Thermomechanical Simulation of an Aerogel/RTV-655 Based Cryogenic Propellant Tank

William Dalton Bowen Jr.

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THERMOMECHANICAL SIMULATION OF AN AEROGEL/RTV-655 BASED CRYOGENIC PROPELLANT TANK

by

William D. Bowen, Jr.

A Thesis
Submitted in Partial Fulfillment of the
Requirements for the Degree of
Master of Science

Major: Mechanical Engineering

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Dedication

I would like to dedicate this work to my family, especially my mother, Jennifer Bowen, who was unable to finish her master’s degree.
Acknowledgments

I would like to give my sincerest thanks to Dr. Jeffrey Marchetta for his role in my research. His involvement in my education has undoubtedly given me skills that I will carry with me throughout my career. I would also like to acknowledge the Tennessee Space Grant for funding my research and Dr. Gladius Lewis who was gracious with his time and lent valuable advise during my research efforts.
Abstract

Developing an effective solution for long duration storage of cryogenic liquids is crucial for future, manned space exploration missions. Current storage tanks are made of metals or composites. Although these materials have a relatively high mechanical strength, their high thermal conductivity is a disadvantage with regards to heat infiltration. The influx of heat causes vaporization, increasing the pressure in the tank. To reduce tank pressurization rates, novel materials with densities and thermal conductivities which are lower than metals, such as RTV-655 and aerogels, have been developed which may be feasible for space applications. Due to the complexity and costs of performing experiments, a thermomechanical computational model is desired to further study the feasibility of using these novel materials. A thermochemical finite element simulation is used to simulate the Cooldown and Pressurization phases of RTV-655 and RTV-655/Aerogel tank experiments and a comparison of the simulation and experiment results are presented.
# Table of Contents

List of Figure................................................................................................. vii  
Nomenclature................................................................................................. xi  
1. Introduction................................................................................................. 1  
   1.1 Background and Literature Review................................................................. 1  
   1.2 Previous Work............................................................................................... 2  
      1.2.1 Material Testing....................................................................................... 3  
      1.2.2 Tank Creation......................................................................................... 6  
   1.3 Experimental Setup..................................................................................... 8  
   1.4 Research Objectives..................................................................................... 14  
2. RTV-655 Tank Finite Element Analysis Model............................................ 14  
   2.1 Governing Equations.................................................................................... 14  
   2.2 RTV-655 Tank Geometry and Mesh............................................................... 15  
   2.3 Cylindrical Coordinate Verification Case.................................................... 17  
   2.4 RTV-655 Material Properties........................................................................ 19  
   2.5 Initial Cooldown RTV-655 Model................................................................. 19  
   2.6 Expansion Coefficient.................................................................................. 23  
   2.7 RTV-655 Pressurization Model.................................................................... 28  
   2.8 Hyperelastic Solver..................................................................................... 32  
   2.9 Young’s Modulus......................................................................................... 33  
   2.10 Poisson’s Ratio......................................................................................... 40  
   2.11 Effect on Cooldown Phase......................................................................... 47  
3. Aerogel/RTV-655 Finite Element Model...................................................... 51  
   3.1 Aerogel/RTV-655 Tank Model Creation/Mesh Convergence Study............. 51  
   3.2 Aerogel/RTV-655 Results........................................................................... 53  
4. Analysis of Cooldown Predictions.................................................................. 62
<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>5. Influence of Aerogel Geometry on Simulation Predictions</td>
<td>71</td>
</tr>
<tr>
<td>6. Summary/Conclusion</td>
<td>72</td>
</tr>
<tr>
<td>7. Study Limitations</td>
<td>75</td>
</tr>
<tr>
<td>8. References</td>
<td>79</td>
</tr>
<tr>
<td>9. Appendix A. RTV-655 FEA Simulation Tutorial</td>
<td>82</td>
</tr>
</tbody>
</table>
List of Figures

Figure 1: Picture RTV-655..............................................................................................................3
Figure 2: Picture Polyimide Aerogel...............................................................................................3
Figure 3: Stress and Strain Graph for RTV-655 at 301 K...............................................................4
Figure 4: Stress and Strain Graph for RTV-655 at 77 K.................................................................5
Figure 5: Stress and Strain Graph for Polyimide Aerogel at Various Temperatures....................5
Figure 6: Aluminum Lid Used for Tank Creation............................................................................6
Figure 7: Base Mold Used for Tank Creation..................................................................................6
Figure 8: V-Channel Formed by Connecting Two Tank Halves....................................................7
Figure 9: Cross Sectional View of Prototype Tank Experimental Setup........................................9
Figure 10: Picture of Experimental Setup for RTV-655.................................................................10
Figure 11: Experimental Results of the Strain During theCooldown Phase.................................11
Figure 12: Pressure inside the RTV-655 Tank During the Pressurization Phase.........................12
Figure 13: Recorded Strain for RTV-655 Tank During the Pressurization Phase.........................13
Figure 14: Meshed RTV-655 Tank.................................................................................................16
Figure 15: RTV Tank Mesh Convergence Study............................................................................17
Figure 16: FEA Results of Thin Pressure Vessel..........................................................................18
Figure 17: Comparison of the Constant Expansion Coefficient (Ca) and Poisson’s Ratio (CPR) with a Linear Temperature Dependent Youngs Modulus (LYM) Model vs. the Experimental Cooldown Phase Results in the Axial Direction..................................................20
Figure 18: Comparison of the Constant Expansion Coefficient (Ca) and Poisson’s Ratio (CPR) with a Linear Temperature Dependent Youngs Modulus (LYM) Model vs. Experimental Cooldown Phase Results in the Diametral Direction..................................................21
Figure 19: Comparison of the Constant Expansion Coefficient (Ca) and Poisson’s ratio (CPR) with a Linear Temperature Dependent Youngs Modulus (LYM) Model vs Experimental Cooldown Phase Results in the Circumferential Direction..............................................................................................................22
Figure 20: Comparison of the Normalized Expansion Coefficient (Na) with a Constant Poisson’s Ratio (CPR) and a Linear Temperature Dependent Youngs Modulus (LYM) Model and the Experimental Cooldown Phase Results in the Axial Direction..........................25
Figure 21: Comparison of the Normalized Expansion Coefficient (Nα) with a Constant Poisson’s Ratio (CPR) and a Linear Temperature Dependent Youngs Modulus (LYM) Model and the Experimental Cooldown Phase Results in the Diametral Direction

Figure 22: Comparison of the Normalized Expansion Coefficient (Nα) with a Constant Poisson’s Ratio (CPR) and a Linear Temperature Dependent Youngs Modulus (LYM) Model and the Experimental Cooldown Phase Results in the Circumferential Direction

Figure 23: Pressure Load in Inner Wall of Tank in FEA Model

Figure 24: Comparison of the Normalized Expansion Coefficient (Nα) with a Constant Poisson’s Ratio (CPR) and a Linear Temperature Dependent Youngs Modulus (LYM) Model and the Experimental Pressurization Results in the Axial Direction

Figure 25: Comparison of the Normalized Expansion Coefficient (Nα) with a Constant Poisson’s Ratio (CPR) and a Linear Temperature Dependent Youngs Modulus (LYM) Model and the Experimental Pressurization Results in the Diametral Direction

Figure 26: Comparison of the Normalized Expansion Coefficient (Nα) with a Constant Poisson’s Ratio (CPR) and a Linear Temperature Dependent Youngs Modulus (LYM) Model and the Experimental Pressurization Results in the Circumferential Direction

Figure 27: Example of Elastomer Young’s Modulus Behavior

Figure 28: Comparison of Different Elastomers and Estimated RTV-655 Value

Figure 29: Comparison of the Normalized Expansion Coefficient (Nα) with a Constant Poisson’s Ratio (CPR) and a Linear Temperature Dependent Youngs Modulus (LYM) Model, the Normalized Expansion Coefficient (Nα) with a Constant Poisson’s Ratio (CPR) and a Normalized Temperature Dependent Youngs Modulus with a Glass Transition Temperature (NYM) Model, and the Experimental Pressurization Phase Results in the Axial Direction

Figure 30: Comparison of the Normalized Expansion Coefficient (Nα) with a Constant Poisson’s Ratio (CPR) and a Linear Temperature Dependent Youngs Modulus (LYM) Model, the Normalized Expansion Coefficient (Nα) with a Constant Poisson’s Ratio (CPR) and a Normalized Temperature Dependent Youngs Modulus with a Glass Transition Temperature (NYM) Model, and the Experimental Pressurization Phase Results in the Diametral Direction
Figure 31: Comparison of the Normalized Expansion Coefficient ($N_\alpha$) with a Constant Poisson’s Ratio (CPR) and a Linear Temperature Dependent Youngs Modulus (LYM) Model, the Normalized Expansion Coefficient ($N_\alpha$) with a Constant Poisson’s Ratio (CPR) and a Normalized Temperature Dependent Youngs Modulus with a Glass Transition Temperature (NYM) Model, and the Experimental Pressurization Phase Results in the Circumferential Direction.................................................................39

Figure 32: Example of Poisson’s Ratio as a Function of Temperature for Structural Epoxy.....41

Figure 33: Comparison of the Normalized Expansion Coefficient ($N_\alpha$) with a Constant Poisson’s Ratio (CPR) and a Normalized Temperature Dependent Youngs Modulus with a Glass Transition Temperature (NYM) Model, the Normalized Expansion Coefficient ($N_\alpha$) with a Normalized Poisson’s Ratio with a Glass Transition Temperature (NPR) and a Normalized Temperature Dependent Youngs Modulus with a Glass Transition Temperature (NYM) Model, and the Experimental Pressurization Phase Results in the Axial Direction.................................................................43

Figure 34: Comparison of the Normalized Expansion Coefficient ($N_\alpha$) with a Constant Poisson’s Ratio (CPR) and a Normalized Temperature Dependent Youngs Modulus with a Glass Transition Temperature (NYM) Model, the Normalized Expansion Coefficient ($N_\alpha$) with a Normalized Poisson’s Ratio with a Glass Transition Temperature (NPR) and a Normalized Temperature Dependent Youngs Modulus with a Glass Transition Temperature (NYM) Model, and the Experimental Pressurization Phase Results in the Diametral Direction.................................................................44

Figure 35: Comparison of the Normalized Expansion Coefficient ($N_\alpha$) with a Constant Poisson’s Ratio (CPR) and a Normalized Temperature Dependent Youngs Modulus with a Glass Transition Temperature (NYM) Model, the Normalized Expansion Coefficient ($N_\alpha$) with a Normalized Poisson’s Ratio with a Glass Transition Temperature (NPR) and a Normalized Temperature Dependent Youngs Modulus with a Glass Transition Temperature (NYM) Model, and the Experimental Pressurization Phase Results in the Circumferential Direction.................................................................45

Figure 36: Comparison of the Normalized Expansion Coefficient ($N_\alpha$) with a Constant Poisson’s Ratio (CPR) and a Linear Temperature Dependent Youngs Modulus (LYM) Model, the Normalized Expansion Coefficient ($N_\alpha$) with a Constant Poisson’s Ratio (CPR) and a Normalized Temperature Dependent Youngs Modulus with a Glass Transition Temperature (NYM) Model, and the Experimental Cooldown Phase Results in the Axial Direction.................................................................47

Figure 37: Comparison of the Normalized Expansion Coefficient ($N_\alpha$) with a Constant Poisson’s Ratio (CPR) and a Linear Temperature Dependent Youngs Modulus (LYM) Model, the Normalized Expansion Coefficient ($N_\alpha$) with a Constant Poisson’s Ratio (CPR) and a Normalized Temperature Dependent Youngs Modulus with a Glass Transition Temperature (NYM) Model, and the Experimental Pressurization Phase Results in the Diametral Direction.................................................................48
Figure 38: Comparison of the Normalized Expansion Coefficient (No) with a Constant Poisson’s Ratio (CPR) and a Linear Temperature Dependent Youngs Modulus (LYM) Model, the Normalized Expansion Coefficient (No) with a Constant Poisson’s Ratio (CPR) and a Normalized Temperature Dependent Youngs Modulus with a Glass Transition Temperature (NYM) Model, and the Experimental Cooldown Phase Results in the Circumferential Direction

Figure 39: Cross-Section View of Meshed Aerogel/RTV-655 Tank Model

Figure 40: Mesh Convergence Study of Aerogel/RTV-655 Tank

Figure 41: Comparison of the Normalized Expansion Coefficient (No) with a Normalized Poisson’s Ratio with a Glass Transition Temperature (NPR) and a Normalized Temperature Dependent Youngs Modulus with a Glass Transition Temperature (NYM) Model vs Experimental Cooldown Phase Results in the Axial Direction for the Aerogel/RTV-655 Tank

Figure 42: Comparison of the Normalized Expansion Coefficient (No) with a Normalized Poisson’s Ratio with a Glass Transition Temperature (NPR) and a Normalized Temperature Dependent Youngs Modulus with a Glass Transition Temperature (NYM) Model vs Experimental Cooldown Phase Results in the Diametral Direction for the Aerogel/RTV-655 Tank

Figure 43: Comparison of the Normalized Expansion Coefficient (No) with a Normalized Poisson’s Ratio with a Glass Transition Temperature (NPR) and a Normalized Temperature Dependent Youngs Modulus with a Glass Transition Temperature (NYM) Model vs Experimental Cooldown Phase Results in the Circumferential Direction for the Aerogel/RTV-655 Tank

Figure 44: Comparison of the Normalized Expansion Coefficient (No) with a Normalized Poisson’s Ratio with a Glass Transition Temperature (NPR) and a Normalized Temperature Dependent Youngs Modulus with a Glass Transition Temperature (NYM) Model vs Experimental Pressurization Phase Results in the Axial Direction for the Aerogel/RTV-655 Tank

Figure 45: Comparison of the Normalized Expansion Coefficient (No) with a Normalized Poisson’s Ratio with a Glass Transition Temperature (NPR) and a Normalized Temperature Dependent Youngs Modulus with a Glass Transition Temperature (NYM) Model vs Experimental Pressurization Phase Results in the Diametral Direction for the Aerogel/RTV-655 Tank

Figure 46: Comparison of the Normalized Expansion Coefficient (No) with a Normalized Poisson’s Ratio with a Glass Transition Temperature (NPR) and a Normalized Temperature Dependent Youngs Modulus with a Glass Transition Temperature (NYM) Model vs Experimental Pressurization Phase Results in the Circumferential Direction for the Aerogel/RTV-655 Tank
Figure 47: Comparison of Thermal and Mechanical Strain in the Axial Direction for Aerogel/RTV-655 Tank Model for the Cooldown Phase .................................................. 63
Figure 48: Comparison of Thermal and Mechanical Strain in the Circumferential Direction for Aerogel/RTV-655 Tank Model for the Cooldown Phase .................................................. 64
Figure 49: Comparison of Thermal and Mechanical Strain in the Diametral Direction for Aerogel/RTV-655 Tank Model for the Cooldown Phase .................................................. 64
Figure 50: Test Cylinder Part .......................................................................................................................................................................................... 66
Figure 51: Total Strain of Test Cylinder .......................................................................................................................................................... 67
Figure 52: Thermal Strain of Test Cylinder .................................................................................................................................................. 67
Figure 53: Total Strain of RTV Tank ................................................................................................................................................................. 68
Figure 54: Thermal Strain of RTV Tank ................................................................................................................................................................. 69
Figure 55: Total Strain of Test Cylinder with a Temperature Gradient ................................................................................................................. 70
Figure 56: Thermal Strain of Test Cylinder with a Temperature Gradient ......................................................................................................... 70
Figure 57: Aerogel with RTV-655 Connecting Layer ............................................................................................................................................. 72
Figure 58: Picture of Meshed Tank with Datum Planes ........................................................................................................................................ 84
Figure 59: Example of Cooldown Step Editor .................................................................................................................................................. 86
Figure 60: Example of the Field Output Selection Box ..................................................................................................................................... 88
List of Tables

Table 1: Characteristics of Each Mesh Size Studied

Table 2: RTV Material Properties at Room Temp (301K)

Table 3: RTV Material Properties at 298K and 75K

Table 4: Cooldown Phase S.O.S Analysis for Case: Cα-LYM-CPR

Table 5: Updated Expansion Coefficients

Table 6: Cooldown Phase S.O.S Analysis for Cases: Cα-LYM-CPR and Nα-LYM-CPR

Table 7: Pressurization Phase S.O.S Analysis for Case: Nα-LYM-CPR

Table 8: Pressurization Phase S.O.S Analysis for Cases: Nα-LYM-CPR and Nα-NYM-CPR

Table 9: Normalized Poisson’s Ratio

Table 10: Comparison of S.O.S Analysis Between Different Models During Pressurization Phase

Table 11: Comparison of S.O.S Analysis Between Different Models During Pressurization Phase

Table 12: Aerogel/RTV-655 Tank Mesh Characteristics

Table 13: Aerogel Properties at Different Temperatures

Table 14: Aerogel Properties at Room Temperature

Table 15: Cooldown Phase Analysis for Case: PA-Nα-NYM-NPR

Table 16: Pressurization Phase S.O.S. Analysis for PA-Nα-LYM-CPR
Nomenclature

RTV - Room Temperature Vulcanizing
psi - Pressure Per Square Inch
Pa - Pascal
W - Watt
m - Meter
K - Kelvin
FEA - Finite Element Analysis
σ - Total Stress
σ_{ii} - Principal Stress
D_{el} - Forth-Order Elasticity Tensor
ε_{el} - Total Elastic Strain
E - Young’s Modulus
ε_{ii} - Principal Strain
ν - Poisson’s Ratio
γ_{ij} - Transverse Strain
σ_{c} - Circumferential Stress
p - Pressure
r - Inner Radius
t - Wall Thickness
ε_{m} - Predicted Strain
ε_{e} - Experimental Strain
n - Number of Model Time Steps
ε_{th} - Thermal Strain
α(θ, f_{β}) - Thermal Expansion Coefficient
θ - Current Temperature
θ^{I} - Initial Temperature
f_{β} - Current Values of the Predefined Field Variables
$f^I_0$ - Initial Value of the Predefined Field Variables

$\theta^0$ - The Reference Temperature for the Thermal Expansion Coefficient

$U_{dev}$ - Deviatoric part

$U_{vol}$ - Volumetric Part

$\bar{I}_1$ - First Deviatoric Strain Invariant

$\bar{\lambda}_d$ - Deviatoric Stretches

$J_{el}$ - Elastic Volume Ratio

$C\alpha$ - Constant Expansion Coefficient

$N\alpha$ - Normalized Temperature Dependent Expansion Coefficient

LYM - Linear Two-Point Young’s Modulus

NYM - Normalized Temperature Dependent Young’s Modulus

CPR - Constant Poisson’s Ratio

NPR - Normalized Poisson’s Ratio

PA - Polyimide Aerogel
1.0 Introduction

1.1 Background and Literature Review

Due to the recent push for manned interplanetary exploration, cryogenic liquid management has become a topic of research of great interest.[18] Since life support and propulsion systems rely on cryogenic liquids, the ability to store them for long periods of time is mission enabling technology for the success of manned interplanetary missions. Today, many cryogenic tanks are made of either metals or composites. These tanks, while having relatively high mechanical strength, have several disadvantages. Metal tanks have a relatively high thermal conductivity, leading to heat infiltration into the tank. Heat infiltration causes the cryogenic liquid inside the tank to vaporize. Since the gas wants to take up more volume than the liquid, pressure increases inside the tank in a process known as self-pressurization. To maintain a safe operating pressure, the vapor is either vented off or cooled. Repeated pressurization and venting cycles can lead to fatigue of the tank wall. In addition to the pressurization and venting cycles, these tanks are also exposed to temperatures that range from 423K to 123K which causes thermal cycling. Thermal and mechanical cycling can lead to microcracks which compromise the mechanical strength of the tank. For long duration mission, cryogenic liquid tanks would likely need to be regularly serviced and/or repaired which would be difficult to accomplish in a space environment. Metals also have an inherently high density. This leads to an increased upmass for the spacecraft which increases the thrust requirements. Any increase in thrust requires more cryogenic propellant and increases the cost of the missions. [1][2]

To mitigate the boiloff of the cryogenic liquid caused by heat infiltration, current cryogenic tanks use passive and active systems. Jets, cryocoolers and thermodynamic vent
systems are all examples of active systems while insulation and vacuum layers are examples of passive systems. Multilayer insulation system, a type of passive system, uses multiple layers of material to insulate the cryogenic storage tank. These materials are usually added to an existing storage tank adding weight to the system. [1] [14]

To overcome these challenges, new novel materials have been developed which may be potentially useful in the construction of cryogenic storage tanks for space applications. RTV-655 is a vulcanized rubber that is space qualified and is easily molded into any shape. Its low thermal conductivity makes it ideal for cryogenic storage. Another class of materials developed within the last twenty years are aerogels. Aerogels possess favorable qualities for this application because they have relatively low densities and thermal conductivities. The first generation of aerogels developed, commonly referred to as native aerogels, have low tensile strength. To improve this, chemically crosslinked aerogels have been developed which increases the strength of the aerogel. Studies have shown that aerogels can be used in space applications as an insulator. Crosslinked polyimide aerogels were recently developed which can be synthesized into relatively thin flexible sheets. [1] [15]

Since these materials show promise as potential alternatives to metals and composites for cryogenic tanks, terrestrial experiments were performed to acquire some essential material properties and to test the feasibility of using these materials at cryogenic temperatures.

1.2 Previous Work

A research study was undertaken to construct two small scale cryogenic liquid tanks and determine whether RTV-655 and polyimide aerogel can be used to hold cryogenic liquids while
undergoing self-pressurization. One tank proposed was to be constructed of RTV-655 (RTV tank) and the other was to be constructed of RTV-655 embedded with polyimide aerogel (Aerogel/RTV-655 tank). For the study, it was hypothesized that the RTV-655 could serve as the primary construction material, in lieu of metals, which would result in tank with a relatively lower mass and lower thermal conductivity. The thin, flexible polyimide aerogel was proposed as an additional insulating layer which would be embedded in RTV-655 tank wall. The polyimide aerogel has an even lower density and thermal conductivity than the RTV-655. In Figures 1 and 2 you can see a sample of RTV-655 and a strip of polyimide aerogel.[1]

Figure 1: Picture RTV-655

Figure 2: Picture Polyimide Aerogel [1]

1.2.1 Material Testing

Prior to the construction of the two proposed tanks, it was necessary to obtain some mechanical property data at a cryogenic temperature. RTV-655 samples were synthesized using molds into dog-bone samples of dimensions of 16.00mm in length, 4.74 mm in width and
2.62mm thickness. These samples were loaded into a MARK-10 ESM301 test stand, and the samples were pulled in the axial direction until the samples broke. Using the deformation and force measurements from the tensile tests, stress and strain graphs can be created for the test samples of RTV-655. The slope of the initial portion of the graph is the Young’s Modulus. A similar process was done for polyimide aerogel to find its Young’s Modulus. The stress strain graphs for RTV-655 and polyimide aerogel can be seen below at both room temperature (301K) and 77 K. [1] [16]

![Stress and Strain Graph for RTV-655 at 301 K](image)

**Figure 3: Stress and Strain Graph for RTV-655 at 301 K** [3]
Figure 4: Stress and Strain Graph for RTV-655 at 77 K [3]

Figure 5: Stress and Strain Graph for Polyimide Aerogel at Various Temperatures [3]


1.2.2 Tank Creation

Since RTV-655 is a two-part compound, the polymer and binder were mixed together with a 10:1 weight ratio and were allowed to partially cure. The RTV-655 was then outgassed in a vacuum chamber to remove bubbles formed during the mixing process. It is outgassed in an aluminum base mold to form it in the proper shape. Once the outgassing process was complete, an aluminum lid is placed on top of the base mold and creates a cavity to form the shape of the tank walls. The base mold and aluminum lid can be seen Figures 6 and 7. The entire assembly is placed in an oven to complete the curing process. The process creates one-half of the tank and must be repeated to complete the second half of the tank. Once both halves of the tanks are created, test fittings are added to the tank. To combine the two halves together, 45° angled cuts were made to the two halves of the tank and the two halves are placed together forming a V-channel seen in Figure 8. This V-channel is then filled with uncured RTV-655 to complete the bonding of the two halves. [1]

![Figure 6: Aluminum Lid Used for Tank Creation](image1)

![Figure 7: Base Mold Used for Tank Creation](image2)
To create the Aerogel/RTV-655 tank, the polymer and binder were once again mixed to make the RTV-655, and two lids were used to mold a gap for the polyimide aerogel layer. The aerogel is embedded by placing the flexible strips on the inner surface of the outer wall of the tank. They are then tacked in place with uncured RTV-655. A second layer is applied with a 1mm layer of RTV to adhere the two aerogel layers together. Once the layers are adhered, the half of tank is placed in the mold to fill out the rest of the inner wall of the tank. These steps are repeated for the other half the tank. The two halves are then cut with a 45-degree angle and then fused together with uncured RTV-655 similarly to the RTV tank. [1]

Figure 8: V-Channel Formed by Connecting Two Tank Halves [1]
1.3 Experimental Setup

To test the viability of the tanks for storing cryogenic liquids, an experiment was designed to test the mechanical and thermal performance of the tanks. The cross-section of the experimental setup can be seen below in Figure 9. The tank sits in a terrestrial environmental chamber resting between two rings designed to keep the tank in place during the different phase of the experiment. Thermocouples were placed on the outer and inner wall of the tank to record the temperature. Extensometers were placed on the outer walls of the tank to measure the strain in three directions: diametral, circumferential, and axial. It is important to note that the circumferential extensometer utilized a bulky chain that was observed to freeze up and slide down the tank. This calls into the question the accuracy of the experimental data for the circumferential direction. To continue with the experimental setup, a flexible hose is attached to the tank below. This hose is where the liquid nitrogen enters the tank. There are union fittings at the top and bottom of the tank connected to the venting and supply piping systems. A pressure transducer is placed behind a safety valve and will be used to record the pressure inside the tank. The experimental setup can be seen below in Figure 10. [3]

Typical cryogenics used in space are liquid hydrogen and liquid oxygen, common propellants for liquid rocket engines such as the RS-25 used in the Space Shuttle Program. However, these propellants are highly reactive and are very expensive, so liquid nitrogen was used in place of liquid hydrogen and liquid oxygen. Liquid nitrogen was chosen as a suitable alternative because it is safer to handle, cheaper, and has a boiling point close to that of oxygen and hydrogen.
Figure 9: Cross Sectional View of Prototype Tank Experimental Setup [2]
The experimental procedure was the same for both the RTV-655 and Aerogel/RTV-655-655 tank. There were four phases of the experiment: Cooldown, Pressurization, Constant Liquid, and Boiloff. The experiment begins with the Cooldown phase to cool the outer wall of the tank and the environmental chamber down to -20°C where the tank can hold liquid nitrogen without it instantly vaporizing. The Cooldown phase begins when a valve is opened, and the liquid nitrogen enters the tank through the flexible hose at the bottom of the tank. The liquid nitrogen then vaporizes and exits the tank through the vent and enters the environmental chamber. This
continues until, eventually, the tank temperature comes down sufficiently to hold twenty-five percent of the tank volume with liquid nitrogen. The temperature and strain caused by the contraction of the tank were recorded during this phase. The results can be seen in Figure 11. [3]

![Figure 11: Experimental Results of the Strain During the Cooldown Phase](image)

Once the liquid nitrogen is filled to twenty-five percent of the total tank volume, the liquid nitrogen supply and vent are closed, and the Pressurization phase begins. Because of heat infiltration, the liquid nitrogen vaporizes causing the tank to self-pressurize. The pressure inside the tank was recorded using the pressure transducer. This pressure inside the tank can be seen in Figure 12. The extensometers also recorded the strain caused by the self-pressurization which can be seen in Figure 13. [3]
Figure 12: Pressure inside the RTV-655 Tank During the Pressurization Phase [3]
After the pressure inside the tank reaches 17 psig, a safety valve is released to allow the nitrogen vapor to escape. The vent is opened to allow the tank to return to atmospheric pressure and the nitrogen supply is reopened to replenish the liquid nitrogen that vaporized during the Pressurization phase. Once the tank returns to twenty-five percent volume of liquid nitrogen, the Constant Liquid phase begins. In this phase the liquid nitrogen supply is controlled to keep the tank at a twenty-five percent fill level. The purpose of this phase is to quantify the heat infiltration through the wall into the nitrogen liquid and ullage.[3]

After twenty minutes of the Constant Liquid phase, the liquid nitrogen supply is shut off and the phase ends and the Boiloff phase begins. In the Boiloff phase, the liquid nitrogen vaporizes, and the vapor is vented from the tank. After the liquid nitrogen is completely vaporized in the tank, the experiment is concluded.[3]
1.4 Objective

The objective of this research is to develop and validate a thermomechanical model of both the RTV-655 and Aerogel/RTV-655 tanks. If the proposed effort is fruitful, accurate simulations will ease the need for complex and expensive experiments in the future. A commercially available finite element method simulation will be used to model the thermomechanical behavior of the tanks. The first two phases of the RTV-655 and Aerogel/RTV-655-655 tank experiments will be the focus of the simulation and validation effort.

2.0 RTV-655 Finite Element Analysis Model

2.1 Governing equations

In order to model both, the thermal and mechanical behavior properly, a coupled-temperature analysis was used. The elastic behavior is modeled using Equations 1 and 2 for the relationship between stress and strain. [19]

\[ \sigma = D^{el} \epsilon^{el} \quad [\text{Eq. 1}] \]

\[
\begin{pmatrix}
\varepsilon_{11} \\
\varepsilon_{22} \\
\varepsilon_{33} \\
\gamma_{12} \\
\gamma_{13} \\
\gamma_{23}
\end{pmatrix} =
\begin{bmatrix}
1/E & -\nu/E & -\nu/E & 0 & 0 & 0 \\
-\nu/E & 1/E & -\nu/E & 0 & 0 & 0 \\
-\nu/E & -\nu/E & 1/E & 0 & 0 & 0 \\
0 & 0 & 0 & 1/G & 0 & 0 \\
0 & 0 & 0 & 0 & 1/G & 0 \\
0 & 0 & 0 & 0 & 0 & 1/G
\end{bmatrix}
\begin{pmatrix}
\sigma_{11} \\
\sigma_{22} \\
\sigma_{33} \\
\sigma_{12} \\
\sigma_{13} \\
\sigma_{23}
\end{pmatrix} \quad [\text{Eq. 2}]
\]
The equation modeling the thermal strain is given in Equations 3 below: [5]

\[ \varepsilon^{th} = \alpha(\theta, f_B)(\theta - \theta^0) - \alpha(\theta^I, f_B^I)(\theta^I - \theta^0) \] [Eq. 3]

### 2.2 RTV-655 Tank Geometry and Mesh

The RTV-655 tank was modeled first since it was constructed of a single material, thus simplifying the model. The tank geometry was created using the sketch feature in a finite element analysis (FEA) software package. It is hypothesized that the FEA software has adequate built-in capabilities necessary to model the thermomechanical behavior of these materials using the tank geometry and the experimental data as boundary conditions.

The geometry was then meshed, and a mesh convergence study was conducted to ensure the solution will be mesh independent. Three different mesh sizes were compared. The characteristics of each mesh can be seen below in Table 1.

<table>
<thead>
<tr>
<th>Global Seed Size (m)</th>
<th>Nodes</th>
<th>Elements</th>
</tr>
</thead>
<tbody>
<tr>
<td>.007</td>
<td>15,160</td>
<td>11,364</td>
</tr>
<tr>
<td>.003</td>
<td>139,482</td>
<td>119,482</td>
</tr>
<tr>
<td>.0025</td>
<td>237,568</td>
<td>267,282</td>
</tr>
</tbody>
</table>

The experimental temperature data recorded during the experiment was used as boundary conditions for the outer and inner walls of the tank. A simulation was conducted using each mesh
size. The comparison of these different mesh size results can be seen below in Figure 15. The .007 mesh was selected because of the minor differences between it and the finer meshes.

Figure 14: Meshed RTV-655 Tank
Although rectangular coordinates are the default setting in the FEA software, cylindrical coordinates were selected to enable a direct comparison with experimental data. As a validation case, a simple thin-wall hollow cylinder was modeled. The cylinder geometry is specified by an inner radius of 0.23 meters and a wall thickness of 0.02 meters which meets the requirements of \( r/t > 10 \) requirement for a thin pressure wall vessel. A pressure of 10 Pa was evenly distributed to the inner wall of the cylinder in cylindrical geometry. The solution for the circumferential stress can be determined analytically with the thin-walled assumption using the equation below.

\[
\sigma_c = \frac{pr}{t} \quad [11]
\]
For the geometry specified, the stress is:

\[ \sigma_c = \frac{(10 \text{ Pa}) \cdot (0.23 \text{ m})}{0.02 \text{ m}} = 115 \text{ Pa} \]

The simulation results, shown in Figure 16, show the circumferential stress is 115 Pa. This confirms that the model and coordinate system are working as intended.

**Figure 16: FEA Results of Thin Pressure Vessel**
2.4 RTV Material Properties

The results obtained from the mechanical material properties testing discussed in the Section 1.2.1 and material properties available in the literature can be seen in the Tables 2 and 3 below. These material properties will be used in the initial thermomechanical simulation presented in Section 2.5. [13]

### Table 2: RTV Material Properties at Room Temperature (301K)

<table>
<thead>
<tr>
<th>Material Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mass Density (kg/m³)</td>
<td>1040</td>
</tr>
<tr>
<td>Expansion Coefficient, α (m/m/K)</td>
<td>3.30E-04</td>
</tr>
<tr>
<td>Specific Heat (J/(kg*K))</td>
<td>1460</td>
</tr>
</tbody>
</table>

### Table 3: RTV Material Properties at 298K and 75K

<table>
<thead>
<tr>
<th>Young’s Modulus (Pa)</th>
<th>Poisson’s Ratio</th>
<th>Thermal Conductivity (W/(m*K))</th>
<th>Temp (K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.08E+08</td>
<td>0.495</td>
<td>.0833</td>
<td>298</td>
</tr>
<tr>
<td>9.65E+05</td>
<td>0.495</td>
<td>.1843</td>
<td>75</td>
</tr>
</tbody>
</table>

2.5 Initial Cooldown Model RTV-655

With the verification case completed, an initial effort was undertaken to model the cooldown phase of the RTV-655 experiment. A zero-displacement boundary condition was applied to the bottom of the tank as well as a displacement condition that would only allow the
top of the tank to move in the vertical direction. It is important to note that the contact influence of the support rings of the experimental apparatus were not measured directly, so the zero-displacement boundary condition was applied as a singular point at the bottom of the tank instead for simplification. It is thought that contact influence of the ring supports could be modeled later to help further refine the model as needed. After the displacement and experimental temperature boundary conditions were applied to the inner and outer wall of the RTV-655 tank, a simulation of the cooldown phase was performed. The results can be seen below in Figures 17, 18, and 19. To effectively differentiate this model from the forthcoming efforts to improve the model, a naming scheme was created to describe how the material properties are applied for each refinement or case study. This model, or case, is named Cα-LYM-CPR. Referring to properties shown in Tables 2 and 3, the “Cα” represents constant expansion coefficient; “LYM” stands for two-point linear Young’s Modulus, and “CPR” represents constant Poisson’s ratio.

![Comparison of the Constant Expansion Coefficient (Cα) and Poisson’s Ratio (CPR) with a Linear Temperature Dependent Young’s Modulus (LYM) Model vs. the Experimental Cooldown Phase Results in the Axial Direction](image)

**Figure 17:** Comparison of the Constant Expansion Coefficient (Cα) and Poisson’s Ratio (CPR) with a Linear Temperature Dependent Young’s Modulus (LYM) Model vs. the Experimental Cooldown Phase Results in the Axial Direction
Figure 18: Comparison of the Constant Expansion Coefficient (Cα) and Poisson’s Ratio (CPR) with a Linear Temperature Dependent Youngs Modulus (LYM) Model vs. Experimental Cooldown Phase Results in the Diametral Direction
To quantitatively compare simulation predictions with the experimental data, an average sum of the squares (S.O.S) is used. An average of the sum of squares (S.O.S) will ensure the number of iterations does not bias the comparison. This will allow for a direct comparison between different models with a different number of time steps. The formula for the average sum of squares can be seen below.

\[
\frac{\sum_{i=0}^{n}(\epsilon_m - \epsilon_e)^2}{n} \tag{17}
\]
Table 4: Cooldown Phase S.O.S Analysis for Case: Cα-LYM-CPR

<table>
<thead>
<tr>
<th></th>
<th>Axial</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Case</td>
<td>Average Sum of Squares</td>
<td></td>
</tr>
<tr>
<td>Cα-LYM-CPR</td>
<td>7.5E-05</td>
<td></td>
</tr>
</tbody>
</table>

|                  | Diametral                 |                            |
| Case             | Average Sum of Squares    |                            |
| Cα-LYM-CPR       | 5.00E-04                  |                            |

|                  | Circumferential           |                            |
| Case             | Average Sum of Squares    |                            |
| Cα-LYM-CPR       | 2.03E-02                  |                            |

2.6 Expansion Coefficient

From the results in Figures 17, 18 and 19, it is apparent that the simulation predicts a near linear relationship between temperature and strain; however, the experimental data show the material does not behave this way. The linear behavior in the thermal strain is a result of the equation used in the FEA model, Equation 3, for temperature dependent strain.

\[
e^{th} = \alpha(\theta, f_B)(\theta - \theta^0) - \alpha(\theta^1, f_B^1)(\theta^1 - \theta^0) \quad \text{[Eq. 3]}
\]
The thermal strain is obtained by multiplying the temperature difference by the expansion coefficient. Since the only expansion coefficient for RTV-655 published in the literature is at a temperature of 301K, the thermal strain rate is constant throughout the phase in the simulation. This leads to the linearity seen in the results. Since the temperature-dependent strain behavior of the experimental data is not linear, the expansion coefficient for RTV-655 is likely a function of temperature.

A challenge arose in finding expansion coefficient values for RTV-655 over a relevant temperature range. Since the objective of the research is to avoid expensive and complicated experiments, finding these values experimentally was not a viable short-term option. Instead, a literature review was conducted to find the expansion coefficient behavior of elastomers considered to be similar to RTV-655 and extrapolate based on the known value at room temperature.

Experiments conducted by the Department of Commerce included the measurement of contraction of a silastic rubber every 20K from 300K to 20K. The expansion coefficient can be derived from the contraction measurement data using Equation 5, which relates the slope of the temperature and the thermal strain. Taking the data provided, the expansion coefficient was derived between each temperature and normalized using the known value of RTV-655. The normalized expansion coefficient values for RTV-655 are presented in Table 4.
Table 5: Updated Expansion Coefficients

<table>
<thead>
<tr>
<th>Temp (K)</th>
<th>Derived Expansion Coefficient (m/m/K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>280</td>
<td>0.00033</td>
</tr>
<tr>
<td>240</td>
<td>0.000355</td>
</tr>
<tr>
<td>200</td>
<td>0.000317</td>
</tr>
<tr>
<td>160</td>
<td>0.000241</td>
</tr>
<tr>
<td>120</td>
<td>0.000171</td>
</tr>
<tr>
<td>80</td>
<td>0.000121</td>
</tr>
<tr>
<td>40</td>
<td>5.71E-05</td>
</tr>
</tbody>
</table>

The results of using the temperature dependent expansion coefficients from Table 4 in the simulation are shown in Figures 20, 21, and 22. This case name is $N_\alpha$-LYM-CPR where “$N_\alpha$” stands for normalized expansion coefficient.

![Comparison of the Normalized Expansion Coefficient ($N_\alpha$) with a Constant Poisson’s Ratio (CPR) and a Linear Temperature Dependent Youngs Modulus (LYM) Model and the Experimental Cooldown Phase Results in the Axial Direction](image)

Figure 20: Comparison of the Normalized Expansion Coefficient ($N_\alpha$) with a Constant Poisson’s Ratio (CPR) and a Linear Temperature Dependent Youngs Modulus (LYM) Model and the Experimental Cooldown Phase Results in the Axial Direction
Figure 21: Comparison of the Normalized Expansion Coefficient ($N_\alpha$) with a Constant Poisson’s Ratio (CPR) and a Linear Temperature Dependent Young’s Modulus (LYM) Model and the Experimental Cooldown Phase Results in the Diametral Direction
As seen below in Table 6, the sum of squares analysis suggests that there is a significant improvement due to the normalized expansion coefficient.

**Figure 22: Comparison of the Normalized Expansion Coefficient (Nα) with a Constant Poisson’s Ratio (CPR) and a Linear Temperature Dependent Youngs Modulus (LYM) Model and the Experimental Cooldown Phase Results in the Circumferential Direction**
Table 6: Cooldown Phase Analysis for Cases: Cα-LYM-CPR and Nα-LYM-CPR

<table>
<thead>
<tr>
<th></th>
<th>Axial</th>
<th></th>
<th>Diametral</th>
<th></th>
<th>Circumferential</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Case</td>
<td>Average Sum of Squares</td>
<td>Case</td>
<td>Average Sum of Squares</td>
<td>Case</td>
<td>Average Sum of Squares</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Cα-LYM-CPR</td>
<td>7.51E-05</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Nα-LYM-CPR</td>
<td>6.76E-05</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Cα-LYM-CPR</td>
<td>5.00E-04</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Nα-LYM-CPR</td>
<td>3.30E-04</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Cα-LYM-CPR</td>
<td>2.03E-02</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Nα-LYM-CPR</td>
<td>1.79E-02</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

With the updated table of temperature dependent expansion coefficients, the average S.O.S. for case Nα-LYM-CPR is lower in all directions when compared to the predictions from the initial case, Cα-LYM-CPR. The simulation still underpredicts the circumferential strain by an order of magnitude, but this is not surprising given the issues with the circumferential extensometer.
2.7 RTV-655 Pressurization Phase

The Pressurization phase is simulated with the same material properties used in the Cooldown phase simulation including the temperature dependent thermal expansion coefficients. For the Pressurization phase, the temperature gradient across the wall at the end of the Cooldown phase is held constant. Thus, there should be no thermal stress and the RTV-655 should be influenced solely by mechanical stress resulting from the increasing pressure inside of the tank. The pressure data obtained by using the pressure transducer in the experiment is applied as a load boundary condition to the entire inner wall of the tank. This pressure load is represented by orange arrows perpendicular to the inner tank wall in Figure 23. Other boundary conditions can be seen as well in Figure 23 such as the yellow squares representing the initial temperature condition and the orange and yellow cones that represent the top and bottom pins of the tank.
The simulation predictions of the axial, diametral, and circumferential strain over time are shown in Figures 24, 25, and 26.
Figure 24: Comparison of the Normalized Expansion Coefficient ($N_\alpha$) with a Constant Poisson’s Ratio (CPR) and a Linear Temperature Dependent Youngs Modulus (LYM) Model and the Experimental Pressurization Results in the Axial Direction
Figure 25: Comparison of the Normalized Expansion Coefficient ($\tilde{\alpha}$) with a Constant Poisson’s Ratio (CPR) and a Linear Temperature Dependent Young’s Modulus (LYM) Model and the Experimental Pressurization Results in the Diametral Direction.

Figure 26: Comparison of the Normalized Expansion Coefficient ($\tilde{\alpha}$) with a Constant Poisson’s Ratio (CPR) and a Linear Temperature Dependent Young’s Modulus (LYM) Model and the Experimental Pressurization Results in the Circumferential Direction.
The simulation predictions do not compare well to the experiment results for the Pressurization phase. In an effort to improve the accuracy of the model for the Pressurization phase, the material properties used in the physical model which will influence the mechanical strain will be further assessed. The sum of squares analysis can be seen below in Table 7.

Table 7: Pressurization Phase S.O.S Analysis for Case: Nα-LYM-CPR

<table>
<thead>
<tr>
<th></th>
<th>Axial</th>
<th>Diametral</th>
<th>Circumferential</th>
</tr>
</thead>
<tbody>
<tr>
<td>Case</td>
<td>Average Sum of Squares</td>
<td>Case</td>
<td>Average Sum of Squares</td>
</tr>
<tr>
<td>Nα-LYM-CPR</td>
<td>1.50E-06</td>
<td>Nα-LYM-CPR</td>
<td>1.00E-06</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Nα-LYM-CPR</td>
</tr>
</tbody>
</table>

2.8 Hyperelastic Solver

The first approach used to obtain a more accurate relationship between mechanical stress and strain in the Pressurization phase was to try a different physical model. The previous simulation used the Young’s Modulus to calculate the mechanical strain. Since it is reasonable to assume that RTV-655 may be more hyperelastic than elastic, a hyperelastic model is considered.
The FEA software includes many different types of hyperelastic solvers such as Ogden, Neo-Hooke, and Mooney-Rivlin.[9] The Marlow hyperelastic model is chosen because it is the only model available in the software which will also allow temperature dependent properties. The formulas for the Marlow model [9] are:

\[ U = U_{dev}(\bar{I}_1) + U_{vol}(J_{el}) \]  
[Eq. 4]

\[ \bar{I}_1 = \lambda_1^2 + \lambda_2^2 + \lambda_3^2 \]  
[Eq. 5]

RTV-655 stress and strain data obtained directly from the tensile test presented in Section 1.2.1 were used as input for the Marlow model simulation at 301 K and 77 K. The results of the simulation show a considerable overestimation of the mechanical strain by a couple magnitudes in all three directions. The poor agreement of the Marlow model predictions with the experiment data suggests that RTV-655 is not a pure hyperelastic material, thus, another approach must be considered.

2.9 Young’s Modulus

The study subsequently returned to a focus on the Young’s Modulus. The initial simulation used a linear interpolation of the Young’s Modulus from the two measured values at 301K and 77K presented in Table 3. To better understand why the simulation might not be accurate using linear interpolation between the two known values, a literature review was conducted to better understand the behavior of Young’s Modulus as a function of temperature for elastomers. Studies from Firestone Tire and Rubber Company, Federal Institute for Material Testing and Research and Institute for Machine Tools and Production Processes were reviewed. It became clear from the studies that in elastomeric materials, Young’s Modulus does not vary
linearly as a function of temperature. Rather, the behavior of the elastomer in terms of Young’s Modulus can be characterized over three different temperature ranges and these ranges are unique from elastomer to elastomer. As shown in Figure 27, the behavior of elastomer as a function of temperature can be characterized by an elastic region, glass transition region and glassy region. The elastic region describes the temperature range in which the elastomer is relatively flexible. The glassy region is the temperature range where elastomer is very stiff. The glass transition region is the temperature range where the elastomer suddenly shifts from being flexible to being stiff or vice versa. [6][10]

Since the two measured values of Young’s Modulus for RTV-655 at 301 K and 77 K differ by several orders of magnitudes, it is reasonable to assume that the point with the highest
magnitude lies in the glassy region and the other point lies in the elastic region. Since the glass transition temperature is not published, the supplier of the RTV-655 was contacted for more information. After receiving no response from the supplier, the specification sheet for RTV-655 was analyzed for any clues on the glass transition temperature. The material specification sheet mentions that “RTV-655 silicone rubber compounds have the capability of remaining flexible at temperatures -115°C [158K]”. The assumption was made that after this temperature, RTV-655 no longer exhibited the behaviors characterized by the elastic region and hence becomes significantly stiffer. It was subsequently assumed that 158 K is the glass transition temperature for RTV-655. The only unknown remaining is temperature that defines the upper bound of the glassy region. With measured values of Young’s Modulus at 301 K and 77 K in the elastic and glassy regions, respectively, and the assumption of the glass transition temperature at 158 K, the behavior of RTV-655 can be estimated over the temperature range of the experiment. RTV-655 was normalized using the behavior of Nitrile-Butadiene-Rubber shown in Figure 27. This elastomer was chosen because of its use in cryogenic applications. A comparison between the normalized RTV-655 temperature dependent Young’s Modulus and other elastomers is shown in Figure 28.
The simulation predictions of the Pressurization phase using the normalized temperature dependent Young’s Modulus values are shown in Figures 29, 30, and 31. The case name is Nα-NYM-CPR, where “NYM” represents normalized Young’s Modulus with a glass transition.

Figure 28: Comparison of Different Elastomers and Estimated RTV-655 Value [6] [13]
temperature. In addition, the Nα-LYM-CPR predictions, which uses a linear fit between the two measured values of Young’s Modulus at 301K and 77K, is included for comparison.

Figure 29: Comparison of the Normalized Expansion Coefficient (Nα) with a Constant Poisson’s Ratio (CPR) and a Linear Temperature Dependent Youngs Modulus (LYM) Model, the Normalized Expansion Coefficient (Nα) with a Constant Poisson’s Ratio (CPR) and a Normalized Temperature Dependent Youngs Modulus with a Glass Transition Temperature (NYM) Model, and the Experimental Pressurization Phase Results in the Axial Direction
Figure 30: Comparison of the Normalized Expansion Coefficient (\(N_\alpha\)) with a Constant Poisson’s Ratio (CPR) and a Linear Temperature Dependent Youngs Modulus (LYM) Model, the Normalized Expansion Coefficient (\(N_\alpha\)) with a Constant Poisson’s Ratio (CPR) and a Normalized Temperature Dependent Youngs Modulus with a Glass Transition Temperature (NYM) Model, and the Experimental Pressurization Phase Results in the Diametral Direction
As shown below in Table 8, the use of the normalized Young’s Modulus using the glass transition temperature, case Nα-NYM-CPR, improved the simulation predictions, in terms of the average S.O.S when compared to case Nα-LYM-CPR. The simulated diametral strain predictions are very close to the experimental values, but the axial, while improved, is still underestimating the experimental strain, so further material property refinement is explored.
### Table 8: Pressurization Phase Analysis for Cases: Nα-LYM-CPR and Nα-NYM-CPR

<table>
<thead>
<tr>
<th>Case</th>
<th>Average Sum of Squares</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Axial</strong></td>
<td></td>
</tr>
<tr>
<td>Nα-LYM-CPR</td>
<td>1.50E-06</td>
</tr>
<tr>
<td>Nα-NYM-CPR</td>
<td>2.65E-07</td>
</tr>
<tr>
<td><strong>Diametral</strong></td>
<td></td>
</tr>
<tr>
<td>Nα-LYM-CPR</td>
<td>1.00E-06</td>
</tr>
<tr>
<td>Nα-NYM-CPR</td>
<td>1.29E-06</td>
</tr>
<tr>
<td><strong>Circumferential</strong></td>
<td></td>
</tr>
<tr>
<td>Nα-LYM-CPR</td>
<td>3.31E-06</td>
</tr>
<tr>
<td>Nα-NYM-CPR</td>
<td>2.46E-06</td>
</tr>
</tbody>
</table>

### 2.10 Poisson’s Ratio

Another material property directly related to mechanical strain is Poisson’s Ratio. A single value of Poisson’s Ratio has been specified at all temperatures in the previous simulations. A literature review was conducted to ascertain whether Poisson’s Ratio, similar to Young’s Modulus, varies significantly with temperatures. The literature shows that that the Poisson’s Ratio can vary significantly with temperature for elastomers as exemplified for a structural epoxy in Figure 32.[7][8][11]
From these studies, Poisson’s Ratio remains relatively constant until the glass transition temperature is reached where there is a significant decrease in the value. Using the glass transition temperature and the known measured value of Poisson’s ratio for RTV-655 at 301 K, the temperature was extrapolated as seen in Table 9. Since there is no known value for Poisson’s ratio after the glass transition temperature, the value of 0.330 was used as a conservative estimate from the literature.[7][8][11]
Table 9: Normalized Poisson’s Ratio

<table>
<thead>
<tr>
<th>Temp K</th>
<th>Poisson’s Ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td>301</td>
<td>0.495</td>
</tr>
<tr>
<td>250</td>
<td>0.495</td>
</tr>
<tr>
<td>158.15</td>
<td>0.495</td>
</tr>
<tr>
<td>125</td>
<td>0.330</td>
</tr>
<tr>
<td>77</td>
<td>0.330</td>
</tr>
</tbody>
</table>

Using these updated material properties, a simulation was performed to ascertain the influence of Poisson’s ratio on the strain predictions during the Pressurization Phase RTV tank. The name of this case is Na-NYM-NPR, where NPR stands for normalized Poisson’s ratio. As shown below in Table 10, case Na-NYM-NPR resulted in improved the simulation predictions of the axial and diametral strains, in terms of the average S.O.S, when compared to case Na-NYM-CPR.
Figure 33: Comparison of the Normalized Expansion Coefficient ($N_\alpha$) with a Constant Poisson’s Ratio (CPR) and a Normalized Temperature Dependent Youngs Modulus with a Glass Transition Temperature (NYM) Model, the Normalized Expansion Coefficient ($N_\alpha$) with a Normalized Poisson’s Ratio with a Glass Transition Temperature (NPR) and a Normalized Temperature Dependent Youngs Modulus with a Glass Transition Temperature (NYM) Model, and the Experimental Pressurization Phase Results in the Axial Direction
Figure 34: Comparison of the Normalized Expansion Coefficient (Nα) with a Constant Poisson’s Ratio (CPR) and a Normalized Temperature Dependent Youngs Modulus with a Glass Transition Temperature (NYM) Model, the Normalized Expansion Coefficient (Nα) with a Normalized Poisson’s Ratio with a Glass Transition Temperature (NPR) and a Normalized Temperature Dependent Youngs Modulus with a Glass Transition Temperature (NYM) Model, and the Experimental Pressurization Phase Results in the Diametral Direction
Figure 35: Comparison of the Normalized Expansion Coefficient ($N_\alpha$) with a Constant Poisson’s Ratio (CPR) and a Normalized Temperature Dependent Young's Modulus with a Glass Transition Temperature (NYM) Model, the Normalized Expansion Coefficient ($N_\alpha$) with a Normalized Poisson’s Ratio with a Glass Transition Temperature (NPR) and a Normalized Temperature Dependent Young's Modulus with a Glass Transition Temperature (NYM) Model, and the Experimental Pressurization Phase Results in the Circumferential Direction.
Table 10: Comparison of S.O.S Analysis Between Different Models During Pressurization Phase

<table>
<thead>
<tr>
<th>Case</th>
<th>Average Sum of Squares</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Axial</strong></td>
<td></td>
</tr>
<tr>
<td>Nα-LYM-CPR</td>
<td>1.50E-06</td>
</tr>
<tr>
<td>Nα-NYM-CPR</td>
<td>2.65E-07</td>
</tr>
<tr>
<td>Nα-NYM-NPR</td>
<td>2.78E-08</td>
</tr>
<tr>
<td><strong>Diametral</strong></td>
<td></td>
</tr>
<tr>
<td>Nα-LYM-CPR</td>
<td>1.00E-06</td>
</tr>
<tr>
<td>Nα-NYM-CPR</td>
<td>1.29E-06</td>
</tr>
<tr>
<td>Nα-NYM-NPR</td>
<td>5.56E-07</td>
</tr>
<tr>
<td><strong>Circumferential</strong></td>
<td></td>
</tr>
<tr>
<td>Nα-LYM-CPR</td>
<td>3.31E-06</td>
</tr>
<tr>
<td>Nα-NYM-CPR</td>
<td>2.46E-06</td>
</tr>
<tr>
<td>Nα-NYM-NPR</td>
<td>1.80E-06</td>
</tr>
</tbody>
</table>
2.11 Effect on Cooldown Phase

After the normalized temperature dependent Young’s Modulus was updated in the Pressurization phase simulation, the Cooldown phase simulation was performed again with the updated properties. The predictions are shown in Figures 36, 37, and 38.

Figure 36: Comparison of the Normalized Expansion Coefficient (Nα) with a Constant Poisson’s Ratio (CPR) and a Linear Temperature Dependent Youngs Modulus (LYM) Model, the Normalized Expansion Coefficient (Nα) with a Constant Poisson’s Ratio (CPR) and a Normalized Temperature Dependent Youngs Modulus with a Glass Transition Temperature (NYM) Model, and the Experimental Cooldown Phase Results in the Axial Direction
Figure 37: Comparison of the Normalized Expansion Coefficient ($N_\alpha$) with a Constant Poisson’s Ratio (CPR) and a Linear Temperature Dependent Youngs Modulus (LYM) Model, the Normalized Expansion Coefficient ($N_\alpha$) with a Constant Poisson’s Ratio (CPR) and a Normalized Temperature Dependent Youngs Modulus with a Glass Transition Temperature (NYM) Model, and the Experimental Pressurization Phase Results in the Diametral Direction
Initially it was believed that the thermal stress would far exceed the mechanical stresses during the Cooldown phase. However, the predictions shown in Figures 36, 37, and 38, clearly show the addition of the normalized temperature dependent Young’s Modulus have significantly affected the results. While the prediction of the strains in the diametral direction are improved when compared to the experiment data, the strains in the axial direction are over predicted as seen in Table 11. After further examination, the reason for the increase in mechanical strain becomes clear. For the temperature range of 301K to 150K the linear fit yields a higher Young’s Modulus than the normalized fit, and therefore, the material exhibits a higher resistance to mechanical strain. Using the normalized temperature dependent Young’s Modulus, the material exhibits elastomeric behavior for temperatures above the glass transition temperature. Below the
glass transition temperature, the Young’s Modulus increases by several orders of magnitude, so the material stiffens considerably. Since much of the Cooldown phase of the experiment occurs in the temperature range of 301K-150K, the simulation predictions using the normalized Young’s Modulus results in higher mechanical strains.

The simulations of the Cooldown phase were also performed using the normalized temperature dependent Poisson’s ratio, however the differences between the Cooldown strain predictions between Na-NYM-CPR and Na-NYM-NPR were negligible. For the Cooldown phase, it was concluded that the variations in the value of Poisson’s ratio did not contribute significantly to any change in the mechanical strain.
Table 11: Comparison of Analysis Between Different Models During Cooldown Phase

<table>
<thead>
<tr>
<th>Case</th>
<th>Average Sum of Squares</th>
</tr>
</thead>
<tbody>
<tr>
<td>Axial</td>
<td></td>
</tr>
<tr>
<td>Cα-LYM-CPR</td>
<td>7.51E-05</td>
</tr>
<tr>
<td>Nα-LYM-CPR</td>
<td>6.76E-05</td>
</tr>
<tr>
<td>Nα-NYM-CPR</td>
<td>3.90E-04</td>
</tr>
<tr>
<td>Diametral</td>
<td></td>
</tr>
<tr>
<td>Cα-LYM-CPR</td>
<td>5.00E-04</td>
</tr>
<tr>
<td>Nα-LYM-CPR</td>
<td>3.30E-04</td>
</tr>
<tr>
<td>Nα-NYM-CPR</td>
<td>1.60E-04</td>
</tr>
<tr>
<td>Circumferential</td>
<td></td>
</tr>
<tr>
<td>Cα-LYM-CPR</td>
<td>2.03E-02</td>
</tr>
<tr>
<td>Nα-LYM-CPR</td>
<td>1.79E-02</td>
</tr>
<tr>
<td>Nα-NYM-CPR</td>
<td>1.87E-02</td>
</tr>
</tbody>
</table>

3.0 Aerogel/RTV-655 Finite Element Model

3.1 Aerogel/Tank Model Creation/Mesh Convergence Study

Following the completion of the RTV-655 tank simulation, a model of the Aerogel/RTV-655 tank was created. The geometry of each layer of material was drawn as its own part and the geometries were merged into a single assembly. The feature avoids the need to use complex
interaction features that are computationally expensive. The final meshed assembly can be seen below in Figure 39.

![Figure 39: Cross-Section View of Meshed Aerogel/RTV-655 Tank](image)

After the tank model was created, a mesh convergence study was conducted. Three different mesh sizes were studied: 0.007m, 0.003m, and 0.0025m. The diametral strain of the outer wall was studied to compare predictions for the different sizes. The same boundary conditions used for the RTV tank mesh convergence study were applied to the Aerogel/RTV-655 tank. The results of the mesh convergence study are shown in Figure 40. The 0.003m seed size was selected because there was negligible difference in strain predictions when compared to the 0.0025m seed size.
Table 12: Aerogel/RTV-655 Tank Mesh Characteristics

<table>
<thead>
<tr>
<th>Global Seed Size (m)</th>
<th>Nodes</th>
<th>Elements</th>
</tr>
</thead>
<tbody>
<tr>
<td>.007</td>
<td>22,260</td>
<td>25,984</td>
</tr>
<tr>
<td>.003</td>
<td>158,832</td>
<td>178,704</td>
</tr>
<tr>
<td>.0025</td>
<td>224,192</td>
<td>252,234</td>
</tr>
</tbody>
</table>

Using the RTV-655 material properties with the temperature-dependent expansion coefficient, Young’s Modulus and Poisson’s ratio as well as the known polyimide aerogel properties seen in Tables 13 and 14, simulations of both the Cooldown and Pressurization phases

3.2 Aerogel/RTV-655 Results

Figure 40: Mesh Convergence Study of Aerogel/RTV-655 Tank
were conducted. The temperature and pressure boundary conditions are taken directly from Aerogel/RTV-655-655 tank experimental data.

Table 13: Aerogel Properties at Different Temperatures

<table>
<thead>
<tr>
<th>Young’s Modulus (MPa)</th>
<th>Thermal Conductivity (W/m*K)</th>
<th>Temperature (K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>23.2</td>
<td>0.0397</td>
<td>293</td>
</tr>
<tr>
<td>37.1</td>
<td>0.0344</td>
<td>273</td>
</tr>
<tr>
<td>75.7</td>
<td>0.0198</td>
<td>77</td>
</tr>
</tbody>
</table>

Table 14: Aerogel Properties at Room Temperature

<table>
<thead>
<tr>
<th>Mass Density (kg/m³)</th>
<th>137</th>
</tr>
</thead>
<tbody>
<tr>
<td>Expansion Coefficient (m/m/K)</td>
<td>3.00E-06</td>
</tr>
<tr>
<td>Specific Heat (J/(kg*K))</td>
<td>1078</td>
</tr>
<tr>
<td>Poisson’s Ratio</td>
<td>0.2</td>
</tr>
</tbody>
</table>

The results of the Cooldown phase simulations can be seen below in Figures 41, 42, 43. This model’s name is PA-Nα-NYM-NPR where the “PA” represent polyimide aerogel.
Figure 41: Comparison of the Normalized Expansion Coefficient (N\(\alpha\)) with a Normalized Poisson’s Ratio with a Glass Transition Temperature (NPR) and a Normalized Temperature Dependent Young’s Modulus with a Glass Transition Temperature (NYM) Model vs Experimental Cooldown Phase Results in the Axial Direction for the Aerogel/RTV-655 Tank
Figure 42: Comparison of the Normalized Expansion Coefficient (Nα) with a Normalized Poisson’s Ratio with a Glass Transition Temperature (NPR) and a Normalized Temperature Dependent Youngs Modulus with a Glass Transition Temperature (NYM) Model vs Experimental Cooldown Phase Results in the Diametral Direction for the Aerogel/RTV-655 Tank
Figure 43: Comparison of the Normalized Expansion Coefficient ($N_\alpha$) with a Normalized Poisson’s Ratio with a Glass Transition Temperature (NPR) and a Normalized Temperature Dependent Young’s Modulus with a Glass Transition Temperature (NYM) Model vs Experimental Cooldown Phase Results in the Circumferential Direction for the Aerogel/RTV-655 Tank
Table 15: Cooldown Phase Analysis for Case: PA-Nα-NYM-NPR

<table>
<thead>
<tr>
<th></th>
<th>Axial</th>
<th>Diametral</th>
<th>Circumferential</th>
</tr>
</thead>
<tbody>
<tr>
<td>Case</td>
<td>Average Sum of Squares</td>
<td></td>
<td></td>
</tr>
<tr>
<td>PA-Nα-NYM-NPR</td>
<td>7.00E-04</td>
<td>7.00E-04</td>
<td>1.41E-02</td>
</tr>
</tbody>
</table>

The results of the Pressurization phase simulation for the Aerogel/RTV-655 Tank can be seen below in Figures 44, 45, and 46. The sum of squares analysis can be seen in Table 15.
Figure 44: Comparison of the Normalized Expansion Coefficient (Nα) with a Normalized Poisson’s Ratio with a Glass Transition Temperature (NPR) and a Normalized Temperature Dependent Youngs Modulus with a Glass Transition Temperature (NYM) Model vs Experimental Pressurization Phase Results in the Axial Direction for the Aerogel/RTV-655 Tank
Figure 45: Comparison of the Normalized Expansion Coefficient ($N_\alpha$) with a Normalized Poisson’s Ratio with a Glass Transition Temperature (NPR) and a Normalized Temperature Dependent Youngs Modulus with a Glass Transition Temperature (NYM) Model vs Experimental Pressurization Phase Results in the Diametral Direction for the Aerogel/RTV-655 Tank
Figure 46: Comparison of the Normalized Expansion Coefficient ($N_\alpha$) with a Normalized Poisson’s Ratio with a Glass Transition Temperature (NPR) and a Normalized Temperature Dependent Young’s Modulus with a Glass Transition Temperature (NYM) Model vs Experimental Pressurization Phase Results in the Circumferential Direction for the Aerogel/RTV-655 Tank.
Table 16: Pressurization Phase S.O.S Analysis for Case: PA-\(\alpha\)-LYM-CPR

<table>
<thead>
<tr>
<th>Case</th>
<th>Average Sum of Squares</th>
</tr>
</thead>
<tbody>
<tr>
<td>PA-(\alpha)-LYM-CPR</td>
<td>1.33E-07</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Case</th>
<th>Average Sum of Squares</th>
</tr>
</thead>
<tbody>
<tr>
<td>PA-(\alpha)-LYM-CPR</td>
<td>1.74E-07</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Case</th>
<th>Average Sum of Squares</th>
</tr>
</thead>
<tbody>
<tr>
<td>PA-(\alpha)-LYM-CPR</td>
<td>3.12E-06</td>
</tr>
</tbody>
</table>

The Aerogel/RTV-655 tank strain predictions are similar to the strain predictions for RTV-655 tank. The simulation overestimates the strain in all directions in the Cooldown phase. A more in-depth analysis of possible causes is presented in the next section. For the Pressurization phase, the strain predictions in the axial direction are in reasonable agreement with the experimental data.

4.0 Analysis of Cooldown Predictions

The discrepancy between the simulation predictions and experimental results in the Cooldown phase highlighted the necessity to differentiate the relative influences of the thermal and mechanical stresses on the behavior of respective materials and tank geometries. Although the ratio of mechanical strain to thermal strain in the experimental results cannot be
differentiated in the available data, the ratio can be ascertained using the model. A breakdown of the contribution of the mechanical strain and thermal strain as a percentage of the total strain for the outer wall of the RTV/Aerogel tank are shown below in Figures 47, 48, and 49. The model predictions show the mechanical stresses clearly influence the total strain more significantly than the thermal stresses. This result was not intuitive since there was no obvious external mechanical load during the Cooldown phase. A few simple test cases were performed to investigate what could be causing mechanical stress.

![Figure 47: Comparison of Thermal and Mechanical Strain in the Axial Direction for Aerogel/RTV-655 Tank Model for the Cooldown Phase](image)
Figure 48: Comparison of Thermal and Mechanical Strain in the Circumferential Direction for Aerogel/RTV-655 Tank Model for the Cooldown Phase

Figure 49: Comparison of Thermal and Mechanical Strain in the Diametral Direction for Aerogel/RTV-655 Tank Model for the Cooldown Phase
To begin the investigation, the displacement boundary conditions were checked to see if they were introducing unwanted mechanical stress. A test case with no boundary conditions (i.e., the tank was unpinned and free to move in any direction) was simulated. The results show that the boundary conditions have zero effect on the predictions of the strain of the tank. With boundary condition checked, a couple of theories were created to explain the cause of the mechanical stresses. The first theory is that the mechanical strain is a result of stress that develops internally due to the geometry of the tank, which is cylindrical with two semi-hemispherical end caps. The different components of tank geometry may contract differently relative to each other which may subsequently introduce mechanical stress concentrations.

The second theory posits that the temperature gradient across the wall may create mechanical stresses since the mechanical properties are temperature dependent. Since the inner wall has direct contact to the cryogenics, it is significantly colder than the outer wall. This difference in temperature then leads to a different rate of contraction due to the thermal stress between the inner and outer walls induces mechanical stress.

To test these theories, several simple test cases were considered. It should be noted that these theories are not mutually exclusive and can both be contributing to the mechanical stress. To test the first theory and see if the mechanical stress is geometry dependent, a cylinder test case was created. The modeled cylinder can be seen below in Figure 50. The cylinder has an outer diameter of .135m and an inner diameter of .100m with a length of 1.00m.
To test the first theory, the cylinder was set to initial temperature of 301 K for all elements. Then all elements were given a boundary condition of 200 K in order to cause contraction in the cylinder. If the theory is correct, the cylinder should only have thermal strains since its cross-section is homogenous and should contract uniformly. Figures 51 and 52 show that the total strain equals the thermal strain, thus there is zero mechanical strain in the cylinder.
Figure 51: Total Strain of Test Cylinder

Figure 52: Thermal Strain of Test Cylinder
To confirm the theory, the tank geometry was revisited. It was given the same boundary conditions as the cylinder to see if the mechanical strain behavior was geometry dependent. The results below show that the strain behavior is in fact geometry dependent as the total strain and thermal strain do not match. Therefore, the mechanical stress is induced internally as the tank is subjected to thermal stress.

Figure 53: Total Strain of RTV Tank
The second theory was also tested using the same cylinder. The same 301K initial temperature condition was used, but instead of applying a single temperature condition to all elements, temperature boundary conditions of 100°C were applied to the inner and 200°C to the outer wall. If the theory is correct, the different rate of contraction on the inner wall should influence the outer wall which is contracting less. This should result in mechanical stress not seen in the previous model where the temperature boundary condition was applied to all elements. As shown in Figure 55 and 56, the thermal strain and total strain do not match. Thus, it can be concluded that both the tank geometry and the difference in thermal strain due to the temperature gradient in the tank wall induce mechanical stress during the Cooldown phase.
Figure 55: Total Strain of Test Cylinder with a Temperature Gradient

Figure 56: Thermal Strain of Test Cylinder with a Temperature Gradient
5.0 Influence of Aerogel Geometry on Simulation Predictions

One possible reason for the inaccuracies of the Aerogel/RTV-655-655 predictions may be due to the simplification made to model the polyimide aerogel layers as one homogeneous, monolithic material embedded in the RTV-655. This is not a geometrically accurate representation of how the aerogel is embedded in RTV-655 in the experimental tank. As described in Section 1.4, the aerogel is composed of two layers of smaller strips instead of a single continuous material. Including geometric details of each strip for would be computationally expensive to model but may increase the accuracy of the model.

A couple of attempts were made to model the polyimide aerogel differently. The first attempt added in the 1mm RTV-655 connecting layer between the two aerogel film strips of .004mm in thickness. The two aerogel layers and the connecting layer of RTV are clearly visible in the geometry’s mesh seen in Figure 57. The second geometry broke up the aerogel layers between the two hemispherical ends of the tank. After simulating both geometries, it became clear that neither of these geometries made a significant difference in the results of the Cooldown phase.
Recent experimentation using two small-scale tanks, one constructed of RTV-655 and another constructed of Aerogel/RTV-655-655, demonstrated the feasibility of using these materials at cryogenic temperatures. The objective of this research was to create thermomechanical models of the two, small-scale cryogenic tanks experiments to enable further study. A secondary objective was to use the simulations to gain a better understanding of the thermal and mechanical properties of both RTV-655 and polyimide aerogel.

The effort began by conducting a literature review of the experiments that would serve as the foundation for creating the thermomechanical model. After the literature review was completed, the RTV-655 tank was modeled first because it is made of a single material. The geometry of the tank was created, and a mesh convergence study was conducted to find the right balance between accuracy and computational time. After an appropriate mesh density was selected, the boundary conditions were specified using data from the Cooldown phase of the

Figure 57: Aerogel with RTV-655 Connecting Layer
experiment. An initial baseline simulation was performed using a linear fit between two measured values of Young’s Modulus at 77K and 301K and known material properties, such as the expansion coefficient and thermal conductivity, which were obtained from the literature. The simulation predicted a constant strain rate which was a poor match to experimental data. The constant strain rate was caused by only having a single expansion coefficient for all temperatures. To correct this, a literature review was undertaken to better understand the behavior of the thermal expansion coefficient for elastomers. During the literature review, it seemed clear the expansion coefficient is temperature dependent, so the temperature dependent coefficients for silastic rubbers derived from published contraction results were used to normalize the expansion coefficient values for RTV-655 using the known values of RTV-655. This updated material behavior was tested in a new simulation and the results showed an improvement in the model predictions compared to experiment data.

A baseline simulation of the Pressurization phase of the experiment was then performed. The baseline predictions underestimated the mechanical strain as compared the experiment data. To resolve this, a literature review was conducted to better understand the temperature dependent behavior for Young’s Modulus for elastomers. The literature review revealed that the Young’s Modulus does not vary linearly with temperature. Thus, the temperature dependent Young’s Modulus behavior of RTV-655 was estimated by using the known values of RTV-655 in the elastic, glass and glass transition temperature region and normalized over the temperature range using values obtained for an elastomer with similar mechanical properties. The use of the normalized temperature dependent Young’s Modulus showed a significant improvement in the model predictions of the Pressurization phase. In an effort to improve the model further, Poisson’s ratio was analyzed. Another literature review was conducted, to better characterize
Poisson’s ratio as a function of temperature for elastomers. This review showed that Poisson’s ratio also varies with temperature. Like Young’s Modulus, the value of Poisson’s ratio does not vary linearly with temperature and changes significantly around the glass transition temperature. The temperature dependent Poisson’s ratio was then updated and showed small improvements in the model predictions.

The Cooldown phase was then revisited to determine how the changes in the material properties would affect the mechanical strain. The normalized temperature dependent material properties significantly improved the model predictions of the strain in the diametral direction but overestimated the strains in the axial direction.

The RTV/Aerogel tank was the next to be simulated. Using all the updated material properties of RTV-655 and the known values of polyimide aerogel obtained from the literature. These results showed that the strain was being overestimated in the Cooldown phase, but relatively accurately predicted in the Pressurization phase. Analysis of the Cooldown phase showed large amounts of mechanical strain. Two test cases were simulated that confirmed that both the geometry of the tank and the temperature gradients in the tank walls contributed to internal mechanical stresses that developed when thermal stresses were present.

In general, the thermomechanical model predicts the strain of the tank relatively well particularly in the Pressurization phase. However, before this model can be used to help in future studies of RTV-655 and polyimide aerogel cryogenic tanks, the discrepancies between the Cooldown phase experimental results and predicted results need to be addressed. The results presented highlight the complex temperature dependence of the material properties for both the RTV-655 and the polyimide aerogel. For both RTV-655 and aerogel, the mechanical properties were estimated by normalizing the behavior of other materials thought to be similar using only a
few known measured values. Normalizing can give a good estimate, but characteristics like the behavior of RTV-655 around glass transition temperature cannot be perfectly normalized as the glass transition property values are unique to each elastomer. It became clear from this work that knowing a few measured property values over a large temperature range, particularly at cryogenic temperatures, was inadequate to accurately model the RTV and RTV/Aerogel tank experiments. The lack of published material properties for both RTV-655 and polyimide aerogel will present a significant challenge in improving the model further. To overcome this, additional material testing should be done to better characterize the material properties of RTV-655 and polyimide aerogel over a range of temperatures.

Continued refinement of the model can be accomplished by including additional features of the experimental apparatus. Features such as the brass and Teflon fittings for the vent and supply hose as well as the rings that hold the tank in place are not modeled in the simulations presented. It is unclear whether these features would have a significant effect on the stresses and strains in tanks, but their inclusion will certainly increase the computational complexity. Before increasing the geometric and computational complexity, however, the results herein suggest the priority should be placed on obtaining a more complete set of accurate mechanical and thermal properties for the RTV-655 and polyimide aerogel.

7.0 Study Limitations

Recognition of limitations and uncertainties is important in the assessment of the simulation and its predictions. The six sources of uncertainty proposed by Kennedy and O’Hagen considered within the context of this research study are: parameter uncertainty, model
inadequacy, residual variability, parametric variability, observation error, and code uncertainties. Parameter uncertainty refers to the uncertainty of the input of values for a computer model. For the present study, parameter uncertainty was certainly introduced with the input of the material properties. One critical example of an assumptions made, which would lead to parameter uncertainty, was the use of the material properties of one material to normalize a set of unknown properties for the materials of interest over a range of temperatures. As seen in Section 2.1, it was assumed that RTV-655 is isotropic, but it is possible that the material properties, such as Poisson’s ratio, are directionally dependent, i.e. anisotropic. Model inadequacy is the discrepancy between the predicted value and the true value. This type of error can be introduced when there is uncertainty around the physical model which is chosen to describe the behavior of a particular material. For example, the material properties for RTV-655 and polyimide aerogel are poorly characterized in the literature, thus, the selection of an appropriate physical model for these materials was uncertain from the onset. A comparison of the mechanical strain simulation predictions using the linear strain model and hyperelastic strain model illustrate the impact of changing the physical model. Residual variability describes the randomness of processes in the real world that are difficult to model. The residual variability for the present study lies in the experiment data which is used for both the input conditions and serves as validation for the simulation predictions. Experiment uncertainty was assessed in terms of repeatability, but only mean experiment values were used for the boundary conditions in the model. The validation of the simulation predictions is considered a posteriori within the context of the experiment uncertainty. Parametric variability occurs when the input parameters are left unspecified leading to uncertainty in the results. For the present study, parameter uncertainty may be introduced with both the initial and boundary conditions imposed. Some examples of assumptions made, which
may lead to parameter uncertainty, include perfect geometric symmetry and displacement constraint positions. Observation errors should be accounted for as well, although the literature describing the experiments did not specify any specific quantifiable observation errors beyond the results presented. For example, it is noted the circumferential extensometer was problematic and unreliable during the experiments, but the researchers did not elaborate on how that observation specifically translated into the experiment uncertainty reported. Code uncertainty can be introduced when a mathematical model is solved numerically using a set of specific initial and boundary conditions. Well known sources of code uncertainty are truncation and round off error. Coding errors, which will introduce code uncertainty, are typically addressed through verification as exemplified by the verification case considered at the beginning of this study. For commercial models, the underlying code cannot be viewed or changed by the users. As such, users are forced to rely on their own verification efforts and must extend some level of trust that the software developers performed rigorous verification studies of their own.[20]

Improvements in the assessing the differences between the experiment data in simulation predictions can also be made. The average sum of squares is used in this research which provides an adequate comparison from simulation to simulation. However, normalizing the average sum of squares values to get a percent error from the experimental results may be more effective at validating the model in future.
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Appendix A. RTV-655 FEA Simulation Tutorial

Creating Tank model

1. Select “With Standard/Explicit Model”
2. To create tank model, select “Parts”
3. Select “3D” under “Modeling Space”, “Deformable” under “Type”, and “Solid” along with “Revolution” under “Base Feature”
4. Use sketch feature to model the half-cross section of tank, and select “Done” when finished
5. Type “360” in “Angle” text box to complete revolution of sketch
6. Select “Materials” under Model tree, and input given material properties (Be sure to keep units consistent)
7. Select “Section” and “Create” and then name section and select “Solid” and “Homogeneous”. Click “Continue” and select material created and click “OK”.
8. Click “Section Assignments” and select entire tank geometry and name the set in the text box under the model and click “Done”. Select section that was created previously and click “OK”. (Note: Part should turn a teal color)
9. Select “Sets” under Part tree and create sets for both inner and outer wall of tank.

Creating Tank Mesh

1. Select “Instance” under “Assembly” and select part and “Independent”. Then click “OK”.
2. Select “Mesh (Empty)” under Part tree under “Assembly”
3. Use the “Datum” tool found under the “Tools” tab to create datum planes to break up the cylindrical section of the tank from the hemispherical ends. (Seen in Figure 58)

4. Use the “Partition Cell: Use Datum plane” tool found on the left-hand side tool bar and follow the prompts. (After the geometry is successfully partitioned the tank will turn green).

5. Select “Seed part instance” found on the left-hand side tool bar and enter the desired seed size. Select “Apply” and “OK”.

6. Select “Mesh part instance” on the left-hand side tool bar. The newly formed mesh should appear.

7. Under the “Mesh” tool bar select “Element Type”. Highlight the entire tank or select the whole tank from the “Sets” button. In the “Family” selection panel, select “Coupled Temperature-Displacement” and then “OK”
Creating Cooldown Phase

1. Under “Steps” select the “Initial” dropdown. Select “BCs” and then “Displacement/Rotation” in the “Types for Selected Step” selection screen and click “Continue”. Select top point of tank and click “Done”. Select all boxes except for “U2” and click “OK”.

2. Select “BCs” again under “Initial”. Select “Symmetry/Antisymmetry/Encastre” and click on bottom point of tank. Then select “ENCASTRE” and “OK”.

3. Select “Predefined Fields” under “Initial”. Under the Category section select “Other” and then “Temperature”. Select the entire tank through the display or the “Sets” button. Input
the desired initial temperature of the tank in the “Magnitude” section and then select “OK”.

4. Select “Amplitudes” and then “Tabular”. Name amplitude “Outer Wall Temp” and click “Continue”. Input experimental temperature data for the outer wall of the tank and click “OK”. Repeat process for the inner wall of the tank.

5. Select “Step” and name new step “Cooldown”. Ensure that the procedure type is “Coupled temp-displacement” and click “Continue”.

6. In the “Time Period” input box, type “11000” and make sure that the “Response” is “Transient”. In the incrementation tab make sure that a reasonable “Max. allowable temperature change per increment” is inputted. In the “Other” tab in the “Default load variation with time” section, select “Ramp linearly over step” and then click “OK”.

7. Select “BCs” under the “Cooldown” step tree. Name BC “Outer Wall Temp” and select “Other” in the “Category” section. Then click “Temperature” and then “Continue”. Either by using “Sets” or the viewport, select the outer surface of the tank and click “Done” or “Continue”. In the “Magnitude” input box, enter “1” and in the Amplitude dropdown menu, select “Outer Wall Temp” and click “OK”. Repeat process for the inner wall boundary condition.
Creating Pressurization Phase

1. Select “Amplitudes” and “Tabular”. Name the amplitude “Pressurization” and click “Continue”. Input pressurization data and click “Continue”. Note: It is okay to leave the experimental data in psi if SI units are being used. The conversion can be done later in the process.

2. Select “Steps” and click “Cooldown” in the “Insert new step after” selection panel. Name the step “Pressurization” and ensure the procedure type is “Coupled temp-displacement” then click “Continue”.

3. In the “Time Period” input box, type “120” and make sure that the “Response” is “Transient”. In the incrementation tab make sure that a reasonable “Max. allowable
temperature change per increment” is inputted. In the “Other” tab in the “Default load variation with time” section, select “Ramp linearly over step” and then click “OK”.

4. Select “Loads” under the “Pressurization” step tree. Name load “Pressure” and select “Mechanical” in the “Category” section. Then click “Pressure” and then “Continue”. Either by using “Surfaces” or the viewport, select the inner surface of the tank and click “Done” or “Continue”. In the “Magnitude” input box, enter “6894.76” and in the Amplitude dropdown menu, select “Pressurization” and click “OK”. Note: The magnitude section converts the amplitude from psi to Pa. The load conditions can be seen in Figure 23.

Running Job and Output

1. Select “Field Output Request” and “Cooldown” in the dropdown menu and name if necessary and click “Continue”. In the section panel, ensure that “E, Total strain components”, “THE, Thermal strain component”, and “Temp, Element temperature” are all selected and then click “OK”. Repeat for Pressurization phase.

2. Select “Jobs” and name job “Test1” then click “Continue”. Click “OK” when “Edit Job” selection pane appears. Note: Using parallelization can decrease computational time, but for the purposes of this tutorial the feature will not be used.

3. Right click on the newly formed “Test1” and select “Data Check” then click “OK”. If the data check is successful, right click on “Test 1” and select “Submit” then “OK”.

4. Once the job has successfully run, right click on “Test 1” and select “Results”.

5. In order the transform the results into cylindrical coordinates, select “Create Coordinate System” in the left-hand side toolbar. Name the coordinate system “Cylindrical” and
select “Cylindrical” in the “Type” selection pane and click “Continue”. Follow prompts to create desired coordinate system.

6. Under “Results” tab, select “Options”. In the “Results Options” window, select the “Transformation” tab and click “User-specified”. Select “Cylindrical” in the selection menu, then click “Apply” and “OK”.

7. Under the “Tools” tab, hover over “XY Data” and click “Create”. Select “ODB field output” and press “Continue”. Select desired variables such as “E11” or “Temp” and select “Element/Nodes”. Select “Edit Selection” and select the desired element and then click “Save” and “Dismiss”.

Figure 60: Example of the Field Output Selection Box
8. Under the “Tools” tab, hover over “XY Data” and click “Create”. Select “Operate on XY data” and click “Continue”. Use the “combine(X,X)” operator in the right selection panel to combine temperature and strain data saved in the previous step. Click “Save As” to save the data and name appropriately. Note: Each element has 8 nodes, so to ensure the right node is used, it is recommended that the “Query” tool found under the “Tools” tab is used. This tool shows the value for each node in an element for a given variable.

9. To export the data to Excel, select the “Plug-ins” tab, and hover over “Tools”. Click “Excel Utilities” and select desired data and click “Apply”. An Excel spreadsheet with the data should appear.