

Thermodynamic Modeling of Solder Melting and Solidification for Proposed Squishbot Design

by

Robert Utz

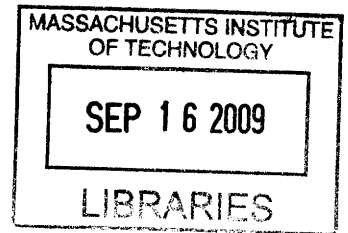
Submitted to the Department of Mechanical Engineering in Partial
Fulfillment of the Requirements for the
Degree of

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ABSTRACT

This thesis develops a thermodynamic simulation of the melting and solidification of a substance resting on a surface. The simulation was created in an effort to develop a single actuator joint locking and unlocking mechanism for Squishbot. The Squishbot is a proposed robot that has the ability to climb walls and change shape in order to gain entry into normally inaccessible areas. By using COMSOL Multiphysics, a simple model was developed and tested. Under these conditions, the solder melting phase transition took 2.25 seconds to melt and 2.65 seconds to solidify. These results, as well as observations about the behavior of the program's numerical solver, seem to suggest that the proposed joint locking system is feasible. A framework is laid out to proceed with improved and more specific models for use as an optimization tool.

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TABLE OF CONTENTS

1	INTRODUCTION	10
1.1	Purpose.....	10
1.2	Squishbot Requirements.....	11
1.3	Organization of the thesis.....	13
2	BACKGROUND	14
2.1	Proposed Squishbot design.....	14
2.2	Thermodynamics	15
2.2.1	Conduction.....	15
2.2.2	Convection.....	16
2.2.3	Heat Capacity	17
2.3	Alloys	18
2.4	Important factors.....	20
3	MODELING APPROACH	22
3.1	COMSOL Overview	22
3.2	Heat transfer module	23
3.3	Conduction mode.....	23
3.3.1	Equation and Variables	23
3.3.2	Geometry and subdomains	25
3.3.3	Boundary Conditions	26
3.4	Numerical Phase Change	27
3.4.1	Apparent Specific Heat	27
3.4.2	Linear Interpolation.....	28
3.4.3	Smooth Dirac delta function.....	29
3.4.4	Application to model.....	30
4	RESULTS.....	32
4.1	Melting	32
4.1.1	Initial conditions	32
4.1.2	Point monitoring	33
4.1.3	Melting time.....	33
4.1.4	Temperature behavior	35
4.2	Solidification	36
4.2.1	Initial conditions	36
4.2.2	Point monitoring	37
4.2.3	Solidification time.....	38
4.2.4	Temperature behavior	39
4.3	Squishbot implications.....	41
4.4	Solver Parameters	42
4.4.1	Time step	43

4.4.2 Bypassing.....	44
4.4.3 Oscillation.....	46
4.4.4 Suggestions for improved performance	49
5 CONCLUSION	50
BIBLIOGRAPHY.....	52

LIST OF FIGURES

Figure 1: Example Results: Temperature distribution along cross-section	10
Figure 2: Squishbot leg with joint show at rest and in bending.....	11
Figure 3: Squishbot Concept: Climbing and Morphing	12
Figure 4: Binary phase diagram of tin and lead.....	19
Figure 5: Copper and solder geometric configuration	25
Figure 6: Linear interpolation method in heat capacity of solder phase change.....	28
Figure 7: Smooth Dirac delta function in heat capacity of solder phase change	29
Figure 8: Heat capacity of a point within the solder during melting	33
Figure 9: Solder enters melting temperature range at $t = 3.75$ seconds.....	34
Figure 10: Progression of liquidus line.....	35
Figure 11: Temperature at a point inside the solder during melting.....	36
Figure 12: Heat capacity of a point within the solder during solidification.....	37
Figure 13: Solder enters melting temperature range and begins solidification.....	38
Figure 14: Progression of solidus line	39
Figure 15: Temperature at a point inside the solder during solidification	40
Figure 16: Example screenshot of solder parameters.....	43
Figure 17: Temperature progression resulting from bypassing problem	45
Figure 18: Heat capacity resulting from bypassing problem.....	46
Figure 19: Temperature resulting from oscillation problem	47
Figure 20: Heat capacity resulting from oscillation problem	48

LIST OF TABLES

Table 1: Melting points of tin-lead solder compositions.....	20
Table 2: Variables used by Conduction Mode in COMSOL Multiphysics	24
Table 3: Constants and expressions used to modify heat capacity	30

1 INTRODUCTION

1.1 Purpose

The purpose of this thesis is to determine the feasibility of using fluid melting and solidification for a proposed joint activation and deactivation system in a soft, small-scale robot currently in development known as Squishbot (Soft QUIet Shape-shifting robot). A method of modeling the thermodynamic behavior of the joint was developed using COMSOL Multiphysics. Temperature data has been generated using solder as the locking agent for a copper joint in a simplified geometry. The results have been analyzed to determine melting and solidification duration, factors paramount to the performance of the joint, dependent upon power input and convective heat transfer coefficient. Using the approach of the established model, more complex geometries and alternative materials can be analyzed so that the optimal joint design can be determined.

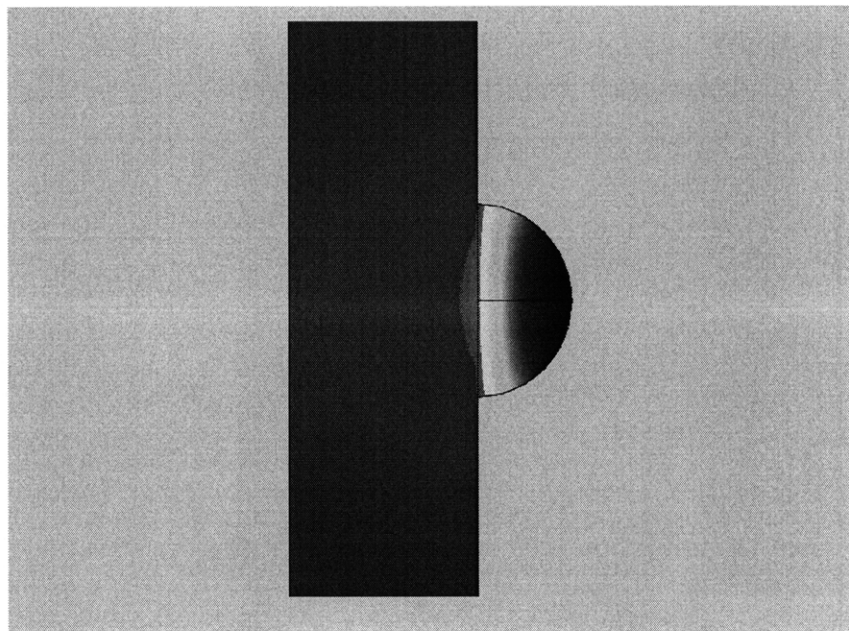


Figure 1: Example Results: Temperature distribution along cross-section

1.2 Squishbot Requirements

The Squishbot must have these characteristics: the ability to climb walls and ceilings, the ability to travel over rough terrain, and the ability to change shape to fit through holes and small spaces. By using locomotion concepts derived from snails and employing a skeleton that can alternate between rigid and flexible states, these desired characteristics could be developed in a Squishbot design. In an effort to simplify the control scheme, a design has been proposed that locks and unlocks all of the joints in the system through a single actuator. One such joint is shown in Figure 2. A portrayal of the overall concept is shown in Figure 3.

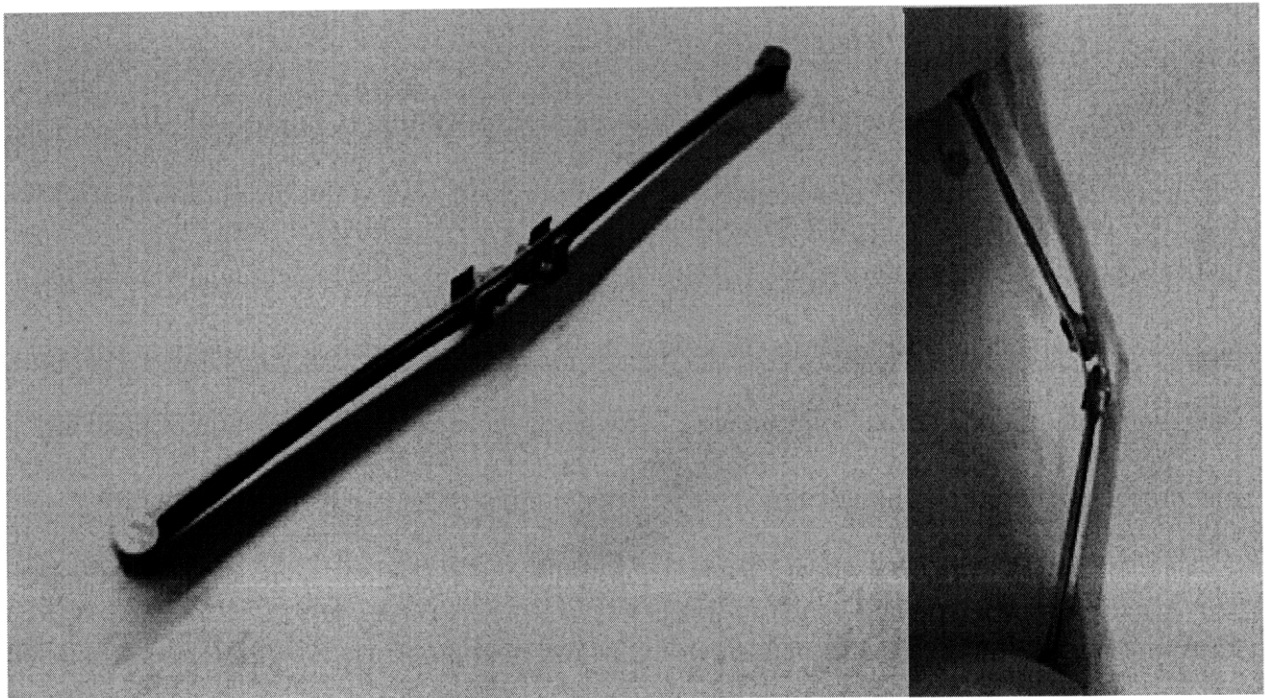


Figure 2: Squishbot leg with joint shown at rest and in bending (Courtesy of [2])

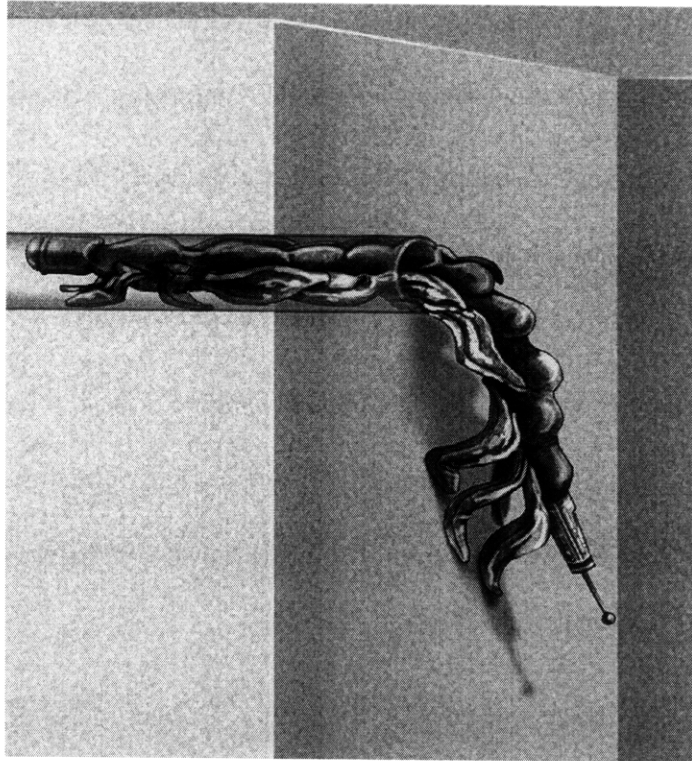


Figure 3: Squishbot Concept: Climbing and Morphing (Courtesy of [1])

The actuator consists of a heat source that, when activated, warms the series of joints and melts a substance that previously had locked the joints. The proposed system must be able to both lock and unlock in a short period of time without exerting an excessive amount of energy. The results suggest that such a solution is possible given an adequate combination of material selection and geometry, although more specific modeling must be completed along with experimental verification to prove this conclusion. Along with the immediate application to the Squishbot problem, methods and analysis from this thesis could be used in other areas or applied to other functions. The thermodynamic modeling of phase change can have other applications in any melting or freezing scenario. Also, the numerical treatment of latent heat and heat capacity during phase change could be used in a similar fashion upon other instantaneous changes in physical properties.

1.3 Organization of the thesis

The thesis will cover the following:

- Squishbot properties and goals pertinent to analysis
- Conduction and convection
- Thermodynamics of melting and solidification
- Phase change in solid solutions
- COMSOL Multiphysics modeling in thermodynamics
- Numerical phase change: Linear interpolation and smooth Dirac delta function
- Melting results
- Solidification results
- Optimizing solver performance

2 BACKGROUND

In order to solve the problem, the concepts behind the Squishbot problem and proposed design must first be understood. The Squishbot has three necessary capabilities with the goal of gaining access to previously inaccessible areas. First, it must be able to climb walls and ceilings. Second, it must be able to travel over rough terrain. Third, it must be able to squeeze into and through small holes and tight spaces. A successful Squishbot design must take into account all factors by incorporating unique engineering features into the same robot.

2.1 Proposed Squishbot design

By mimicking the motion of snails, the Squishbot can satisfy the first two requirements. Known as adhesive locomotion, the foot of the Squishbot would move as a displacement wave along the length of the robot [1]. This occurs when segments of the foot slide forward one-by-one while the rest of the foot stays stationary [1]. In a snail, this motion requires excretion of a thin film of non-Newtonian fluid for proper function [1]. The snail pushes against the fluid with its foot, creating stresses in the fluid that propel it forward [1]. An equivalent non-Newtonian fluid is needed to recreate similar conditions in the Squishbot that will allow for adhesive locomotion.

The Squishbot must alternate between rigid and flexible structures for efficient movement, changing direction, and fitting through small spaces. Composing the structure through a series of rigid elements connected through joints allows for both rigidity and flexibility when the series of joints are locked and unlocked. Furthermore, the controls can be simplified by connecting the entire series of joints to one actuator [2]. By alternately locking and unlocking the joints, the Squishbot can achieve basic locomotion as well as movement in a variety of

directions [2]. The proposed method of joint locking and unlocking is through the use of thermally controlled fluids [2]. Alternately heating and cooling the fluid cycles the joint through locking and unlocking as the fluid goes through the solid-liquid phase change. The thermally controlled fluid method would be considered successful if the transition between locking and unlocking can occur relatively quickly without requiring excessive power.

2.2 Thermodynamics

The thermodynamics of the joint are essential to the understanding of the system behavior during melting and solidification. Throughout both the heating and cooling cycle of the system, the problem is governed thermodynamically by conduction through the copper strip and solder bead and by convection off of the solder-air interface. During phase change from both solid to liquid and liquid to solid, the latent heat of fusion must be captured or released before the material can proceed as normal thermodynamically. How the material behaves during phase change depends upon its material composition. Since the majority of solders used are alloys, the behavior of alloys during phase change, namely eutectic point and melting temperature ranges, describes the behavior of the system during melting and solidification.

2.2.1 Conduction

Three modes of heat transfer exist: conduction, convection, and radiation. Conduction and convection are the dominant modes of heat transfer in the system and thus only those two modes will be discussed here. Conduction is defined as the transfer of energy between particles of the same substance from particle interaction [3]. The temperature of a substance is a measurement of the energy of the particles around the point of measurement, and thus is closely linked to the translational, rotational, and vibrational movement of those particles [3]. When

molecules with high temperature and likewise high energy move, they collide with molecules with lower energy. Energy is transferred from the higher temperature molecules to the lower temperature molecules, consequently raising their temperature. This intuitively works in gases and liquids. In solids, the process carries on in much the same way, with lattice vibrations and electron movement performing the energy transfer [3].

Mathematically, the heat transfer through the substance can be modeled in one dimension by Fourier's law [3].

$$q_x = -k \frac{dT}{dx} \quad (1)$$

In this equation, q_x is the conductive heat flux per unit area, k is the thermal conductivity, and dT/dx is the temperature gradient in the x -direction. Fourier's law can be extended to three dimensions by making the heat flux a vector as follows [3].

$$q = -k \nabla T \quad (2)$$

2.2.2 Convection

Convection employs two different mechanisms into one heat transfer mode describing the thermodynamic behavior of a fluid. Like conduction, energy is transferred due to molecular motion interactions. Additionally, energy is also transmitted through the bulk motion of the fluid. The superposition of the two mechanisms combines to govern the entire heat transfer mode [3]. More specifically, convection describes the interaction between a moving fluid and an adjacent surface. At the interface between the fluid and the surface, the fluid is stationary and shares the same temperature as the surface. At some finite distance away from the surface, the fluid reaches a uniform maximum velocity and an ambient temperature. The area of the fluid progressing from stationary to uniform velocity is known as the velocity boundary layer.

Likewise, as long as the ambient temperature does not equal the surface temperature, the area of the fluid progressing from surface temperature to ambient temperature is known as the thermal boundary layer. The velocity and thermal boundary layers are often not necessarily identical. Nevertheless, the boundary layers govern convective heat transfer with molecular motion dominant near the surface and fluid motion dominant further from the surface [3].

Convection is classified in two different ways depending upon the nature of the flow. Forced convection occurs when external forces generate the flow. Natural convection occurs when buoyancy forces generate the flow. The fluid near the surface decreases in density when heated, causing the warmer fluid to rise and cooler fluid to replace it. The system in question is dominated by natural convection, although forced convection could apply in some instances. Regardless of the type, convection can be modeled using the same equation [3].

$$q = h(T_s - T_\infty) \quad (3)$$

In Equation 3, q is the convective heat flux, T_s and T_∞ are the surface and ambient temperatures, and h is the convective heat transfer coefficient. Both convection and conduction control the heat fluxes that take place during the melting period and the solidification period, as well as in a single phase.

2.2.3 Heat Capacity

Heating or cooling a substance affects the internal energy of the material. The internal energy of the system changes with the following equation [3].

$$\frac{dE_{st}}{dt} = -\rho c_p \frac{\partial T}{\partial t} \quad (4)$$

Equation 4 describes the time rate of change of the thermal energy of the system through the density ρ and specific heat capacity c_p of the material. The heat capacity is a property of the

material that determines how much heat is necessary to raise the temperature of a certain quantity of the material by a specified amount [3]. This equation is valid when the change in internal energy of the system includes only sensible energy, or the thermal energy in states outside of phase changes. During phase change, an additional amount of energy must be released or captured in order to weaken or strengthen the intermolecular forces required for the new phase. Known as the latent heat, this finite amount of energy must be added to the material before any temperature change [3]. For instance, when a solid melts, intermolecular forces must be weakened through the addition of latent heat before the temperature can continue to increase. No matter in which direction the phase transition is occurring, the latent energy change between two specific phases is a finite quantity dependent upon the material. The behavior of the system can be completely described by combining convection and conduction with internal energy behavior determined by heat capacity and the latent heat of solidification.

2.3 Alloys

The melting and solidification of substances and compounds are easily defined in this manner. Solid solutions composed of two or more chemically separate but physically mixed materials behave differently in comparison. Since solder is an alloy composed of tin and lead, only binary alloys will be reviewed here. For binary alloys, phase and phase transition behavior is best understood through phase diagrams showing phase regions on a graph of temperature versus concentration of one of the elements. The binary phase diagram of tin and lead is shown below in Figure 4. Figure 4 shows the phase composition of all tin-lead solders at relevant temperatures.

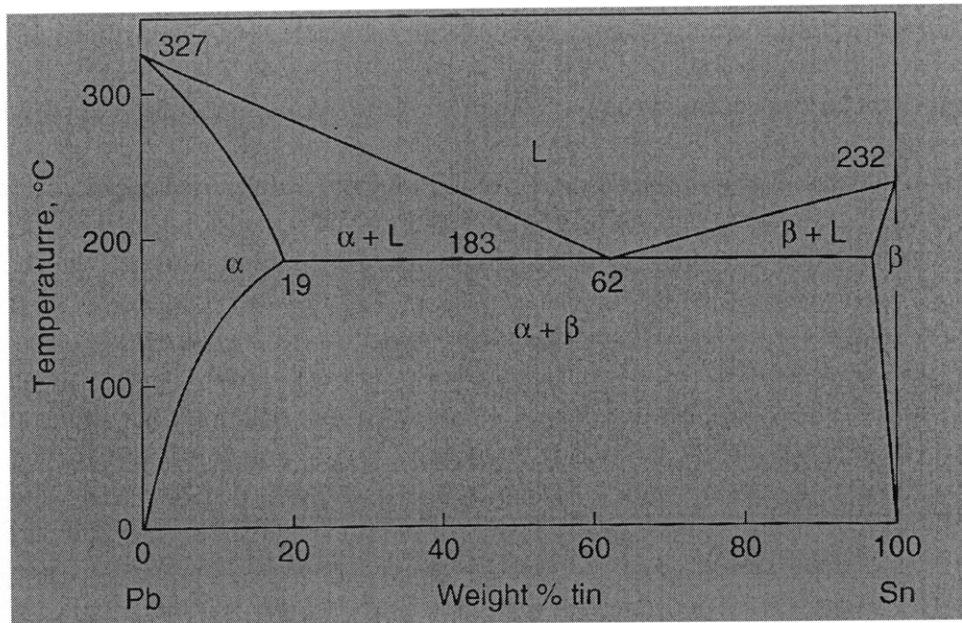


Figure 4: Binary phase diagram of tin and lead. Eutectic transition occurs at 62% tin by weight. All other compositions have melting and solidification processes over a finite temperature range (Courtesy of [4])

In the figure, α represents regions where solid lead is present, β represents regions where solid tin is present, and L represents regions where some of either tin or lead exist in liquid form. A point on the diagram that exists in a two-phase region contains both phases simultaneously. Tin-lead solders are specified by percent composition by weight of each element. A vertical line in Figure 4 represents how tin-lead solder of a specific composition behaves as it is heated or cooled. For some binary alloys, a composition exists where a smooth and instantaneous transition occurs between solid and liquid, much like that of a basic element. This point is known as the eutectic point [4]. At all other compositions, the transition between liquid and solid is not instantaneous but rather occurs over a temperature range. Melting and freezing occur between the solidus, the line that borders the phase transition and 100% solid regions, and the liquidus, the line that borders the phase transition and 100% liquid regions [4]. The solution is

not completely liquid until the temperature at the liquidus is reached. Likewise, the solution is not completely solid until the temperature at the solidus is reached. The existence of this transition range has an impact upon the performance of the system depending upon which solder concentration is chosen. Table 1 shows the melting ranges of both tin-lead solders as well as solders composed of combinations of other elements listed by composition.

Table 1: Melting points of tin-lead solder compositions, organized by percent weight (Courtesy from [5])

Lead (% weight)	Tin (% weight)	Melting Range (°C)
37	63	183
40	60	183-190
45	55	183-203
50	50	183-214
55	45	183-225
60	40	183-238
65	35	183-247
70	30	183-258
75	25	183-268
80	20	268-302
90	10	268-302
95	5	301-314

2.4 Important factors

With both the background of the project and the governing thermodynamics in mind, a few concepts pertinent to the problem are clear. Above all else, the phase transition time, both melting and solidification, must be minimized. Choosing a solder at its eutectic point would be preferred over any other composition given the same elements since the solid-liquid phase

transition is virtually instantaneous with temperature and thus with time as well. If a solder at eutectic composition cannot be used, then a composition that minimizes the temperature range between the solidus and liquidus is preferred. Using a non-eutectic composition in the proposed locking joint could have undesirable effects. When the solder is solidified and entering the phase transition region, the joint will likely unlock very rapidly since a solder composition that is both liquid and solid will likely not keep the joint locked under stress. When the solder is in the liquid state and entering the phase transition region, the joint will not lock completely until the solder has completely solidified. All things being equal, the solidification process could take longer than the melting process in terms of the behavior of the overall system. Secondary considerations include minimizing the heat source required in order to minimize energy usage.

3 MODELING APPROACH

The heat transfer of the system was analyzed through COSMOL Multiphysics 3.5.

COMSOL uses a built-in heat transfer module to model heat transfer situations. In the heat transfer module, the conduction mode is sufficient to model all aspects of the system.

Conduction mode employs the heat equation with a set of variables, constants, and boundary conditions. Once a specific set of initial conditions are introduced, COMSOL can determine the temperature at small, finite elements of the system. Modeling the effects of latent heat during the phase change of the solder poses a unique challenge that can be solved though modifying the heat capacity of the solder over a small but finite temperature range around the melting temperature. By producing heat capacity as a function of temperature in COMSOL, the effect of phase change upon the thermodynamics of the system is included in the model.

3.1 COMSOL Overview

COMSOL Multiphysics uses sets of partial differential equations to solve a wide range of engineering problems. COMSOL employs a set of built-in modes to perform numerical analysis in several areas of physics, including fluid mechanics, acoustics, diffusion, structural mechanics, electromagnetics, and heat transfer. Multiple physics modes can be combined with each other or with user created differential equations to analyze complex problems that undergo changes in multiple ways. For modeling the joint locking mechanism of the Squishbot, the fluid behavior of solder during liquid phase was not considered. The solder bead retains a similar shape in the transition from solid to liquid then back to solid. The heat transfer mode sufficiently models the system under these conditions.

3.2 Heat transfer module

The version of COMSOL Multiphysics used contains two heat transfer modes: conduction mode and conduction and convection mode. Conduction and convection mode is primarily used to model thermodynamics in moving fluids. The mode uses input regarding the velocity field of the fluid to control the convection heat transfer term of the governing equation. Since the solder is considered completely stationary throughout both melting and solidification, the conduction and convection mode cannot be used to correctly analyze the behavior of the locking joint. Although the conduction mode is designed to primarily analyze heat transfer through solids, defining boundary conditions allows for convective heat transfer to be included at surfaces in contact with the surrounding air. Since the thermodynamics of the system are dominated by conduction through the copper and solder as well as convection between the solder surface and the air, the conduction application mode sufficiently defines temperatures throughout the system.

3.3 Conduction mode

3.3.1 Equation and Variables

COMSOL uses a set of equations, variables, geometry divided into subdomains, constants, and boundary conditions. The conduction mode uses the version of the heat equation shown below [6].

$$\delta_{ts}\rho C_p \frac{\partial T}{\partial t} - \nabla \cdot (k \nabla T) = Q + \frac{h_{trans}}{dA} (T_{ext} - T) + \frac{C_{trans}}{dA} (T_{ambtrans}^4 - T^4) \quad (5)$$

In Equation 5, δ_{ts} is a time-scaling coefficient, ρ is the density, C_p is the heat capacity, k is the thermal conductivity, Q is the heat flux, h_{trans} is the convective heat transfer coefficient, and T_{ext}

is the external temperature. The variable T , defining the temperature of a particular element, is dictated by this partial differential equation. The final term of the equation pertains to radiation and is not considered in the analysis. In steady state, the first term of the equation is removed. Since times to melt and solidify are important results of the analysis, the first term cannot be ignored.

Table 2 lists the variables used by the conduction mode in solving the partial differential equation.

Table 2: Variables used by Conduction Mode in COMSOL Multiphysics (Courtesy of [6])

NAME	DOMAIN/TYPE	DESCRIPTION	EXPRESSION
T	S/B	Temperature	T
gradT, Txi	S/V	Temperature gradient	$ \nabla T , \frac{\partial T}{\partial x_i}$
flux	S	Heat flux	$ \underline{k}\nabla T $
nflux_T	B	Normal heat flux	$\mathbf{n} \cdot (-\underline{k}\nabla T)$
fluxxi	V	Heat flux, x_i component	$\sum_j -k_{ij} \frac{\partial T}{\partial x_j}$
Dts	S	Time-scaling coefficient	δ_{ts}
rho	S	Density	ρ
c	S	Heat capacity	C_p
k, kxi xj	S	Thermal conductivity	k, k_{ij}
Q	S	Heat source	Q
htrans	S	Transversal convective heat transfer coefficient	h_{trans}
Text	S	Transversal external temperature	T_{ext}
Ctrans	S	User-defined constant	C_{trans}
Tambtrans	S	Transversal ambient temperature	$T_{ambtrans}$
T0	B	Prescribed temperature	T_0
h	B	Convective heat transfer coefficient	h
Tinf	B	Ambient bulk temperature	T_{inf}
Const	B	Radiation constant: product of emissivity and Stefan-Boltzmann constant	Const
Tamb	B	Temperature of the surrounding radiating environment	T_{amb}

The column “Domain/Type” refers to where the variable applies in the geometry. S represents a subdomain, B represents boundary conditions, and V represents a universal variable. Temperature is dependent upon the results of the simulation. The rest of the variables can be defined as constants or functions dependent upon other variables during the simulation. Any variable defined above can be observed in the post-processing mode at defined points, boundaries, or surfaces for analysis.

3.3.2 *Geometry and subdomains*

For the present analysis, a simplified geometry was created with the joint design in mind. A square slab 10 mm on each side was extruded to a thickness of 1 mm. On top of and at the center of the slab, a hemisphere 1 mm in diameter was generated with the flat side in contact with the top surface of the square slab. The slab represents the joint structure and the hemisphere represents the solder joint locking fluid. Figure 5 displays the produced geometry from an isometric and cross-sectional angle.

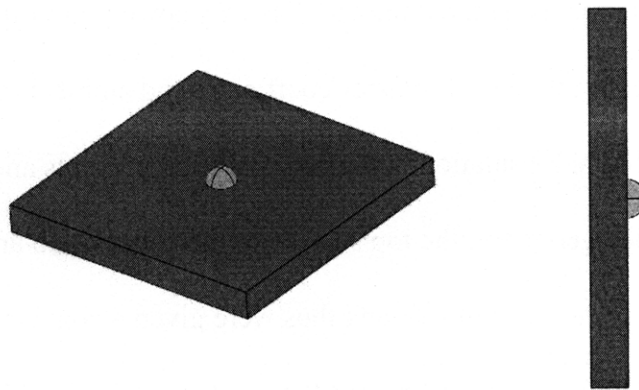


Figure 5: Copper and solder geometric configuration

Each individual geometric section in COMSOL is considered a subdomain. Subdomains have their own material properties used to dictate their behavior by specific variables according to the governing equation of the model. Through the built-in material library available in COMSOL, the square slab subdomain was given the material properties of copper and the hemisphere subdomain was given the material properties of 60Sn-40Pb solder. If desired, the user can enter individual properties to model subtle changes and differences in materials or define a material that does not exist in the COMSOL library. Although material properties are often constant or considered constant for ease of calculation, COMSOL allows for properties to change with time, temperature, or other variables if desired.

3.3.3 Boundary Conditions

Furthermore, conditions at subdomain boundaries must be defined. The behavior at each individual boundary can be defined as a heat flux, thermal insulation, set temperature, zero temperature, or thermally resistive layer [6]. For analyzing the system, only heat flux and thermal insulation were used. The heat flux at the boundary can be defined as a conductive, convective, or radiative flux as well as any combination of the three according to Equation 5. A conductive heat flux can simply be entered numerically as a power per unit area in W/m^2 . To set a convective heat flux, a convective heat transfer coefficient and ambient temperature must be specified. Conversely a thermal insulation boundary condition prevents any heat flux across that boundary. On the generated geometry, the top surface of the copper slab and the top surface of the solder hemisphere are in contact with air and thus were given a convective flux with a heat transfer coefficient of $10 \text{ W/m}^2\text{-K}$ and an ambient temperature of 25°C . All of the sides of the copper slab are thermally insulated. In the melting analysis, a conductive heat flux of 2.5 W/in^2 (3875 W/m^2) was assigned to the bottom face of the copper slab whereas the solidification

analysis treats the bottom face as open to air under the same conditions outlined previously. Setting these boundary conditions effectively defines the heat fluxes into and out of the system.

3.4 Numerical Phase Change

3.4.1 *Apparent Specific Heat*

Using COMSOL with the above settings and characteristics effectively models the behavior of the system outside of phase change. Adjustments must be made before the model can be applied to phase transitions. The governing equations of the conduction mode have no provisions for latent heat. Moreover, the latent heat required to melt or solidify a substance has no direct relationship to the specific heat capacity, making it difficult to include into the heat capacity term of the equation. The latent heats of solidification for several materials have been determined experimentally and are known quantities. Since integrating heat capacity with respect to temperature results in the enthalpy change, modifying the heat capacity can account for the additional latent heat necessary to undergo phase change. In this way, phase change can be modeled through the conduction mode in COMSOL with the existing equation. For the case of pure materials or binary solid solutions at eutectic composition, the melting process takes place instantaneously with respect to temperature. A plot of heat capacity versus temperature would resemble a delta function with an instantaneous increase at the melting temperature. Attempting to model phase change in this manner proves to be virtually impossible because numerical solvers compute solutions in finite intervals. The solver will likely bypass the melting temperature without taking the latent heat into account. Assuming that the transition actually takes place over a narrow but finite temperature range, the heat capacity can increase up to a maximum and then decrease again to the post transition value at finite temperatures [7]. If the

time steps of the solver allow for a slow rate of change in temperature during phase change, the solver will recognize the increased heat capacity and incorporate the results into the output temperatures.

3.4.2 Linear Interpolation

There are multiple methods of depicting a delta over a finite domain. Two methods were explored: the linear interpolation method and the smooth Dirac delta function method. The linear interpolation method models the heat capacity of the material during phase change as a linear increase to a maximum followed by a linear decrease at an identical but negative slope back to the original value. Choosing the maximum heat capacity requires first determining the temperature range of the phase transition. Once the range is set, matching the integral of heat capacity over the finite melting temperature range to the known latent heat value determines the maximum heat capacity value. This method has previously been applied in COMSOL to pure materials with point melting temperatures adapted from analysis of the heat capacities of biological materials [8]. Figure 6 shows how this method would be applied in the Squishbot joint analysis to the melting and solidification of solder.

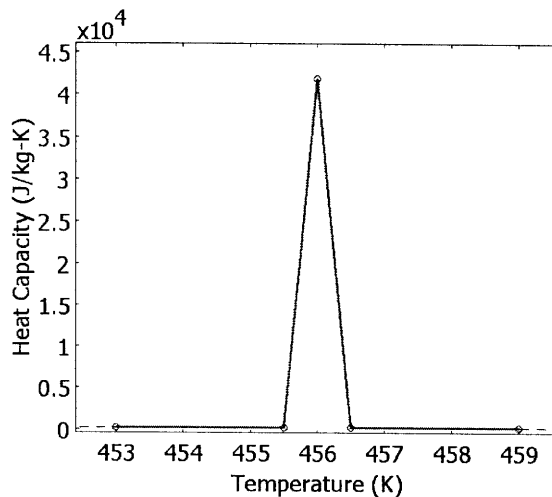


Figure 6: Linear interpolation method in heat capacity of solder phase change

3.4.3 Smooth Dirac delta function

The smooth Dirac delta function method provides an alternative approach to portraying the operation of heat capacity during phase change. The Dirac delta function is the derivative of the Heaviside step function. Since the change in enthalpy versus temperature during phase change resembles a step function and heat capacity is the derivative of enthalpy, the Dirac delta function serves as a valid model for heat capacity. A smoothed Dirac delta acts as a distribution over a finite range whose integral over that range is equal to one [9]. COMSOL has built-in delta functions for use in modeling. One such function $fldc2hs(x, scale)$ has been used previously in the thermodynamic modeling of the solidification of liquid metals [10]. The entry $T - T_m$ takes the place of the x term where T_m is the single point melting temperature of the material. A proposed finite melting temperature range takes the place of the $scale$ term. This function is then multiplied by the latent heat to generate a latent heat capacity term that is added to the steady-state heat capacity to create a total heat capacity during phase change. Figure 7 shows how heat capacity is modeled in the smooth Dirac delta function case.

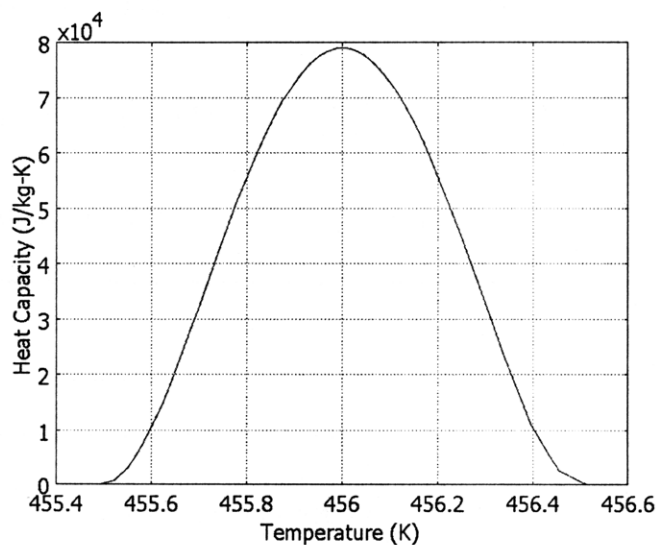


Figure 7: Smooth Dirac delta function in heat capacity of solder phase change

3.4.4 Application to model

The smooth Dirac delta function method was chosen to model the heat capacity of the solder during phase change. COMSOL has the ability to define a set of constants and expressions available for implementation wherever the user deems that it is necessary. COMSOL can compensate for the latent heat of phase change by generating an expression for heat capacity dependent upon temperature and substituting that expression for the given heat capacity. The set of constants and expressions outlined below in Table 3 were entered into the model.

Table 3: Constants and expressions used to modify heat capacity

Name	Value	Meaning
cpS	150 [J/(kg*K)]	normal heat capacity
e	1 [K]	transition temperature range
Tm	456 [K]	melting temperature
L	4.20e4 [J/kg]	latent heat of melting
cpL	$L \cdot \delta(T - T_m, e)$	latent heat capacity added
Cpt	cpL+cpS	total heat capacity

The constants in Table 3 were chosen with a eutectic or near-eutectic solder in mind. The melting temperature matches that of eutectic solder and the transition temperature is rather narrow. For clarification, expressions cpL and Cpt were entered as subdomain expressions that

only apply to the solder subdomain. The heat capacity of copper remains unchanged from the value obtained from the material library.

4 RESULTS

Successful results from both melting and solidification scenarios were obtained. Careful manipulation of the solver parameters was necessary in order to establish valid results. Results show that phase change can readily occur over a short amount of time using the given materials. Furthermore, the model can be used for a wide range of materials, geometries, initial conditions, and boundary conditions, although optimization of solver parameters will likely be necessary for each arrangement.

4.1 Melting

4.1.1 *Initial conditions*

For the melting scenario, the initial temperatures of both the copper and solder subdomains were set at 180°C, three degrees below the established melting temperature. The finite element mesh of the geometry was generated at default conditions. The settings of the solver were adjusted to accommodate the specific problem and facilitate analysis of important factors. The solver was changed from stationary to transient mode. Analysis of steady-state conditions is of no benefit or interest to the Squishbot design. The Squishbot will likely never reach the steady-state solution in practice. Furthermore, the steady-state analysis does not provide any information regarding the rate of phase change or how the temperature, heat capacity, and other factors were affected during phase change. Transient mode monitors and evaluates conditions at each time step, allowing for analysis through time of temperature, heat capacity, and the phase change itself. Data was taken at intervals of every 0.05 seconds for 20 seconds. The maximum time step allowed was 0.2 seconds. All other solver settings remained default.

4.1.2 Point monitoring

The results of the simulation are shown below in Figures 8-11. Figure 8 depicts the heat capacity throughout the simulation of a point in the solder hemisphere 0.25 mm above the solder-copper interface. The heat capacity remains at a small, baseline level before and after melting. Like the smooth Dirac delta function, the heat capacity sharply rises and falls in a short timeframe within $\pm 0.5^\circ$ of the melting temperature.

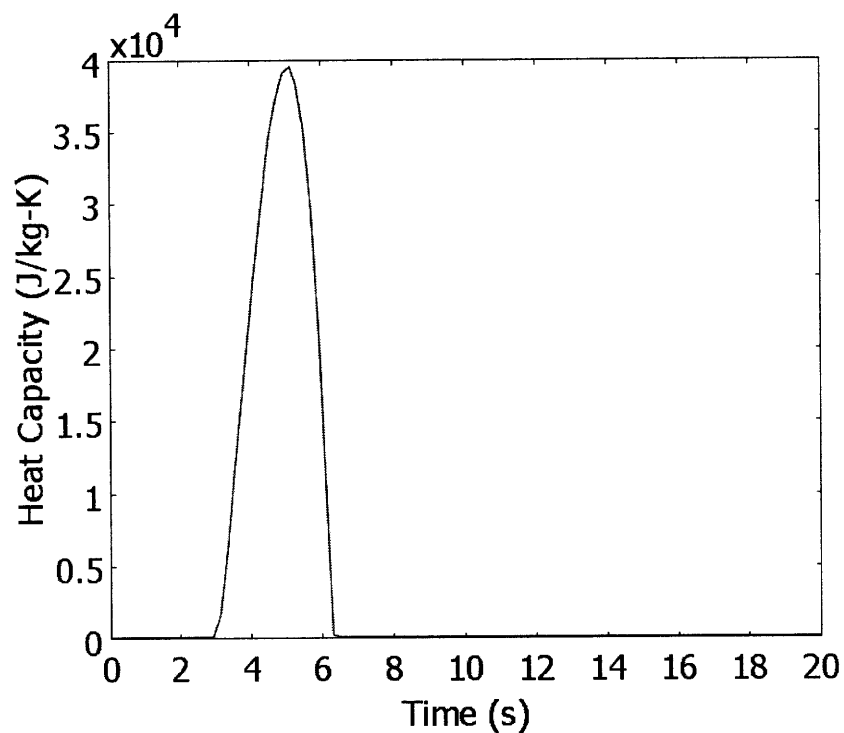


Figure 8: Heat capacity of a point within the solder during melting

4.1.3 Melting time

The time it takes for a point to make the complete phase transition is a rough indication of how long it takes for the solder to melt completely. This point within the solder took roughly 3.25 seconds to melt completely. This is a slight overestimate of the actual time to melt since the smooth Dirac delta function has a finite values slightly outside of the designated range as seen in

Figure 7. By visualizing thin temperature bands along the cross-section of the solder, it is possible to pinpoint the beginning and end times of melting for the entire solder subdomain.

Figure 9 was constructed by assigning a color to all temperatures $1/100^{\text{th}}$ of a degree above and below the lower bound of the melting range. Figure 9 demonstrates that the solder has begun to melt 3.75 seconds into the simulation. Note that any part of the copper subdomain marked is still in the solid phase since copper is a solid at this temperature.

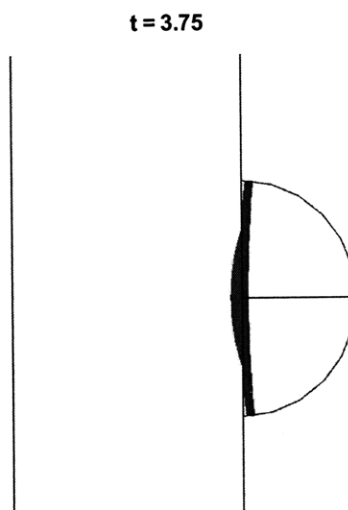


Figure 9: Solder enters melting temperature range at $t = 3.75$ seconds

A similar procedure involving the upper bound of the melting range demonstrates the end of the melting process. Figure 10 shows the progression of the liquidus line through the solder subdomain. Any points to the left of the marked line indicate an area composed of 100% liquid. By time $t = 6$ seconds, the liquidus line has left the solder and the entire solder subdomain exists at temperatures above the melting temperature range. According to this simulation, the solder melts in 2.25 seconds under the established conditions.

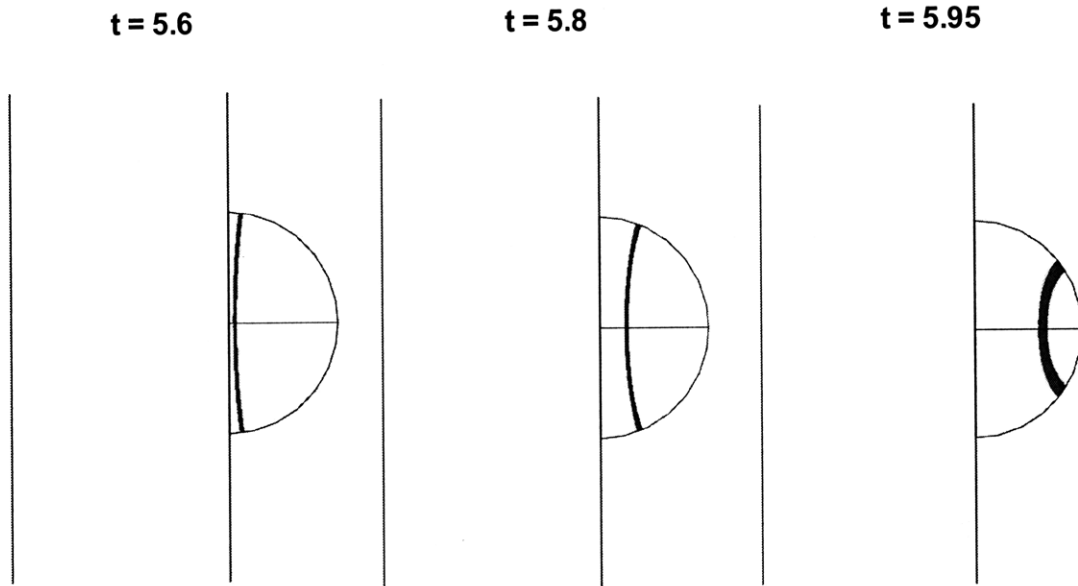


Figure 10: Progression of liquidus line, which signifies the boundary between material within the transition range and 100% liquid

4.1.4 Temperature behavior

To verify the results, the temperature inside the solder must behave appropriately throughout the simulation. Figure 11 shows the temperature of the same point analyzed in Figure 9. The rate of temperature change slows down as expected when the point enters the melting phase. Once the point leaves the melting temperature range, the rate of temperature range briefly exceeds the normal rate and then settles back down to the original rate. There are two possible explanations for this behavior. First, a point stuck inside the phase transition remains at a slightly lower temperature than the liquid material adjacent to it. Once that point escapes the melting range, the material sees a higher conductive heat flux than it normally would

and experiences a sharper temperature rise. This is a real-life phenomenon experienced in materials with high latent heats relative to the heat fluxes present. The more likely reason points to the behavior of the numerical modeling itself, which will be explained later in this section.

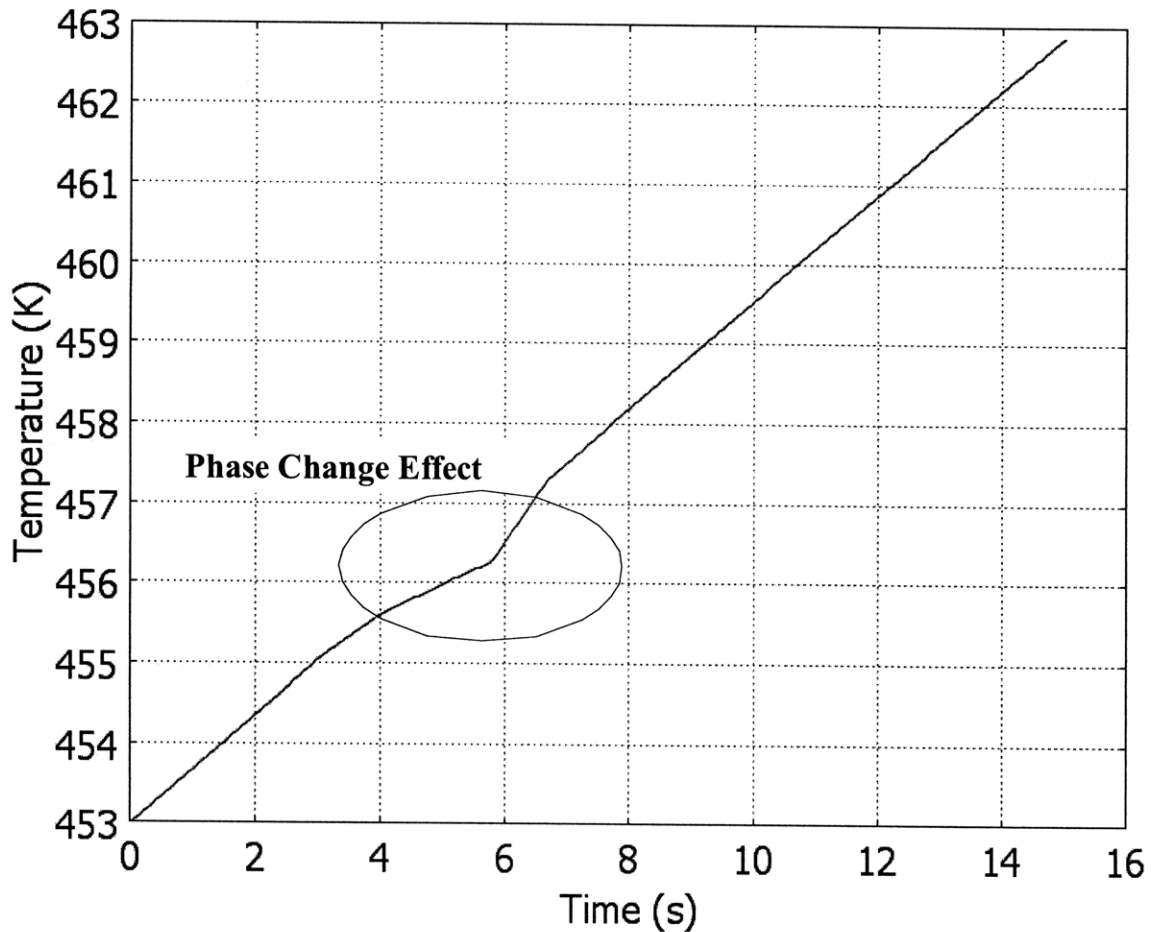


Figure 11: Temperature at a point inside the solder during melting

4.2 Solidification

4.2.1 Initial conditions

The solidification analysis followed very similar criteria as the melting analysis. This time, the initial temperatures of the copper and solder subdomains were set to 186°C. The heat flux boundary condition on the bottom of the copper slab was replaced by a thermal insulation

boundary condition. Data was taken at intervals of every 0.05 seconds for 25 seconds. The maximum time step allowed was 1 second. Transient and mesh settings remained the same and all other settings remained as their default configurations.

4.2.2 Point monitoring

The results of the solidification simulation are shown in Figures 12-15. Figure 12 depicts the heat capacity throughout the simulation of a point in the solder hemisphere 0.25 mm above the solder-copper interface. The heat capacity behaves in a similar fashion to the melting simulation, remaining at a small, baseline level before and after melting and sharply rising and falling in a short timeframe during the phase transition.

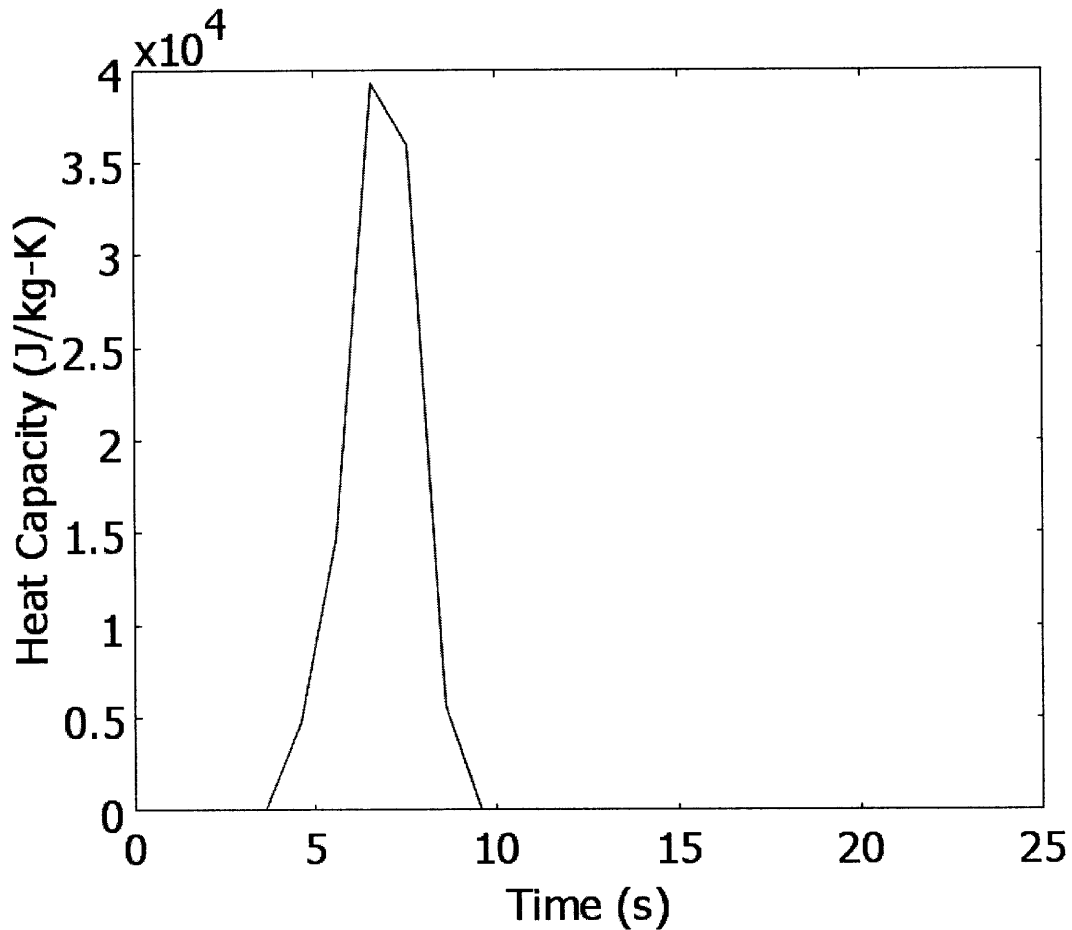


Figure 12: Heat capacity of a point within the solder during solidification

4.2.3 Solidification time

For comparison, the operation of the heat capacity during solidification will be compared to the melting results. This point within the solder took roughly 5.5 seconds to melt completely. Visualization of thin temperature bands along the cross-section of the solder as in the previous case enables the establishment of the beginning and end times of solidification for the entire solder subdomain. Figure 13 was constructed by assigning a color to all temperatures $1/100^{\text{th}}$ of a degree above and below the upper bound of the melting range. Figure 13 demonstrates that the solder has begun to solidify 5.5 seconds into the simulation.

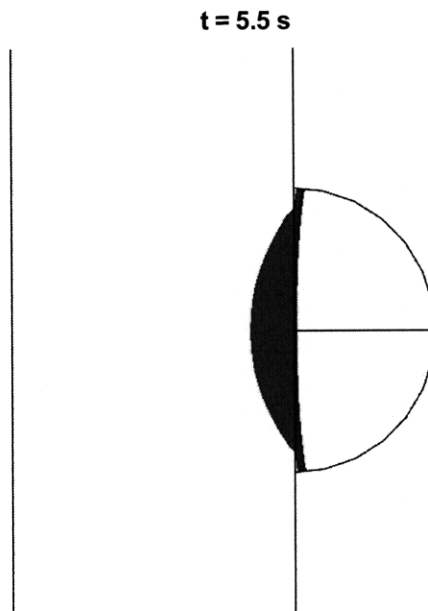


Figure 13: Solder enters melting temperature range and begins solidification at 5.5 seconds

Using the same process on the lower bound of the melting range demonstrates the end of the solidification process. Figure 14 shows the progression of the solidus line through the solder subdomain. Any points to the left of the red line indicate an area composed of 100% solid. By

time $t = 8.2$ seconds, the solidus line has left the solder and the entire solder subdomain exists at temperatures below the melting temperature range. According to this simulation, the solder solidifies in 2.65 seconds under the established conditions.

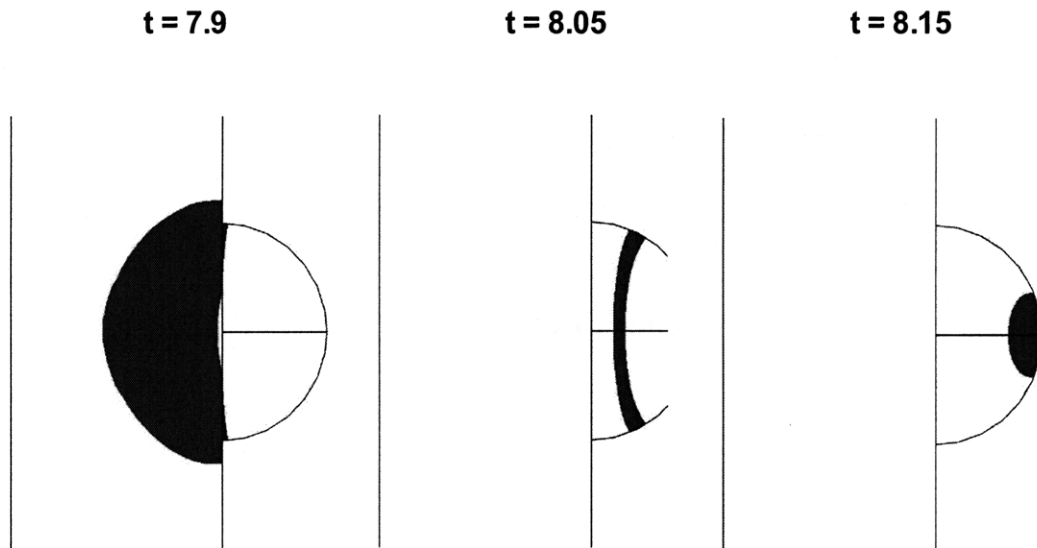


Figure 14: Progression of solidus line, which signifies the boundary between material within the transition range and 100% solid

4.2.4 Temperature behavior

Once again, the temperature inside the solder must be monitored throughout the simulation so that the results can be confirmed. Figure 15 shows the temperature of the same point analyzed in Figure 12. The results closely follow the same tendencies in rate of temperature decrease as do the melting results in rate of temperature increase. The rate of temperature change slows down as expected when the point enters the solidification stage. Once

the point leaves the melting temperature range, the rate of temperature change briefly exceeds the normal rate and then settles back down to the original rate. Similar effects in melting and solidification show that the effect is pertinent to phase change in both directions. The physical phenomenon mentioned in melting also occurs in solidification but with adjacent solid material cooling the material just leaving the transition temperature range at a higher rate instead of heating.

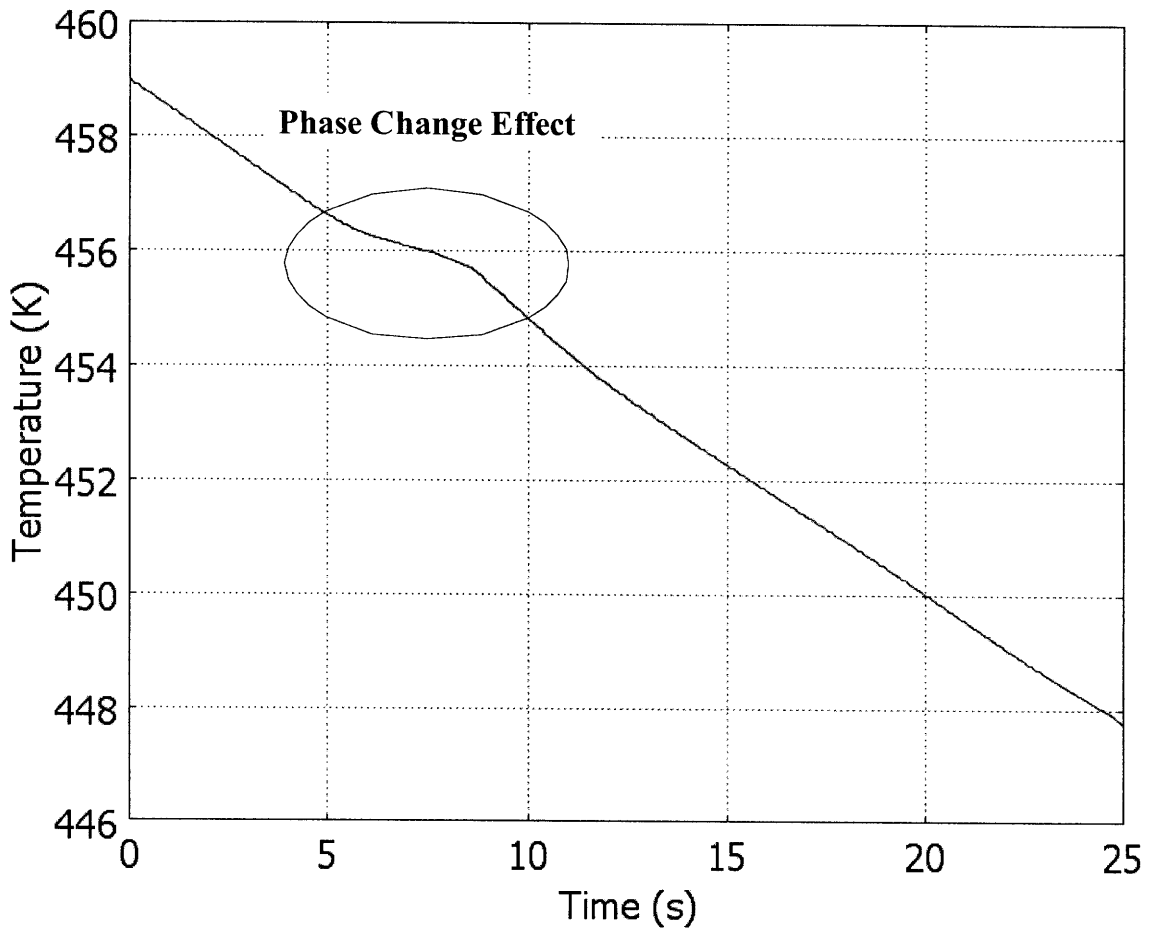


Figure 15: Temperature at a point inside the solder during solidification

4.3 Squishbot implications

The melting and solidification results have important implications for the Squishbot joint design. With all relevant settings equal, the unlocking of the joint (melting) occurs faster than locking (solidification). This is due a larger net heat flux into the solder during melting than the net heat flux out of the solder during solidification. Adjustments can be made to the joint design to decrease either melting or solidification time. Using a higher power heater will decrease melting time while increasing the convective heat transfer coefficient will decrease the solidification time. Although there are space and energy restrictions, decreasing melting time only requires a simple design change whereas improving the design to allow for higher convective heat transfer would be more difficult with less net reward. Moreover, increasing the convective heat transfer coefficient works against the conductive heat transfer during melting. Thus, decreasing the solidification time in this manner has the unfortunate side effect of increasing the melting time.

The solidification cycle contains another inherent disadvantage. As a joint locking device, solder or any solid solution for that matter will naturally unlock faster than lock due to the existence of the melting temperature range. When solidified, the solder resists joint movement up to a certain amount of torque. Once the solder begins to melt and both liquid and solid are present, the solder begins to lose its holding torque. Regardless of the level of completion of the melting cycle, the joint is free to move as soon as the solder can no longer hold the torque being applied to the joint. This will likely happen early in the melting cycle, since the formation of liquid begins on the surface of the joint itself. On the other hand, the locking process requires that the solder reach a level of solidification where a minimum holding torque is applied. Although solidification also starts along the joint surface, a thin layer of solid solder

will likely break under the torques applied due to heightened stresses upon a small cross-section. Whereas unlocking will likely occur earlier in the melting cycle, locking will likely occur later in the solidification cycle. In the real application of the joint, unlocking will take less time than the simulation indicates while the locking time will more closely resemble the maximum solidification time found in the simulation.

4.4 Solver Parameters

The correct selection of solver parameters and initial conditions determines the success of the simulation. Time step must be chosen to prevent the solver from inaccurately modeling the phase transition. The original conditions of the problem must place the model directly before the phase change in both melting and solidification to decrease solver run time and improve the accuracy of the results. Two forms of inaccurate results arise from improper solver and initial condition settings. The oscillation problem emerges when the time step used by the solver during phase transition is too small. The bypassing problem occurs when the time step used by the solver throughout the simulation is too large or the initial conditions prompt a long run time before phase transition. The correct combination of settings for a given set of heat fluxes and geometry is difficult to determine beforehand and generally are only discovered through trial and error. Monitoring the temperature and heat capacity behavior of the solder during the simulation reveals whether the results are valid or whether they run into one of the aforementioned problems.

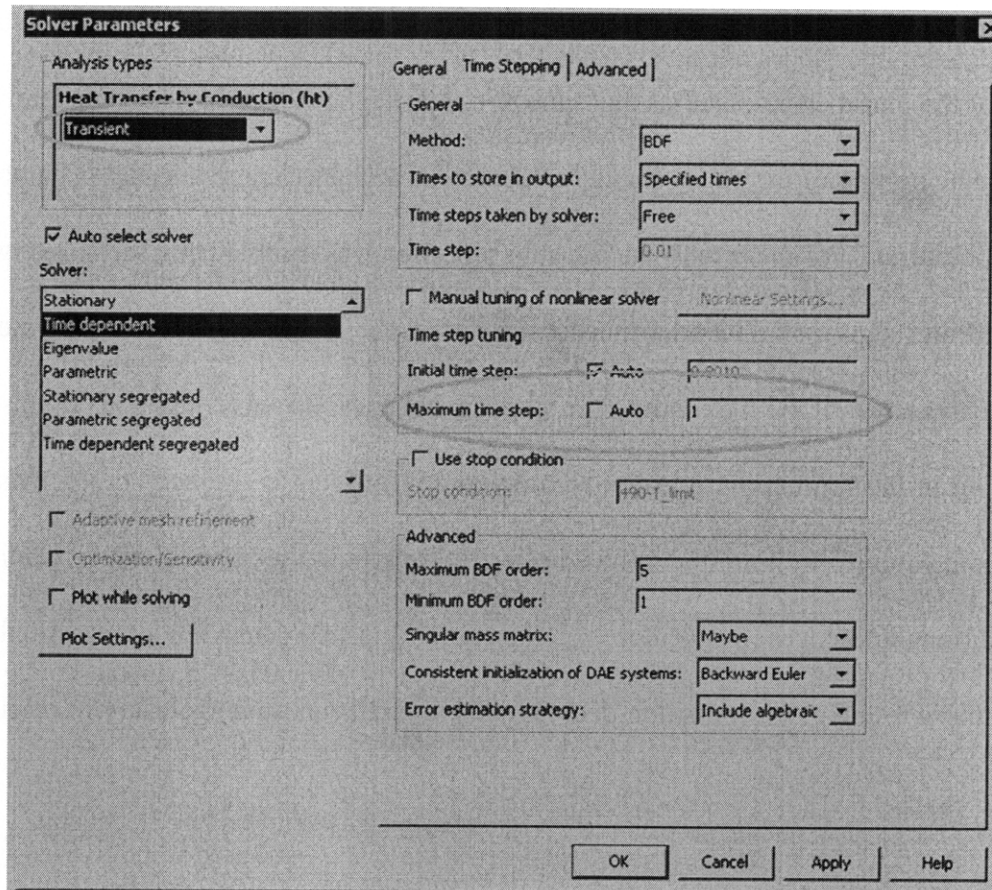


Figure 16: Example screenshot of solder parameters, transient mode and max time step

4.4.1 Time step

More so than the other solver parameters, choice of time step often decides the validity of the results. Large time steps run the danger of including only a few data points from the phase transition in the solution or even none at all. Small time steps risk influencing the results too heavily in the favor of sharp changes in properties, thus corrupting the temperature outputs. The default setting of the solver applies an automatic time step functionality. The auto-step option leaves the choice of time step up to the solver as it progresses through the simulation, resulting in small time steps in the beginning with increasingly larger time steps as the solver proceeds. The large variability in time step makes it difficult to capture the thermodynamic effects of phase change correctly. If the phase change occurs too late in the simulation, the solver likely will

breeze through the phase change without much effect. If the time steps are small enough at the beginning of the phase change, increasing time slices throughout the phase change lead to results favoring the beginning of the phase change over the end and encourage unusual behavior in the output temperatures. For these reasons, the auto time step was disabled and the solver was given a maximum time step instead. Under this configuration, the solver starts at a small time step and gradually increases until the maximum time step is reached. The solver uses this time step for the remainder of the simulation. Ideally, the maximum time step is reached before phase change occurs, causing a uniform time step to be employed throughout the phase change. Choice of initial conditions influences results more so when auto time step is used. Picking initial conditions close to the phase transition decreases the overall run time necessary to reach a solution.

4.4.2 Bypassing

As mentioned above, large time steps can produce results that only lightly include or completely ignore the latent heat effects of phase change in what has been called a bypassing problem. Figure 17 shows what can happen to the temperature of a point inside the solder if this is the case. The increased heat capacity during phase change has virtually no impact upon the rate of temperature increase. The rate of temperature change only slightly decreases over the course of roughly ten seconds before returning to the normal rate of change.

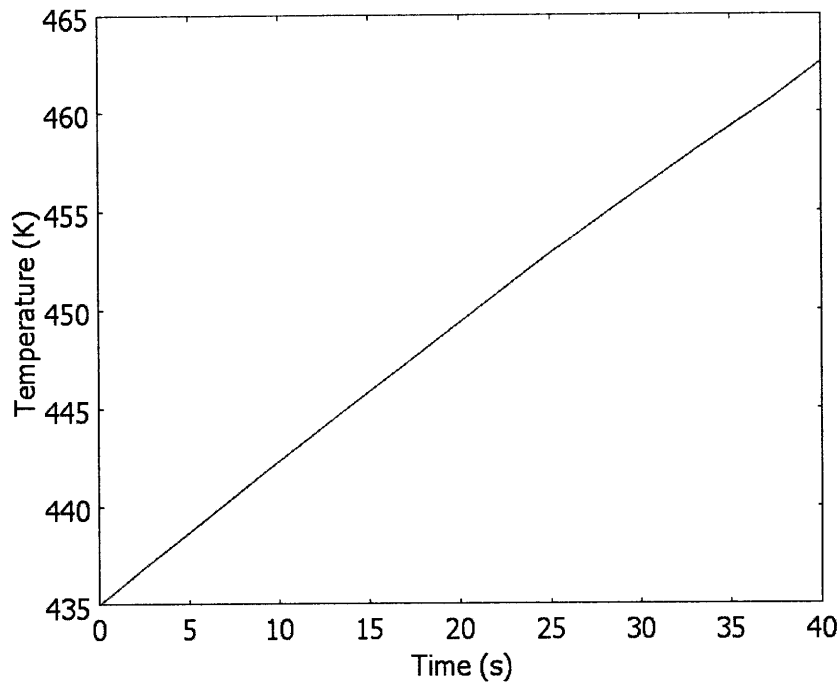


Figure 17: Temperature progression resulting from bypassing problem

Observing the heat capacity during the simulation provides a better understanding of what is actually occurring. Figure 18 shows the heat capacity of the same point during the simulation. The heat capacity is uniform throughout the simulation except for one point just short of 30 seconds, where the value is approximately an order of magnitude less than the maximum value seen in normal simulations. The time step at this point of the simulation has reached four seconds. By increasing the time step, the phase transition has been stretched out longer in time and temperature than it actually occurs. The simulation no longer closely mimics the actual system and no definite conclusions can be drawn from any analysis.

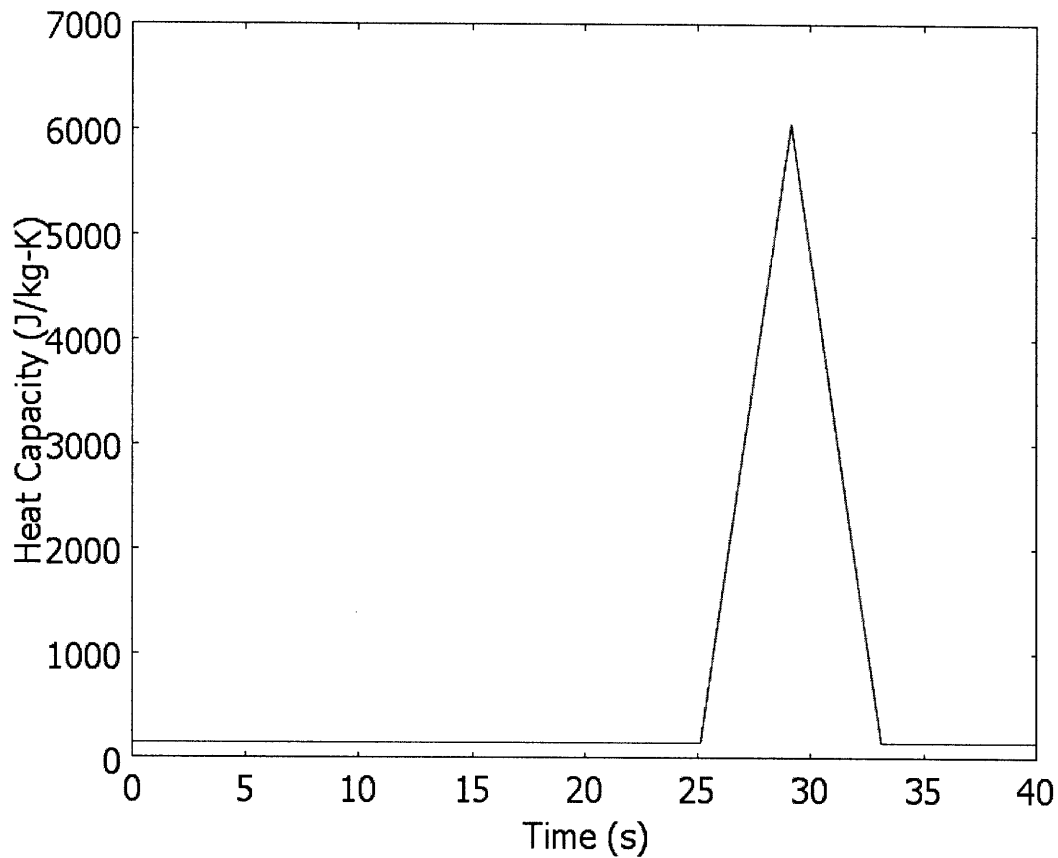


Figure 18: Heat capacity resulting from bypassing problem

4.4.3 Oscillation

Small time steps can also produce undesirable temperature results for different reasons. Figure 19 displays the temperature results from a melting case with a time step of 0.1 seconds. After experiencing the phase transition, the temperature begins to oscillate about the path extended from the original temperature increase line. The oscillation has grown out of control by $t = 13$ seconds and experiences a minimum of 453 K and a maximum of 482 K over a the course of a second.

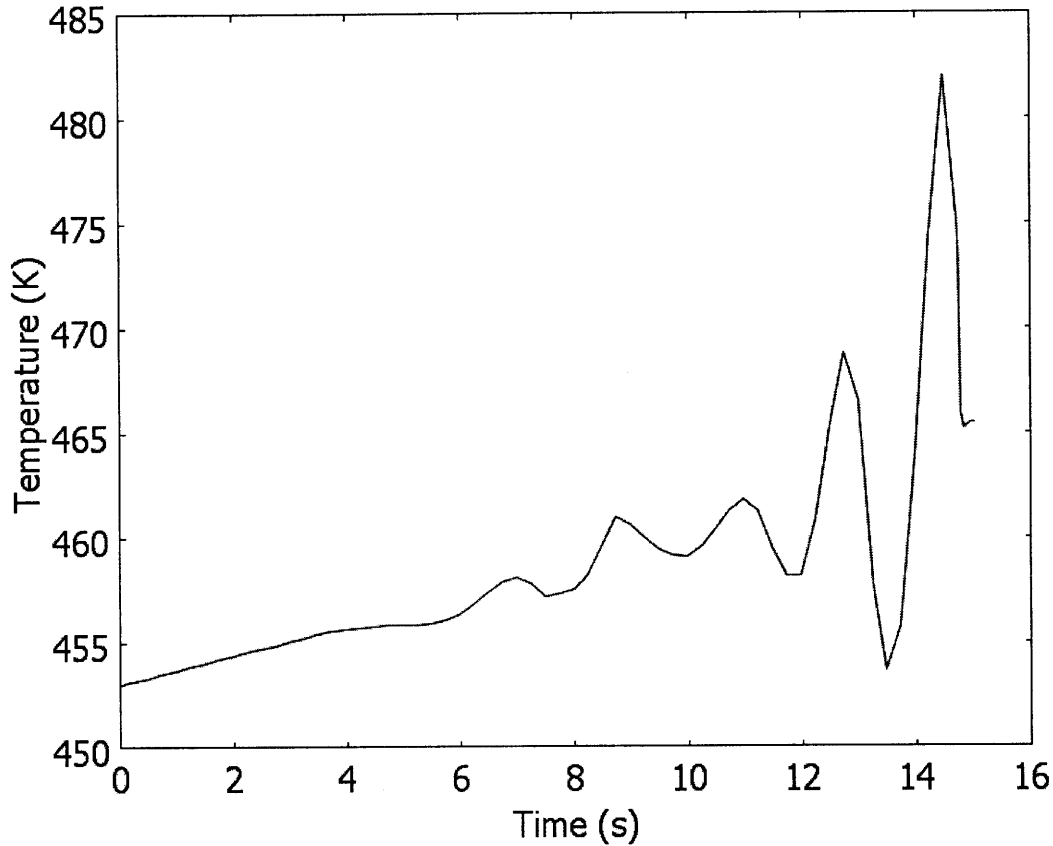


Figure 19: Temperature resulting from oscillation problem

This effect has been documented before in numerical modeling of phase change as it applies to optical rewritable recording [7]. The problem arises because the latent heat factor is suddenly taken into account when a point enters the melting temperature range. An initial overshoot occurs in the first step involving an increased heat capacity. Afterwards, the output temperature proceeds to oscillate back and forth over the actual temperature. For materials with wide melting temperature ranges, the more gradual rise and fall of heat capacity means that this is less likely to be a problem [7]. For materials with narrow melting temperature ranges or single melting point materials modeled as having a very narrow melting range, the problem can significantly affect the results. This numerical phenomenon explains why the previous results experienced slight

elevations of the rate of temperature change beyond the normal rate immediately after leaving the transition region. Even though it cannot be avoided, the effect can certainly be minimized through the correct choice of time step.

It is unclear from Figure 19 whether or not severe temperature oscillation after phase change has a significant impact upon performance during phase change. Analysis of the heat capacity during phase change in Figure 20 reveals more about how it affects phase change itself. The increase is rather sharp for a short period and then starts oscillating itself, changing concavity again to overshoot after already beginning to peak. After finally reaching a peak, the heat capacity takes a sudden dive in value at around $t = 6$ seconds. Such a severe drop despite the rise and fall occurring in a period longer than two seconds exacerbates the oscillation problem in temperature output. The oscillation problem can have an impact upon the behavior during phase change itself and should be minimized whenever possible.

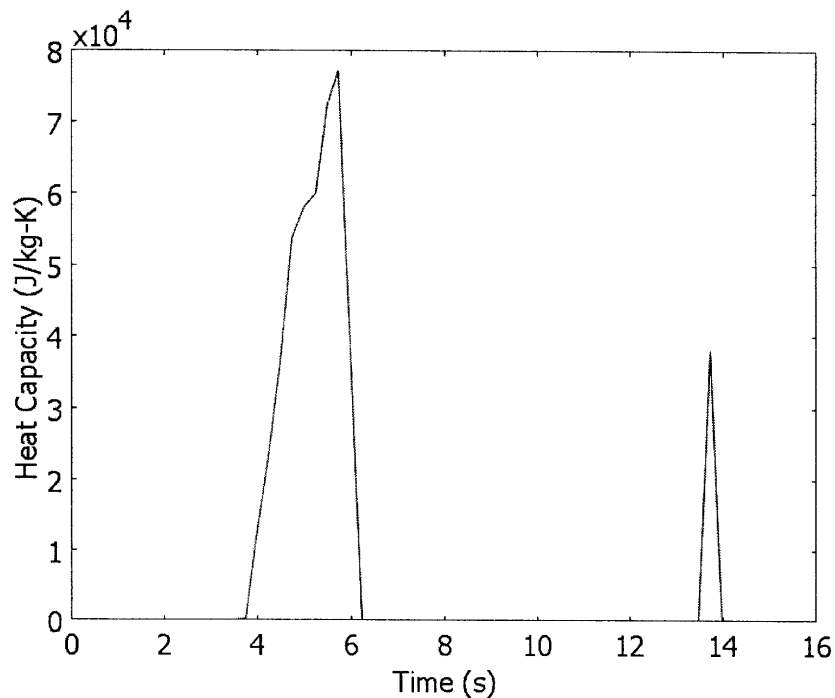


Figure 20: Heat capacity resulting from oscillation problem

4.4.4 Suggestions for improved performance

A healthy balance between capturing multiple points within the phase change and avoiding amplifying the overshoot problems inherent in the numerical modeling must be obtained. A maximum time step must be found that exhibits little to no overshoot effects without sacrificing accurate simulation of the phase transition. Since so many variables and conditions are present in the model, this can only be achieved through trial and error. For materials with large melting temperature ranges, the bypassing problem can easily be avoided without putting the simulation in danger of excessive oscillation error. The narrower the melting temperature range, the more difficult it becomes to balance these two effects. This poses a problem for the Squishbot joint locking system because materials with narrower melting temperature ranges are preferred for their speed in phase transition. This becomes even more of a problem when the chosen material possesses a rather high latent heat of melting. A practical solution to this dilemma is to model narrow melting range materials as having larger melting ranges. Both errors will be less likely to occur and the modeling of latent heat effects should not suffer. Instead of observing the expanded melting range phase change fronts, the melting and solidification fronts of the actual temperature range can be observed using the same analysis techniques applied previously in the melting and solidification models. Analysis of time to melt and solidify does not suffer from the expanded melting range if this procedure is followed. These results could potentially be more accurate than the simplified results obtained in this thesis.

5 CONCLUSION

The purpose of this thesis has been satisfied. An effective tool was created in COMSOL to model melting and solidification. This tool was created with the modeling of joint locking fluid in the Squishbot in mind. The model uses an equivalent heat capacity approach to incorporate the effect of latent heat into the thermodynamic behavior of the system. Successful data was obtained for both melting and solidification scenarios involving a small solder hemisphere on top of a thin copper plate. Care must be taken when choosing the solver parameters since inadequate representation of latent heat or uncontrollable temperature oscillation can occur when solver step size becomes too big or too small. From this data, efforts can be made to improve the design in terms of power required and joint locking and unlocking speed to meet Squishbot requirements. The methods used to numerically model phase change can also be applied to other thermodynamic problems involving phase change under similar conditions.

The results of this thesis mark the beginning of a continuing effort to design an effective Squishbot joint mechanism. Several steps must be taken to utilize the model effectively toward achieving this goal. First, the suggestions for removing error outlined in the solver parameters section must be incorporated into any further analysis. Second, geometry more closely resembling that of the actual joint must be imported into the model and all boundary conditions redefined to match the conditions present. Third, basic experiments of systems closely resembling those analyzed in COMSOL must be conducted to determine the validity of the simulation. If the computer simulation results can be matched reasonably well to empirical data, the model can be used to optimize material and geometric design choices for the Squishbot. Material and geometric design features would be chosen to minimize locking and unlocking

without using an excessive amount of energy. The current results seem to suggest that the proposed joint locking fluid design could work for the Squishbot. Using more desirable materials manufactured into an optimal geometry, it is speculated that the joint locking fluid design is feasible under the existing restrictions. Extension of this thesis along the suggested guidelines will answer this question definitively.

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