated. The ideal gas law was used to establish a baseline performance. The performance when using the van der Waals (VDW) equation of state and when using a real gas equation of state provided by the National Institute of Standards and Technology (NIST) were then evaluated. When using the van der Waals equation of state the SIMPLE code required about twice the time required for the ideal gas law. The NIST equation of state needed about 12 times longer than the ideal gas law. When using the ideal gas law the program spent about 41% of the time in the fluids property section. This increased to 74% for the VDW equation of state and 95% for the NIST equation of state. This identified the fluids property code as the major time consumer during execution of the computer code.

The thermophysical properties used in the SIMPLE algorithm are the density, viscosity, thermal conductivity, constant volume specific heat, isothermal compressibility (the
inverse of the isothermal bulk modulus), and the volume expansivity. Except for the
density all the fluid properties are given as functions of temperature and density. The
equation of state gives the pressure as a function of temperature and density. The ideal
gas law allows for the direct solution of density given the pressure and temperature. The
van der Waals equation of state is a cubic polynomial in density. It is possible to directly
solve for the density but common practice is to iterate on the density until sufficient
accuracy is achieved. The van der Waals equation was rewritten as

$$\rho = \frac{-ab\rho^3 + a\rho^2 + P}{b\rho + RT} \quad (3-187)$$

Six hundred (600) iterations provided six significant digits of accuracy on the density.

The real gas equation of state provided by NIST\(^1\) is a 33-term polynomial, which gives
the pressure as a function of temperature and density.

$$P = \rho RT + \rho^3 \left( C_1 T + C_2 \sqrt{T} + C_3 + \frac{C_4}{T} + \frac{C_5}{T^2} \right) + \rho^4 \left( C_6 T + C_7 + \frac{C_8}{T} + \frac{C_9}{T^2} \right)$$

$$+ \rho^5 \left( C_{10} T + C_{11} + \frac{C_{12}}{T} \right) + C_{13} \rho^6 + \rho^6 \left( \frac{C_{14}}{T} + \frac{C_{15}}{T^2} \right) + C_{16} \frac{\rho^7}{T} + \rho^8 \left( \frac{C_{17}}{T} + \frac{C_{18}}{T^2} \right)$$

$$+ C_{19} \frac{\rho^9}{T^2} + \exp(C_0 \rho^3) \{ C_{20} \frac{\rho^3}{T^2} + C_{21} \frac{\rho^3}{T^3} + C_{22} \frac{\rho^5}{T^2} + C_{23} \frac{\rho^5}{T^3} + C_{24} \frac{\rho^7}{T^2} + C_{25} \frac{\rho^7}{T^3} \}$$

$$+ C_{26} \frac{\rho^9}{T^2} + C_{27} \frac{\rho^9}{T^4} + C_{28} \frac{\rho^{11}}{T^2} + C_{29} \frac{\rho^{11}}{T^3} + C_{30} \frac{\rho^{13}}{T^2} + C_{31} \frac{\rho^{13}}{T^3} + C_{32} \frac{\rho^{13}}{T^4} \} \quad (3-188)$$

In order to solve for the density a root solver is used to find the density as a function of
temperature and pressure. This is where the computer code spent the majority of its time
for the real gas density.
After reviewing the SIMPLE algorithm it was determined that the fluid properties only change twice during one pass through the algorithm. The fluid properties are updated after the pressure update and again after solving the energy equation. The SIMPLE computer code was therefore modified to store all fluid properties in a matrix. The SIMPLE computer code would access the matrix to get the fluid properties when any nodal property was required. The matrix would be updated after the pressure update and again after solving the energy equation. This reduced the number of calls to the equation of state from $12N + 4$ to $2N + 4$. The number of calls to the fluid property subroutine was reduced by a factor of six. The performance of the modified SIMPLE code with the storage matrix is shown in Figure 3-3. The VDW equation of state still runs about twice as long as the ideal gas law and the NIST equation of state still takes 12 times longer than the ideal gas law. The total time per iteration is reduced significantly. Storing the fluid properties in a matrix resulted in getting a factor of seven improvement in the time per iteration. The SIMPLE code still spends about 58% of the time evaluating the VDW equation of state and about 89% of the time evaluating the NIST equation of state. The memory requirement of the code is twice as large as before but this is offset by the factor of seven improvement in speed.
Figure 3-2 SIMPLE algorithm performance for the three different equations of state when accessing the fluids code each time a fluid property is required
Figure 3-3 SIMPLE algorithm performance for the three different equations of state when accessing the fluid property from a storage matrix.
Further improvements in performance could be accomplished by either using an equation of state that gives the density directly as a function of temperature and pressure or employing a look-up table to provide the density as a function of temperature and pressure.

The next chapter discusses the results from a series of one-dimensional analyses conducted to compare the pressure sensitivity of oxygen based on using the van der Waals equation of state and the NIST equation of state. These analyses show the influence that the equation of state has on the pressure response of a fluid at the critical point. Then analyses were conducted to compare the pressure response of oxygen and hydrogen near the critical point. These analyses show the influence of the thermophysical properties on the pressure response.
Chapter 4 – Analysis Results

The previous research into the fast thermal equalization of a fluid at the critical point used only the van der Waals equation of state at temperatures within mK of the critical point. This will be the starting point for this research effort. The thermophysical properties involved in the energy equation are the density, thermal conductivity, constant volume specific heat, isothermal compressibility (the inverse of the isothermal bulk modulus), and the volume expansivity. The properties of oxygen will be examined to determine what differences in behavior are noticeable when using either the van der Waals equation of state or the NIST equation of state. This comparison is performed to determine the effect that the selection of the equation of state has on the pressure and temperature response of a fluid near the critical point. The temperature of the bulk fluid will also be examined at conditions well below the critical temperature. The most important properties for the piston effect were determined to be the thermal conductivity, the volume expansivity, and the isothermal compressibility. The thermal conductivity and the volume expansivity determine the thickness of the thermal penetration region. Experimental and numerical analyses have shown that the thermal penetration region can be considered to be a piston compressing or expanding the bulk fluid. The isothermal compressibility determines the pressure response of the bulk fluid to the change in volume of the thermal penetration region.
The variation of the density and the pressure derivative, \( \left( \frac{\partial p}{\partial T} \right)_p \), with temperature based on the use of the van der Waals and NIST equations of state are compared in Figure 4-1. The pressure is held constant at the critical pressure of oxygen, 5043 kPa. The density prediction from the van der Waals equation of state underpredicts the actual density by approximately 30 percent over most of the temperature range. The van der Waals equation of state became unstable for temperatures below 100 K. The density is solved by iterating on the van der Waals equation of state. This iterative process fails to converge to a stable solution below 100 K. This is expected since the van der Waals equation of state is a modification of the ideal gas law and does not provide a good density prediction for the subcooled liquid state. The van der Waals equation provides a good estimate for the saturated liquid state but the error increases as the fluid conditions get farther away from the saturation condition. In the compressed gas region, above 156 K, the correlation is much closer. The 30 percent reduction in density would require a corresponding increase in the velocity in order to satisfy the conservation of continuity. Therefore it is expected that the velocity of the bulk fluid after the passage of the pressure wave will exhibit higher velocities when using the van der Waals equation of state. The van der Waals equation of state overpredicts the pressure derivative by a factor of two. The pressure derivative is used in the energy equation source term and therefore it is expected to observe less heating in the bulk fluid when using the van der Waals equation of state compared to the NIST equation of state.
Figure 4-1 Variation of the density and the pressure derivative with temperature for oxygen at 5043 kPa. The solid lines represent values from the NIST equation of state and the dashed lines represent values using the van der Waals equation of state.
The pressure derivative can be decomposed into the isothermal compressibility and the
volume expansivity. The variation of the isothermal compressibility and the volume
expansivity with temperature based on the use of the van der Waals and NIST equations
of state are compared in Figure 4-2. The isothermal compressibility is shown multiplied
by $-1$ to simplify the plot. The pressure is again held constant at the critical pressure of
oxygen, 5043 kPa. The volume expansivity determines how much the thermal
penetration region will expand due to the temperature increase at the boundary. The van
der Waals equation of state does a fairly good job of reproducing the volume expansivity.
It even predicts the divergence at the critical temperature. The isothermal compressibility
determines the pressure response of the bulk fluid due to the change in volume of the
thermal boundary layer. The van der Waals equation of state reproduces the divergence
in the isothermal compressibility at the critical point. Over the majority of the subcooled
liquid region the van der Waals equation of state overpredicts the compressibility by a
factor of two. This shows that the error in the pressure derivative caused by using the van
der Waals equation of state is entirely due to the error in the isothermal compressibility.
A larger absolute value of the isothermal compressibility indicates a greater
compressibility of the fluid. A larger volume change would therefore occur for a small
pressure change when near the critical point. The inverse would also hold true, for a
large volume change the pressure would change only a small amount when near the
critical point. If the fluid is much colder than the critical temperature then the fluid will
respond as an incompressible liquid. Therefore the compressibility effects will be
isolated to the thermal penetration region. The van der Waals equation of state will
underpredict the pressure response of the bulk liquid by a factor of two.
Figure 4-2 Variation of the isothermal compressibility and the volume expansivity with temperature for oxygen at 5043 kPa. The solid lines represent values from the NIST equation of state and the dashed lines represent values using the van der Waals equation of state. The isothermal compressibility is shown multiplied by $-1$ for plotting purposes.
This effect had not been encountered in prior research since all the previous numerical investigations of the piston effect were evaluated using only the van der Waals equation of state at conditions very close to the critical point.

All the remaining fluid properties are evaluated from the NIST computer program. The variation of the thermal conductivity and the specific heat at constant volume with temperature are shown in Figure 4-3. The pressure is again held constant at the critical pressure of oxygen, 5043 kPa. The thermal conductivity of the liquid oxygen decreases by a factor of four as the temperature increases towards the critical temperature. There is a large divergence at the critical point and then the thermal conductivity continues to decrease as the oxygen temperature continues to increase. The specific heat at constant volume shows only a slight variation in the liquid region. There is a large divergence at the critical temperature and then the value continues to decrease as the temperature is increased. The van der Waals numerical analyses and the NIST numerical analyses using fixed fluid properties use the same thermal conductivity so the thickness of the penetration depth region will be the same. The NIST numerical analyses using variable fluid properties will result in a higher thermal conductivity in the penetration depth region due to the divergence of the thermal conductivity at the critical point. This will result in a thinner penetration depth compared to using fixed fluid properties. The thinner penetration depth will result in a lower pressure increase compared to the analyses using fixed fluid properties.
Figure 4-3 Variation of the thermal conductivity and the specific heat at constant volume with temperature for oxygen at 5043 kPa. Both functions are from values given by the NIST.
The variation of the viscosity and the speed of sound with temperature are shown in Figure 4-4. The pressure is again held constant at the critical pressure of oxygen, 5043 kPa. The viscosity of oxygen decreases by a factor of four as the oxygen is heated up. There is a sharp decrease in the viscosity at the critical temperature and then a gradual decrease as the gaseous oxygen is heated further. The speed of sound decreases as the fluid is heated to the critical temperature and then stabilizes at approximately 200 m/s for the gas phase. For each numerical simulation the speed of sound was evaluated based on the initial temperature of the bulk fluid and was held constant for each run. The values used in the numerical analyses are shown in Table 4-1.

Table 4-1 Speed of sound for oxygen and acoustic times used for the numerical simulations.

<table>
<thead>
<tr>
<th>Temperature, K</th>
<th>Reduced Temperature, T/Tc</th>
<th>Speed of Sound, M/s</th>
<th>Acoustic time, μsec</th>
<th>Thermal Diffusivity, cm²/s</th>
<th>Diffusion time, Secs</th>
</tr>
</thead>
<tbody>
<tr>
<td>154.581</td>
<td>1.00</td>
<td>154.15</td>
<td>16.22</td>
<td>5.799 x 10⁻³</td>
<td>1.08 x 10⁻¹</td>
</tr>
<tr>
<td>146.85</td>
<td>0.95</td>
<td>388.19</td>
<td>6.44</td>
<td>3.366 x 10⁻⁴</td>
<td>185.68</td>
</tr>
<tr>
<td>139.12</td>
<td>0.90</td>
<td>492.08</td>
<td>5.08</td>
<td>4.548 x 10⁻⁴</td>
<td>137.42</td>
</tr>
<tr>
<td>131.39</td>
<td>0.85</td>
<td>576.40</td>
<td>4.34</td>
<td>5.385 x 10⁻⁴</td>
<td>116.06</td>
</tr>
<tr>
<td>123.66</td>
<td>0.80</td>
<td>650.98</td>
<td>3.84</td>
<td>6.057 x 10⁻⁴</td>
<td>103.19</td>
</tr>
<tr>
<td>115.94</td>
<td>0.75</td>
<td>719.60</td>
<td>3.47</td>
<td>6.627 x 10⁻⁴</td>
<td>94.31</td>
</tr>
<tr>
<td>108.21</td>
<td>0.70</td>
<td>784.49</td>
<td>3.19</td>
<td>7.126 x 10⁻⁴</td>
<td>87.71</td>
</tr>
<tr>
<td>100.48</td>
<td>0.65</td>
<td>846.82</td>
<td>2.95</td>
<td>7.566 x 10⁻⁴</td>
<td>82.61</td>
</tr>
<tr>
<td>92.75</td>
<td>0.60</td>
<td>907.54</td>
<td>2.78</td>
<td>7.953 x 10⁻⁴</td>
<td>78.59</td>
</tr>
<tr>
<td>85.02</td>
<td>0.55</td>
<td>967.37</td>
<td>2.58</td>
<td>8.292 x 10⁻⁴</td>
<td>75.37</td>
</tr>
<tr>
<td>77.29</td>
<td>0.50</td>
<td>1026.72</td>
<td>2.44</td>
<td>8.585 x 10⁻⁴</td>
<td>72.80</td>
</tr>
</tbody>
</table>
Figure 4-4 Variation of the viscosity and the speed of sound with temperature for oxygen at 5043 kPa. Both functions are from values given by the NIST.
Having looked at the temperature variation of the thermophysical properties of oxygen, a number of numerical analyses were conducted to compare the pressure and temperature response to the predictions based on the above observations. The pressure and temperature increases in oxygen contained between two infinite parallel plates were evaluated at the critical pressure of 5043 kPa. The plates were fixed with a separation distance of 2.5 mm. The bulk fluid was initialized to various temperatures ranging from 0.50 to 0.95 times the critical temperature, $T_c$, of 154.58 K and then one plate would undergo a step change to 1 K above the critical temperature. Reflection boundary conditions are applied at both the left and right boundaries which gives zero pressure gradient and zero velocity at each boundary. If the bulk fluid is initialized at temperatures very close to the critical temperature then the pressure boundary condition at the right plate has to be change from a reflection condition to an outflow boundary condition\textsuperscript{50}. The conditions encountered during this research effort did not require this change in the pressure boundary condition. The right boundary is maintained at the bulk fluid temperature while the left boundary is set to 1 K above the critical temperature. The fluid is initially at rest with the pressure at the critical pressure and the fluid temperature at $T_{\text{bulk}}$.

Initializing the bulk fluid temperature at the critical temperature resulted in problems when using the NIST equation of state. The pressure wave created by the step change in the left boundary temperature was very small due to only having a 1 K temperature difference. Also, the very large compressibility in the bulk fluid at the critical point resulted in the pressure wave being dissipated by the time it had traveled only 30 – 40%
of the distance between the two plates. The large compressibility means that the pressure wave compresses the fluid immediately in front of the pressure wave but only a small portion of the pressure wave is transmitted to the near by fluid. This same behavior was observed when the same problem was attempted using a commercially available CFD code that also used the SIMPLE algorithm. Further research is needed to investigate this behavior.

The simulations employed a time step of half the acoustic time period, \( t_a/2 \), and ran for a total of five acoustic time periods, \( 5t_a \), which was sufficient for the pressure to return to a nearly uniform condition after the temperature disturbance at the boundary. The acoustic time period was adjusted for each run based on the speed of sound in the bulk fluid. A smaller time step was investigated but reducing the time step from half the acoustic time period to one-tenth the acoustic time period changed the peak pressure and velocity by only a few percent but greatly increased the computational time. It was decided to proceed with the larger time step. A grid sensitivity study was performed to determine the number of nodes required to get an acceptable accuracy. The peak pressure showed a 5% change when the number of nodes was increased from 5,000 to 10,000 but showed a change of less than 1% when increased further to 15,000. It was, thus, determined that 10,000 nodes would provide an acceptable accuracy. A large number of nodes was required to resolve the thermal profile at the boundaries. The use of a non-linear grid distribution would allow for resolution of the thermal profile using much fewer nodes. The use of a non-linear grid will be used in future research efforts.
Three sets of conditions were studied in this research effort. First, the van der Waals equation of state was used to evaluate the density, volume expansivity and isothermal compressibility. The thermal conductivity, specific heat and viscosity were held constant at the initial conditions of the bulk fluid, using values provided by the NIST.\textsuperscript{1} This is the procedure used by the previous researchers who used only the van der Waals equation of state. Repeating their procedures gives a direct comparison to the prior research efforts. Next, the NIST equation of state was used to evaluate the density, volume expansivity and isothermal compressibility. The thermal conductivity, specific heat and viscosity were again held constant at the initial conditions of the bulk fluid, using values provided by the NIST. This provides a direct assessment of how the equation of state affects the pressure and temperature response of a fluid. Finally, all fluid properties were evaluated as a function of pressure and temperature, based on equations provided by the NIST. This final condition evaluates the effect of variable fluid properties on the pressure and temperature response. Predictions of the pressure and temperature changes due to a thermal disturbance were made by evaluating the thermophysical properties and then the predictions were compared to the numerical results.

The following numerical results were all evaluated using a reduced temperature of the bulk fluid of 0.85. The reduced temperature is defined as the fluid temperature divided by the critical temperature. The velocity and pressure profile after half an acoustic time period are presented in Figures 4-5 and 4-6, respectively. The peak velocity from the van der Waals run is 43 percent higher than the velocity from the NIST run using fixed fluid properties.
Figure 4-5 Velocity profiles after half the acoustic time period. Solid line is data from the van der Waals equation of state. Short dashes are data using the NIST equation of state with fixed fluid properties. Long dashes are data using the NIST equation of state with variable fluid properties.
Figure 4-6 Pressure increase after half the acoustic time period. Solid line is data from the van der Waals equation of state. Short dashes are data using the NIST equation of state with fixed fluid properties. Long dashes are data using the NIST equation of state with variable fluid properties.
This increase in the velocity was predicted based on the lower density given by the van der Waals equation of state. The peak pressure for the van der Waals run is seen to also be 30 percent lower compared to the NIST run with fixed fluid properties. The peak pressure for the van der Waals run using fixed fluid properties is seen to be 8 percent higher than the NIST run using variable fluid properties. The van der Waals equation of state overpredicts the peak velocity by 123 percent compared to the NIST run using variable fluid properties. From the previous discussion of the thermal conductivities it was predicted that the pressure rise would be larger when using fixed fluid properties.

The pressure rise and temperature rise was nearly uniform after five acoustic time periods. The total pressure rise from the van der Waals run was 20 kPa while the pressure rise from the NIST run using fixed fluid properties was 40 kPa. The total pressure rise from the van der Waals run is half of the pressure rise from the NIST run using fixed fluid properties. This is in agreement with the factor of two underprediction of the isothermal compressibility by the van der Waals equation of state. The total pressure rise from the NIST run using variable fluid properties was 32 kPa. The van der Waals run underpredicted the pressure rise by 38 percent compared to the NIST run using variable fluid properties. The total temperature rise in the bulk fluid from the van der Waals run was 21 mK while the temperature rise from the NIST run using fixed fluid properties was 23 mK. The factor of two decrease in the isothermal compressibility offsets the 44 percent lower velocity to result in underpredicting the bulk heating from the van der Waals run by nine percent compared to the NIST run with fixed fluid properties. The temperature rise of the bulk fluid was 18 mK for the NIST run using variable fluid
properties. The van der Waals run with fixed fluid properties overpredicts the
temperature rise by 17 percent compared to the NIST run with variable fluid properties.

The resulting pressure rise after five acoustic time periods is shown in Figure 4-7 as a
function of the amount of subcooling of the bulk fluid. The temperature difference is
defined as the difference between the heater temperature and the bulk fluid temperature.
For all runs the heater temperature was set at 1 K above the critical temperature. It is
seen that the van der Waals equation of state consistently underpredicts the magnitude of
the pressure rise by approximately 38 percent while using the NIST equation of state with
fixed fluid properties consistently overpredicts the pressure rise by approximately 25
percent. Pressure increases of multiple kPa are achievable with subcooling as low as 20
K below the critical temperature. A supercritical liquid oxygen tank loaded with normal
boiling point oxygen and then pressurized to the critical pressure will have a bulk fluid
temperature of 90 K or 64 K of subcooling. A pressure increase greater than 10 kPa
could result if a submerged heater surface is then heated to the critical temperature.
Zappoli et.al.\textsuperscript{14} reported a pressure rise of 0.01 Pa at a 1 K subcooled condition. The
pressure rise observed in this research effort is six orders of magnitude larger than
previously reported values.

The temperature increase in the bulk fluid after five acoustic time periods is shown in
Figure 4-8 as a function of the amount of subcooling of the bulk fluid. It is seen that both
the van der Waals runs and the NIST runs using fixed fluid properties overpredict the
extent of the acoustic heating.
Figure 4-7 Pressure increase after five acoustic time periods. Solid line is data from the van der Waals equation of state. Short dashes are data using the NIST equation of state with fixed fluid properties. Long dashes are data using the NIST equation of state with variable fluid properties.
Figure 4-8 Bulk fluid temperature increase after five acoustic time periods. Solid line is data from the van der Waals equation of state. Short dashes are data using the NIST equation of state with fixed fluid properties. Long dashes are data using the NIST equation of state with variable fluid properties.
The van der Waals equation of state with fixed fluid properties overpredicts the amount of acoustic heating by approximately 13 percent. Using fixed fluid properties with the NIST equation of state overpredicts the acoustic heating by approximately 40 percent. At 64 K of subcooling the temperature increase is over 20 mK compared to 2 µK at 1 K of subcooling. The temperature rise observed during this research effort is four orders of magnitude larger than any temperature rise reported in the literature.

The use of the van der Waals equation of state for numerical simulation of the piston effect results in underpredicting the magnitude of the pressure wave by approximately 38 percent while overpredicting the acoustic heating by approximately 13 percent compared to using all fluid properties from the NIST. When evaluating the piston effect at conditions typical of cryogenic storage systems the pressure response of the fluid was observed to be six orders of magnitude larger than had been previously reported. The extent of the acoustic heating resulted in temperature increases in the bulk fluid that were four orders of magnitude larger. The impact of the selection of the equation of state on the magnitude of the piston effect is discussed in Wagner et.al.

Having evaluated the effect that the equation of state has on the pressure and temperature response of the fluid, the NIST equation of state was selected for further investigation. Oxygen and hydrogen were selected for this study to examine fluid behavior near the critical point for a “poor” heat transfer fluid and a “good” heat transfer fluid, respectively. The variation of density as functions of temperature and pressure for both fluids near the
critical point is shown in Figure 4-9. The critical pressure, $P_c$, and the critical temperature, $T_c$, respectively, for oxygen are 5043 kPa and 154.58 K and for hydrogen are 1315 kPa and 33.19 K. To more directly compare the two fluids, the reduced temperature is defined as the fluid temperature divided by the critical temperature for that fluid. The density of both fluids decreases as the temperature is increased, with a steep gradient at the critical temperature. There is a slight increase in density as the pressure is increased. The density of oxygen is about 16 times larger than that of hydrogen. From the continuity equation it would be expected to encounter higher velocities in hydrogen than in oxygen.

The variation of viscosity as functions of temperature and pressure for both fluids near the critical point is shown in Figure 4-10. The viscosity of both fluids decreases as the temperature is increased, with a steep gradient at the critical temperature. There is a slight increase in viscosity as the pressure is increased. The viscosity of oxygen is about eight times that of hydrogen. The NIST program$^1$ did not include the viscosity of hydrogen so a curve fit was performed on the published NBS tables$^2$ to generate the needed equations. The details of the curve fit results are discussed in Wagner et.al.$^{3,4}$

The variation of the specific heats at constant volume as functions of temperature and pressure for both fluids near the critical point is shown in Figure 4-11. The specific heat, and therefore the heat transfer capability, of oxygen decreases as the temperature is increased while that of hydrogen increases. Both fluids exhibit a sharp increase in the specific heat at the critical point.
Figure 4-9 Variation of density with temperature and pressure. Solid line is data from the NIST equation of state at the critical pressure. Short dashes are data from the NIST equation of state at 1.1 times the critical pressure. Long dashes are data from the NIST equation of state at 1.2 times the critical pressure.
Figure 4-10 Variation of viscosity with temperature and pressure. Solid line is data from the NIST equation of state at the critical pressure. Short dashes are data from the NIST equation of state at 1.1 times the critical pressure. Long dashes are data from the NIST equation of state at 1.2 times the critical pressure.
Figure 4-11 Variation of specific heat with temperature and pressure. Solid line is data from the NIST equation of state at the critical pressure. Short dashes are data from the NIST equation of state at 1.1 times the critical pressure. Long dashes are data from the NIST equation of state at 1.2 times the critical pressure.
This behavior supports the observation that most fluids become extremely good heat transport fluids near the critical point. The specific heat of hydrogen is approximately seven times greater than that of oxygen.

The variation of the isothermal compressibility as functions of temperature and pressure for both fluids near the critical point is shown in Figure 4-12. The isothermal compressibility is the inverse of the isothermal bulk modulus and is shown multiplied by \(-1\) to simplify the plot. Both fluids show an extreme sensitivity to pressure changes near the critical point. The magnitude of the divergence at the critical point decreases as the pressure increases. For a small pressure change both fluids would undergo a large volume change when near the critical point. The inverse also holds true, for a large volume change the pressure would change only a small amount when near the critical point. If the fluid is much colder than the critical temperature it will respond as an incompressible fluid. Therefore, the compressibility effects will be isolated to the thermal penetration region. The isothermal compressibility of hydrogen is about an order of magnitude larger than that of oxygen, such that the same change in volume of the bulk fluid produces for hydrogen one-tenth the pressure change of oxygen.

The variation of the volume expansivity as functions of temperature and pressure for both fluids near the critical point is shown in Figure 4-13. Both fluids show an extreme sensitivity to temperature changes near the critical point, where a large volume change results from a small temperature change in the fluid. The magnitude of the divergence at the critical point decreases as the pressure increases.
Figure 4-12 Variation of isothermal compressibility with temperature and pressure.

Shown multiplied by \(-1\) for plotting purposes. Solid line is data from the NIST equation of state at the critical pressure. Short dashes are data from the NIST equation of state at 1.1 times the critical pressure. Long dashes are data from the NIST equation of state at 1.2 times the critical pressure.
Figure 4-13 Variation of volume expansivity with temperature and pressure. Solid line is data from the NIST equation of state at the critical pressure. Short dashes are data from the NIST equation of state at 1.1 times the critical pressure. Long dashes are data from the NIST equation of state at 1.2 times the critical pressure.
The volume expansivity determines the thickness of the thermal penetration region, which may experience a sudden increase or decrease resulting from a temperature disturbance at the boundary. A temperature increase at the boundary will result in an expansion of the thermal penetration region and an increase in the pressure. A temperature decrease at the boundary or forced fluid mixing between the thermal penetration region and the bulk fluid will result in shrinkage of the thermal penetration region and a pressure decrease in the bulk fluid. This effect is very significant when near the critical point but reducing the fluid temperature in the thermal penetration region to only a few degrees below the critical temperature the fluid will exhibit normal volume expansivity. Any fluid mixing would then result in small changes in both the thermal penetration region thickness and pressure. The volume expansivity of hydrogen is twice that of oxygen. For a given change in temperature at the boundary the thermal penetration depth of hydrogen would change twice as much as it would for oxygen.

The variation of the thermal conductivity as functions of temperature and pressure for both fluids near the critical point is shown in Figure 4-14. The NIST program\(^1\) did not include the thermal conductivity of hydrogen so a curve fit was performed on the published NBS tables\(^2\) to generate the needed equations. The details of the curve fit results are discussed in Wagner et.al.\(^3,4\) The thermal conductivity of hydrogen is an order of magnitude larger than that of oxygen. The magnitude of the divergence at the critical point decreases as the pressure increases. The thermal conductivity of oxygen decreases as the fluid temperature is increased while the thermal conductivity of hydrogen shows little variation for temperatures less than the critical temperature.
Figure 4-14 Variation of thermal conductivity with temperature and pressure. Solid line is data from the NIST equation of state at the critical pressure. Short dashes are data from the NIST equation of state at 1.1 times the critical pressure. Long dashes are data from the NIST equation of state at 1.2 times the critical pressure.
The decreasing thermal conductivity will result in an increasing thickness of the thermal penetration region. The thermal conductivity of hydrogen shows a much larger divergence at the critical point than does oxygen. As the hydrogen temperature approaches the critical point the thermal conductivity will rapidly increase, resulting in a thinner thermal penetration depth. This means there will be a much smaller volume change in the bulk fluid when the thermal penetration region thickness is decreased. Therefore, it can be expected to see a large pressure change in oxygen but only a small pressure change in hydrogen when the thermal penetration depth is decreased.

The pressure sensitivity near the critical point was investigated by performing a number of one-dimensional numerical analyses using the properties of oxygen and hydrogen. The pressure and bulk fluid temperature increases in hydrogen were compared to the respective increases in oxygen. The numerical analyses using the real gas equation of state for oxygen were repeated but this time using the properties of hydrogen. The pressure and temperature increases in hydrogen contained between two infinite parallel plates were evaluated at the critical pressure of 1315 kPa. The plates were fixed with a separation distance of 2.5 mm. The bulk fluid was initialized to various temperatures ranging from 0.50 to 0.95 times the critical temperature, $T_c$, of 33.19 K and then one plate would undergo a step change to 1 K above the critical temperature. The simulations employed a time step of half the acoustic time period, $t_a/2$, and ran for a total of five acoustic time periods, $5t_a$, which sufficient for the pressure to return to a nearly uniform condition after the temperature disturbance at the boundary. The acoustic time period was adjusted for each run based on the speed of sound in the bulk fluid. The values used
in the numerical analyses of hydrogen are shown in Table 4-2. For the simulations a grid of 10,000 nodes was used.

**Table 4-2** Speed of sound of hydrogen and acoustic times used for the numerical simulations.

<table>
<thead>
<tr>
<th>Temperature, K</th>
<th>Reduced Temperature, T/T&lt;sub&gt;c&lt;/sub&gt;</th>
<th>Speed of Sound, m/s</th>
<th>Acoustic time, μsec</th>
<th>Thermal Diffusivity, cm&lt;sup&gt;2&lt;/sup&gt;/s</th>
<th>Diffusion time, secs</th>
</tr>
</thead>
<tbody>
<tr>
<td>32.938</td>
<td>1.00</td>
<td>379.05</td>
<td>6.60</td>
<td>12.67 x 10&lt;sup&gt;-4&lt;/sup&gt;</td>
<td>4.93 x 10&lt;sup&gt;7&lt;/sup&gt;</td>
</tr>
<tr>
<td>31.29</td>
<td>0.95</td>
<td>660.97</td>
<td>3.78</td>
<td>6.720 x 10&lt;sup&gt;-4&lt;/sup&gt;</td>
<td>93.01</td>
</tr>
<tr>
<td>29.64</td>
<td>0.90</td>
<td>785.97</td>
<td>3.18</td>
<td>9.153 x 10&lt;sup&gt;-4&lt;/sup&gt;</td>
<td>68.28</td>
</tr>
<tr>
<td>28.00</td>
<td>0.85</td>
<td>879.08</td>
<td>2.84</td>
<td>10.870 x 10&lt;sup&gt;-4&lt;/sup&gt;</td>
<td>57.50</td>
</tr>
<tr>
<td>26.35</td>
<td>0.80</td>
<td>955.42</td>
<td>2.62</td>
<td>12.261 x 10&lt;sup&gt;-4&lt;/sup&gt;</td>
<td>50.97</td>
</tr>
<tr>
<td>24.70</td>
<td>0.75</td>
<td>1020.19</td>
<td>2.45</td>
<td>13.452 x 10&lt;sup&gt;-4&lt;/sup&gt;</td>
<td>46.46</td>
</tr>
<tr>
<td>23.06</td>
<td>0.70</td>
<td>1076.41</td>
<td>2.32</td>
<td>14.504 x 10&lt;sup&gt;-4&lt;/sup&gt;</td>
<td>43.09</td>
</tr>
<tr>
<td>21.41</td>
<td>0.65</td>
<td>1127.28</td>
<td>2.22</td>
<td>15.464 x 10&lt;sup&gt;-4&lt;/sup&gt;</td>
<td>40.42</td>
</tr>
<tr>
<td>19.76</td>
<td>0.60</td>
<td>1174.83</td>
<td>2.13</td>
<td>16.323 x 10&lt;sup&gt;-4&lt;/sup&gt;</td>
<td>38.29</td>
</tr>
<tr>
<td>18.12</td>
<td>0.55</td>
<td>1221.47</td>
<td>2.05</td>
<td>16.992 x 10&lt;sup&gt;-4&lt;/sup&gt;</td>
<td>36.78</td>
</tr>
<tr>
<td>16.47</td>
<td>0.50</td>
<td>1270.41</td>
<td>1.97</td>
<td>17.110 x 10&lt;sup&gt;-4&lt;/sup&gt;</td>
<td>36.53</td>
</tr>
</tbody>
</table>

**Acoustic Time Period**

The following results were all evaluated using a reduced temperature of the bulk fluid of 0.75, where the reduced temperature is the fluid temperature divided by the critical temperature. Results at other bulk fluid temperatures demonstrate similar trends. The pressure and velocity profiles after half an acoustic time period for oxygen and hydrogen are shown in Figure 4-15. The peak pressure for oxygen is about five times that of hydrogen, as predicted in the discussion on the isothermal compressibility and the thermal conductivity.
Figure 4-15 Velocity and pressure profiles after half the acoustic time period. Solid lines are for hydrogen and dashed lines are for oxygen.
The discussion on density of the two fluids suggested higher velocities in hydrogen than in oxygen and the peak velocity in hydrogen is almost twice that of oxygen.

After five acoustic time periods, the pressure rise and temperature rise in the bulk fluid were nearly uniform. The pressure rise in oxygen was 57 kPa while hydrogen experienced only 17% of that value, 10 kPa. The ratio of the isothermal compressibility's predicted that the pressure rise in oxygen would be an order of magnitude larger than in hydrogen, assuming both bulk fluids experience the same volume change. The temperature rise in the bulk fluid in oxygen was 20 mK while the temperature rise in hydrogen was 6 mK, 30% of that of oxygen.

The pressure and temperature increases in both fluids after five acoustic time periods are shown in Figure 4-16 as a function of the reduced fluid temperature. As the bulk fluid temperature approaches the critical temperature the compressibility of the bulk fluid increases significantly due to the divergence of the isothermal compressibility at the critical point. This means a very large volume change is required in order to create any significant pressure change. As a result, the pressure increase goes to zero as the reduced temperature approaches one. The pressure rise in oxygen is an order of magnitude larger than in hydrogen, corresponding to the order of magnitude difference in the isothermal compressibilities of the two fluids. The bulk fluid temperature rise in the liquid oxygen decreases as the oxygen temperature is increased. The temperature rise in the liquid hydrogen shows a slight increase as the hydrogen temperature is increased. This trend is similar to the trends in the thermal conductivity of the two fluids shown in Figure 4-14.
Figure 4-16 Pressure and temperature increase after five acoustic time periods. Solid lines are for hydrogen and dashed lines are for oxygen.
**Diffusion Time Period**

The computer simulations were allowed to continue for hundreds of time steps to determine the pressure and temperature response of the bulk fluid on the diffusion time scale. The pressure and temperature increases in oxygen are compared to the respective increases in hydrogen for various thermal penetration depths in Figure 4-17. The results shown are for a representative value of the reduced temperature of 0.55. Similar trends occur at the other bulk fluid temperatures. Both fluids demonstrate a linear pressure rise versus the penetration depth. When the bulk fluid temperature is near the critical temperature the response begins to deviate from this linear response. As the thermal penetration depth is doubled the pressure rise is doubled. The pressure rise in the oxygen is an order of magnitude larger than the pressure rise in hydrogen for the same thermal penetration depth. This is in agreement with the discussion on the isothermal compressibilities of the two fluids. The temperature rise in both fluids also demonstrates a linear response to the thermal penetration depth. When the bulk fluid temperature is near the critical temperature the response begins to deviate from this linear response. As the thermal penetration depth is doubled the temperature rise is doubled. The temperature rise in oxygen is four times greater than the temperature rise in hydrogen.
Figure 4-17 Temperature and pressure increase versus thermal penetration depth at a bulk fluid reduced temperature of 0.55. Solid lines are for hydrogen and dashed lines are for oxygen.
**Space Shuttle Observations**

The order of magnitude difference in the pressure response of oxygen and hydrogen is in agreement with observations of the supercritical cryogen tanks on the space shuttle. Pressure decays of up to 2000 kPa are common in the supercritical liquid oxygen tanks. The liquid oxygen tanks will be operating around the 5516 kPa storage pressure when fluid mixing due to a thruster firing would result in the pressure dropping 500 to 2000 kPa in the tank. Conversely, no noticeable pressure decays have been observed in the supercritical liquid hydrogen tanks. The comparison of the piston effect in oxygen versus hydrogen is discussed in Wagner and Bayazitoglu.⁵⁵
Chapter 5 - Summary

A new means of heat transfer known as the piston effect was identified in the late 1980’s by experimenters studying the specific heat of a fluid very close to the critical point. The temperature of the bulk fluid was observed to be increasing in temperature faster than could be explained by diffusion alone. The piston effect is where an expanding thermal boundary layer acts like a piston, which compresses the bulk fluid. The expansion of the thermal boundary layer also creates a pressure wave traveling at near the speed of sound in the fluid, which transfers energy into the bulk fluid causing a temperature rise in the bulk fluid. Previous research into the piston effect considered only the van der Waals equation of state for conditions very close to the critical point and focused on the fast thermal equilibration of a fluid. This research effort compares the pressure response of oxygen using the van der Waals equation of state and a real gas equation of state. The real gas equation of state is then used to compare the pressure response of liquid oxygen to the pressure response of liquid hydrogen.

The density prediction from the van der Waals equation of state underpredicts the actual density by approximately 30 percent over most of the temperature range. The van der Waals equation provides a good estimate for the saturated liquid state but the error increases as the fluid conditions get farther away from the saturation condition. The van der Waals equation of state overpredicts the pressure derivative by a factor of two. The pressure derivative can be decomposed into the isothermal compressibility and the volume expansivity. The van der Waals equation of state does a fairly good job of
reproducing the volume expansivity. It even predicts the divergence at the critical
temperature. The van der Waals equation of state reproduces the divergence in the
isothermal compressibility at the critical point. Over the majority of the subcooled liquid
region the van der Waals equation of state overpredicts the compressibility by a factor of
two. The error in the pressure derivative caused by using the van der Waals equation of
state is entirely due to the error in the isothermal compressibility. The van der Waals
equation of state will underpredict the pressure response of the bulk liquid by a factor of
two. This effect had not been encountered in prior research since all the previous
numerical investigations of the piston effect were evaluated using only the van der Waals
equation of state at conditions very close to the critical point.

A number of numerical analyses were conducted to compare the pressure and temperature
response of oxygen based on the selection of the equation of state. Three sets of
conditions were studied in this research effort. First, the van der Waals equation of state
was used to evaluate the density, volume expansivity and isothermal compressibility.
The thermal conductivity, specific heat and viscosity were held constant at the initial
conditions of the bulk fluid, using values provided by the NIST. This is the procedure
used by the previous researchers who used only the van der Waals equation of state.
Repeating their procedures gives a direct comparison to the prior research efforts. Next,
the NIST equation of state was used to evaluate the density, volume expansivity and
isothermal compressibility. The thermal conductivity, specific heat and viscosity were
again held constant at the initial conditions of the bulk fluid, using values provided by the
NIST. This provides a direct assessment of how the equation of state affects the pressure
and temperature response of a fluid. Finally, all fluid properties were evaluated as a function of pressure and temperature, based on equations provided by the NIST. This final condition evaluates the effect of variable fluid properties on the pressure and temperature response. Predictions of the pressure and temperature changes due to a thermal disturbance were made by evaluating the thermophysical properties and then the predictions were compared to the numerical results.

After half the acoustic time period, the peak velocity from the van der Waals equation of state is 43 percent higher than the velocity from the NIST equation of state using fixed fluid properties. This increase in the velocity was predicted based on the lower density given by the van der Waals equation of state. The peak pressure for the van der Waals run is seen to also be 30 percent lower compared to the NIST run with fixed fluid properties. The peak pressure for the van der Waals run using fixed fluid properties is seen to be 8 percent higher than the NIST run using variable fluid properties. The van der Waals equation of state overpredicts the peak velocity by 123 percent compared to the NIST run using variable fluid properties. From the thermal conductivities it was predicted that the pressure rise would be larger when using fixed fluid properties. The pressure rise and temperature rise was nearly uniform after five acoustic time periods. The total pressure rise from the van der Waals run was 20 kPa while the pressure rise from the NIST run using fixed fluid properties was 40 kPa. The total pressure rise from the van der Waals run is half of the pressure rise from the NIST run using fixed fluid properties. This is in agreement with the factor of two underprediction of the isothermal compressibility by the van der Waals equation of state. The total pressure rise from the
NIST run using variable fluid properties was 32 kPa. The van der Waals run
underpredicted the pressure rise by 38 percent compared to the NIST run using variable
fluid properties. The total temperature rise in the bulk fluid from the van der Waals run
was 21 mK while the temperature rise from the NIST run using fixed fluid properties was
23 mK. The factor of two decrease in the isothermal compressibility off-sets the 44
percent lower velocity to result in underpredicting the bulk heating from the van der
Waals run by nine percent compared to the NIST run with fixed fluid properties. The
temperature rise of the bulk fluid was 18 mK for the NIST run using variable fluid
properties. The van der Waals run with fixed fluid properties overpredicts the
temperature rise by 17 percent compared to the NIST run with variable fluid properties.

The van der Waals equation of state consistently underpredicts the magnitude of the
pressure rise by approximately 38 percent while using the NIST equation of state with
fixed fluid properties consistently overpredicts the pressure rise by approximately 25
percent. Pressure increases of multiple kPa are achievable with subcooling as low as 20
K below the critical temperature. A supercritical liquid oxygen tank loaded with normal
boiling point oxygen and then pressurized to the critical pressure will have a bulk fluid
temperature of 90 K or 64 K of subcooling. A pressure increase greater than 10 kPa
could result if a submerged heater surface is then heated to the critical temperature.
Previous researchers reported a pressure rise of 0.01 Pa at a 1 K subcooled condition.
The pressure rise observed in this research effort is six orders of magnitude larger than
previously reported values. Both the van der Waals runs and the NIST runs using fixed
fluid properties overpredict the extent of the acoustic heating. The van der Waals
equation of state with fixed fluid properties overpredicts the amount of acoustic heating by approximately 13 percent. Using fixed fluid properties with the NIST equation of state overpredicts the acoustic heating by approximately 40 percent. At 64 K of subcooling the temperature increase is over 20 mK compared to 2 µK at 1 K of subcooling. The temperature rise observed during this research effort is four orders of magnitude larger than any temperature rise reported in the literature.

Having evaluated the effect that the equation of state has on the pressure and temperature response of the fluid, the NIST equation of state was selected for further investigation. Oxygen and hydrogen were selected for this study to examine fluid behavior near the critical point for a “poor” heat transfer fluid and a “good” heat transfer fluid, respectively. The pressure sensitivity near the critical point was investigated by performing a number of one-dimensional numerical analyses using the properties of oxygen and hydrogen. The pressure and bulk fluid temperature increases in hydrogen were compared to the respective increases in oxygen. The numerical analyses using the real gas equation of state for oxygen were repeated but this time using the properties of hydrogen.

**Acoustic Time Period**

After half the acoustic time period, the peak pressure for oxygen is about five times that of hydrogen, as predicted in the discussion on the isothermal compressibility and the thermal conductivity. The discussion on density of the two fluids suggested higher velocities in hydrogen than in oxygen and the peak velocity in hydrogen is almost twice
that of oxygen. After five acoustic time periods, the pressure rise and temperature rise in
the bulk fluid were nearly uniform. The pressure rise in oxygen was 57 kPa while
hydrogen experienced only 17% of that value, 10 kPa. The ratio of the isothermal
compressibility’s predicted that the pressure rise in oxygen would be an order of
magnitude larger than in hydrogen, assuming both bulk fluids experience the same
volume change. The temperature rise in the bulk fluid in oxygen was 20 mK while the
temperature rise in hydrogen was 6 mK, 30% of that of oxygen. The pressure rise in
oxygen is an order of magnitude larger than in hydrogen, corresponding to the order of
magnitude difference in the isothermal compressibilities of the two fluids. The bulk fluid
temperature rise in the liquid oxygen decreases as the oxygen temperature is increased.
The temperature rise in the liquid hydrogen shows a slight increase as the hydrogen
temperature is increased. This trend is similar to the trends in the thermal conductivity of
the two fluids.

Diffusion Time Period

The computer simulations were allowed to continue for hundreds of time steps to
determine the pressure and temperature response of the bulk fluid on the diffusion time
scale. Both fluids demonstrate a linear pressure rise versus the penetration depth. The
pressure rise in the oxygen is an order of magnitude larger than the pressure rise in
hydrogen for the same thermal penetration depth. This is in agreement with the
discussion on the isothermal compressibilities of the two fluids. The temperature rise in
both fluids also demonstrates a linear response to the thermal penetration depth. The
temperature rise in oxygen is four times greater than the temperature rise in hydrogen.
Space Shuttle Observations

The order of magnitude difference in the pressure response of oxygen and hydrogen is in agreement with observations of the supercritical cryogen tanks on the space shuttle. Pressure decays of up to 2000 kPa are common in the supercritical liquid oxygen tanks. The liquid oxygen tanks will be operating around the 5516 kPa storage pressure when fluid mixing due to a thruster firing would result in the pressure dropping 500 to 2000 kPa in the tank. Conversely, no noticeable pressure decays have been observed in the supercritical liquid hydrogen tanks.

This research was initiated after years of personally observing the pressure behavior in the supercritical liquid oxygen and liquid hydrogen tanks on the space shuttle. Numerous occurrences of a pressure collapse have been observed in the liquid oxygen tanks. A pressure collapse is a sudden drop in the tank pressure, usually associated with a maneuvering thruster firing. At the same time, no pressure collapses were observed in the liquid hydrogen tanks. Unfortunately, no theory was available to explain the physical mechanism that was causing these sudden pressure collapses. A detailed review of the data available from the space shuttle indicated that the heater temperatures were always near the critical temperature at the time of the pressure collapse. This was independent of the bulk fluid temperature in the tank. This initiated this investigation into the heat transfer to a fluid near the critical point. The piston effect provides a mechanism to explain the sudden pressure collapse. The thermophysical properties of the liquid oxygen show that the thickness of the thermal boundary layer can change rapidly when near the
critical temperature. Fluid mixing with the colder bulk fluid can result in a rapid decrease in the thermal boundary layer, causing a rapid expansion of the bulk fluid. The rapid expansion of the bulk fluid results in a large pressure collapse. A comparison of the thermophysical properties of oxygen and hydrogen explains why large pressure collapses have been observed in the liquid oxygen tanks but not in the liquid hydrogen tanks.

The 2-D SIMPLE algorithm described herein needs to be extended to a 3-D arbitrary geometry in order to model the actual geometry for the space shuttle tanks. This is required in order to establish the relationship between the magnitude of the pressure collapse, the bulk fluid density and tank discharge flow rate. A simplified model could be developed but it requires knowledge of the fluid velocity profile inside the tank and the boundary layer thickness around the heater. There has been no documented research into the velocity profile inside of a tank during a pressure blowdown. This would require developing a CFD model of a spherical tank to determine the time varying velocity field internal to the tank while the pressure is being slowly decreased. The mass flow rate for each pressure blowdown would be maintained at a constant value during each pressure blowdown. The only heat transfer correlation for flow past a cylinder was developed using data for air. No documented data exists for liquid flow past a cylinder. Using cryogenic fluids a series of forced convection CFD experiments would be conducted to develop a method of predicting the Nusselt number over a range of Reynolds numbers and pressures of the cryogenic flow stream. The thickness of the thermal boundary layer as a function of the heat flux and fluid properties could be evaluated. A series of parametric curves could then be developed to predict the magnitude of the pressure
collapse as a function of the tank discharge mass flow rate and the bulk fluid density.

The data could also be used to redesign the tanks to minimize the potential for a pressure collapse.
REFERENCES


Appendix

Energy Equation Source Term

The energy equation was given in chapter 2 as

$$\frac{\partial \rho T}{\partial t} + \frac{\partial}{\partial x} \left( \rho u T - \frac{k}{C_v} \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left( \rho v T - \frac{k}{C_v} \frac{\partial T}{\partial y} \right) = \frac{k}{C_v^2} \left( \frac{\partial T}{\partial x} \frac{\partial C_v}{\partial x} + \frac{\partial T}{\partial y} \frac{\partial C_v}{\partial y} \right)$$

$$- \frac{u}{C_v} \frac{\partial P}{\partial x} - \frac{v}{C_v} \frac{\partial P}{\partial y} - \frac{T}{C_v} \left( \frac{\partial P}{\partial T} \right)_p \left( \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right) - \frac{1}{C_v} \frac{\partial}{\partial x} \left[ \frac{\rho}{2} (u^2 + v^2) \right]$$

$$- \frac{1}{C_v} \frac{\partial}{\partial x} \left[ \frac{\rho u}{2} (u^2 + v^2) \right] - \frac{1}{C_v} \frac{\partial}{\partial y} \left[ \frac{\rho v}{2} (u^2 + v^2) \right]$$

$$+ \frac{1}{C_v} \frac{\partial}{\partial x} \left[ \mu u \left( \frac{4}{3} \frac{\partial u}{\partial x} - \frac{2}{3} \frac{\partial v}{\partial y} \right) + \mu v \left( \frac{4}{3} \frac{\partial v}{\partial x} + \frac{2}{3} \frac{\partial u}{\partial y} \right) \right]$$

$$+ \frac{1}{C_v} \frac{\partial}{\partial y} \left[ \mu u \left( \frac{\partial v}{\partial x} + \frac{\partial u}{\partial y} \right) + \mu v \left( \frac{4}{3} \frac{\partial v}{\partial y} - \frac{2}{3} \frac{\partial u}{\partial x} \right) \right]$$ \quad (A-1)

The source term can be defined as

$$S = \frac{k}{C_v^2} \left( \frac{\partial T}{\partial x} \frac{\partial C_v}{\partial x} + \frac{\partial T}{\partial y} \frac{\partial C_v}{\partial y} \right) - \frac{u}{C_v} \frac{\partial P}{\partial x} - \frac{v}{C_v} \frac{\partial P}{\partial y} - \frac{T}{C_v} \left( \frac{\partial P}{\partial T} \right)_p \left( \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right)$$

$$- \frac{1}{C_v} \frac{\partial}{\partial x} \left[ \frac{\rho}{2} (u^2 + v^2) \right] - \frac{1}{C_v} \frac{\partial}{\partial y} \left[ \frac{\rho u}{2} (u^2 + v^2) \right] - \frac{1}{C_v} \frac{\partial}{\partial y} \left[ \frac{\rho v}{2} (u^2 + v^2) \right]$$

$$+ \frac{1}{C_v} \frac{\partial}{\partial x} \left[ \mu u \left( \frac{4}{3} \frac{\partial u}{\partial x} - \frac{2}{3} \frac{\partial v}{\partial y} \right) + \mu v \left( \frac{4}{3} \frac{\partial v}{\partial x} + \frac{2}{3} \frac{\partial u}{\partial y} \right) \right]$$

$$+ \frac{1}{C_v} \frac{\partial}{\partial y} \left[ \mu u \left( \frac{\partial v}{\partial x} + \frac{\partial u}{\partial y} \right) + \mu v \left( \frac{4}{3} \frac{\partial v}{\partial y} - \frac{2}{3} \frac{\partial u}{\partial x} \right) \right]$$ \quad (A-2)
The viscous, kinetic and diffusion heating terms were neglected in the energy equation with respect to the acoustic heating term. Their derivation in finite difference notation is shown below.

The viscous contribution to the source term is given by

\[
\text{Visc} = \frac{1}{C_v} \frac{\partial}{\partial x} \left[ \mu u \left( \frac{4}{3} \frac{\partial u}{\partial x} - \frac{2}{3} \frac{\partial v}{\partial y} \right) + \nu \left( \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) \right] + \frac{1}{C_v} \frac{\partial}{\partial y} \left[ \mu u \left( \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) + \nu \left( \frac{4}{3} \frac{\partial v}{\partial y} - \frac{2}{3} \frac{\partial u}{\partial x} \right) \right]
\]

Expressing the viscous contribution in finite difference representation gives

\[
\text{Visc} = \frac{\mu_e}{C_v} \frac{u_e}{\Delta X} \left( \frac{4}{3} \frac{u_e - u_p}{\Delta X} - \frac{2}{3} \frac{v_{se} - v_{sw}}{\Delta Y} \right) + \frac{\mu_e}{C_v} \frac{v_e}{\Delta X} \left( \frac{u_{ne} - u_{se}}{\Delta Y} + \frac{v_{E} - v_{P}}{\Delta X} \right)
\]

\[
- \frac{\mu_w}{C_v} \frac{u_w}{\Delta X} \left( \frac{4}{3} \frac{u_p - u_w}{\Delta X} - \frac{2}{3} \frac{v_{sw} - v_{sw}}{\Delta Y} \right) - \frac{\mu_w}{C_v} \frac{v_w}{\Delta X} \left( \frac{u_{nw} - u_{sw}}{\Delta Y} + \frac{v_{P} - v_{w}}{\Delta X} \right)
\]

\[
+ \left[ \frac{\mu_n}{C_v} \frac{u_n}{\Delta Y} \left( \frac{u_n - u_p}{\Delta Y} + \frac{v_{se} - v_{nw}}{\Delta X} \right) + \frac{\mu_n}{C_v} \frac{v_n}{\Delta Y} \left( \frac{4}{3} \frac{v_{N} - v_{P}}{\Delta Y} - \frac{2}{3} \frac{u_{ne} - u_{nw}}{\Delta Y} \right) \right]
\]

\[
- \left[ \frac{\mu_s}{C_v} \frac{u_s}{\Delta Y} \left( \frac{u_p - u_s}{\Delta Y} + \frac{v_{sw} - v_{sw}}{\Delta X} \right) + \frac{\mu_s}{C_v} \frac{v_s}{\Delta Y} \left( \frac{4}{3} \frac{v_{P} - v_{S}}{\Delta Y} - \frac{2}{3} \frac{u_{se} - u_{sw}}{\Delta Y} \right) \right]
\]

(A-3)

Which simplifies to

\[
\text{Visc} = \frac{4}{3} \frac{\mu_e}{C_v} \frac{u_e}{\Delta X \Delta Y} (u_e - u_p) - \frac{2}{3} \frac{\mu_e}{C_v} \frac{u_e}{\Delta X \Delta Y} (v_{se} - v_{sw}) + \frac{\mu_e}{C_v} \frac{v_e}{\Delta X \Delta Y} (u_{ne} - u_{se})
\]

\[
+ \frac{\mu_e}{C_v} \frac{v_e}{\Delta X \Delta Y} (v_{E} - v_{P}) - \frac{4}{3} \frac{\mu_w}{C_v} \frac{u_w}{\Delta X \Delta Y} (u_p - u_w) + \frac{2}{3} \frac{\mu_w}{C_v} \frac{u_w}{\Delta X \Delta Y} (v_{nw} - v_{sw})
\]

(A-4)
\[- \frac{\mu_w v_w}{C_v \Delta X \Delta Y} (u_{nw} - u_{sw}) - \frac{\mu_w v_w}{C_v \Delta X \delta X_w} (v_p - v_w) + \frac{\mu_s u_s}{C_v \Delta Y \delta Y_s} (u_N - u_p) \]

\[+ \frac{\mu_s u_s}{C_v \Delta Y \delta Y_s} (v_{se} - v_{sw}) + \frac{4}{3} \frac{\mu_s v_s}{C_v \Delta Y \delta Y_s} (v_N - v_p) - \frac{2}{3} \frac{\mu_s v_s}{C_v \Delta Y \delta Y_s} (u_{se} - u_{sw}) \]

\[- \frac{\mu_s u_s}{C_v \Delta Y \delta Y_s} (u_p - u_s) - \frac{\mu_s u_s}{C_v \Delta Y \delta Y_s} (v_{se} - v_{sw}) - \frac{4}{3} \frac{\mu_s v_s}{C_v \Delta Y \delta Y_s} (v_p - v_s) \]

\[+ \frac{2}{3} \frac{\mu_s v_s}{C_v \Delta Y \delta Y_s} (u_{se} - u_{sw}) \quad (A-5) \]

The kinetic energy contribution to the source term is given by

\[\text{KE} = - \frac{1}{C_v} \frac{\partial}{\partial t} \left( \frac{\rho}{2} (u'^2 + v'^2) \right) - \frac{1}{C_v} \frac{\partial}{\partial x} \left( \frac{\rho u}{2} (u'^2 + v'^2) \right) - \frac{1}{C_v} \frac{\partial}{\partial y} \left( \frac{\rho v}{2} (u'^2 + v'^2) \right) \quad (A-6)\]

Expressing the viscous contribution in finite difference representation gives

\[\text{KE} = - \frac{1}{2C_v \Delta t} \left( \rho_p (u_p'^2 + v_p'^2) - \rho_p \left( u_p'^2 + v_p'^2 \right) \right) - \frac{\rho_e u_e}{2C_v \Delta X} (u_e^2 + v_e^2) + \frac{\rho_s u_s}{2C_v \Delta X} (u_s^2 + v_s^2) \]

\[- \frac{\rho_s v_s}{2C_v \Delta Y} (u_s^2 + v_s^2) - \frac{\rho_s v_s}{2C_v \Delta Y} (u_s^2 + v_s^2) \quad (A-7) \]

The diffusion contribution is given by

\[\text{DIFF} = - \frac{u}{C_v} \frac{\partial P}{\partial x} - \frac{v}{C_v} \frac{\partial P}{\partial y} \quad (A-8)\]

Expressing the diffusion contribution in finite difference representation gives

\[\text{DIFF} = - \frac{u_p}{C_v} \frac{P_p - P_w}{\Delta X} - \frac{v_p}{C_v} \frac{P_p - P_t}{\Delta Y} \quad (A-9)\]