Analysis of Thermal Conductivity in Composite Adhesives

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Abstract

Thermally conductive composite adhesives are desirable in many industrial applications, including computers, microelectronics, machinery and appliances. These composite adhesives are formed when a filler particle of high conductivity is added to a base adhesive. Typically, adhesives are poor thermal conductors. A thorough understanding of heat transfer through a composite adhesive would aid in the design of an efficient thermally conductive composite adhesive.

In this work, we provide theoretical foundations for use in design of thermally conductive composite adhesives. For proof of concept, we consider a two dimensional model.

We prove existence, uniqueness and continuous dependence theorems for the model. We formulate a probability based parameter estimation problem and present numerical results.

Motivated by the results of the parameter estimation problem, we are led to derive sensitivity equations for our system. We investigate the sensitivity of composite silicones with respect to the thermal conductivity of both the base silicone polymer and the filler particles. Numerical results of this investigation are also presented.

Keywords: thermal conductivity, composite adhesives, well-posedness, inverse problems, sensitivity equations

1 Introduction and Motivation

Adhesives such as epoxies, gels, and greases have numerous commercial and industrial applications. They are found in computers, machinery, home appliances, etc. In general, these adhesives are very poor conductors while in many applications it would be advantageous for them to possess significant thermal conductivity. Consequently, researchers have been studying thermally conductive composites or filled materials: base materials such as epoxies, gels, and greases, which are filled with thermally conductive particles. Filler particles, such as diamond dust, carbon fibers, or aluminum particles, with higher thermal conductivities are added to create a composite material that is a better thermal conductor than the original material. These thermally conductive composites could then replace the poorly conducting adhesives currently in use in applications such as microelectronics, circuit boards, heat exchangers, machinery, and appliances.

Adding particles with a high thermal conductivity has not had as significant an impact on the overall or effective thermal conductivity of the composite as anticipated. In order to address this issue, we investigate design methodologies for these composite materials. Our goal is an improved understanding of heat transfer through a composite material and an increased knowledge of the impact the composite design has on this thermal process.

The goal in creating a thermally conductive composite is a significant increase in the thermal conductivity of the composite over the thermal conductivity of the unfilled material. There are several design considerations, including the choice of particle, the particle geometry and the size and shape of the particles. We concentrate our presentation here on a composite material with a fixed geometry and consider the role of the particles. (For the effects of varying the geometry see [8].)

In the sections below we present a mathematical model to describe the heat transfer through a composite silicone. We show that the mathematical model is well-posed. In particular, we show there exist unique weak solutions to this mathematical model. Furthermore, these solutions are continuously dependent on the initial conditions, forcing function, and parameters.

We formulate a probability based parameter estimation problem based on results in [1] where the parameters are viewed as realizations of random variables. This approach allows for uncertainty in the model parameters as well as the data, e.g., see [9, 12]. We introduce a formulation for this approach in the context of our model and present some numerical results.

Finally, we rigorously derive sensitivity equations for our mathematical model. We then numerically solve these equations and show that the model is more sensitive to some model parameters than others. These results provide insight into the results of our parameter estimation problem.

The silicone system used as the base for our composite silicone has a thermal conductivity of approximately 0.12 W/mK (Watts per meter-Kelvin). The base silicone consists of a vinyl-functional siloxane (commonly referred to as a resin or polymer) and a hydride-functional siloxane (commonly called a crosslinker). When these two liquid components are cured the hydride adds to the double bond in the vinyl group to form a linkage

$$\mathrm{SiCH{=}CH_2} \ + \ \mathrm{H{-}Si} \ \ - - - - > \ \mathrm{SiCH_2{-}CH_2Si}$$

which is sufficient to form a solid. For ease of reference, we refer to the silicone system as the silicone polymer. In hopes of creating a composite silicone with a higher thermal conductivity, filler particles with a greater thermal conductivity are added to the silicone polymer. A wide variety of filler particles, including aluminum particles, carbon fibers and diamond dust, can be added in varying concentrations. For our sample composite silicone, we use Grade 6 aluminum which has a thermal conductivity of 217 W/mK and concentrate here on composites with 25% by volume concentration of particles.

There are a variety of methods available to measure thermal conductivity. For our data collection we employed a Holometrix Model Microflash. The Microflash uses a laser flash method which allows measurements to be taken at room temperature. The software used in conjunction with the machine is Microflash-RT, version 2.25.

This method works well for materials of uniform density, i.e., non-composites. However, we are using composite materials and it is known that this results only in some measure of the "average" or "effective" thermal properties of the composite material. It is difficult to answer design questions about the composite silicone based only on these effective properties of the composite.

Analysis on a single test piece yields the "effective" diffusivity, specific heat and thermal conductivity of the sample based on an average of three trials. In addition to these three averaged values, the Microflash outputs the diffusivity, specific heat and thermal conductivity of each trial and the voltage at eight different times for each of the three trials. The eight times recorded are the time in milliseconds (msecs) to reach 0, 20, 30, 40, 50, 70, 80, and 100 percent of the temperature rise (equivalently voltage rise, see [8]). For further details on the data collection method and experimental results, see [8].

2 Problem Formulation

2.1 Model

Since the fundamental process of our problem is heat transfer through the composite silicone, the foundation of our model is the transient heat equation [11]. While keeping the composition of the composite silicone and the data collection process in mind, it is necessary to make a few simplifying assumptions. First, we assume all heat from the heat source (a laser) flows through the composite silicone and into the heat sink (an IR detector), as depicted in Figure 1. Second, since the composite silicone slice is very thin, we assume there is no heat loss through the sides. Thus in our model we assume the sides of the composite silicone are insulated. We use a flux boundary condition to describe the heating on the source side of the composite silicone due to the laser. On the sink side of the composite silicone, where the IR detector is located, we use Newton cooling to describe the boundary condition since that face of the composite silicone is in contact with the ambient air.

However, for our initial study of the problem we elected to reduce the three dimensional model to a two dimensional model (solely to facilitate numerous computational simulations). The two dimensional model can be thought of as a very thin interior slice (in the direction

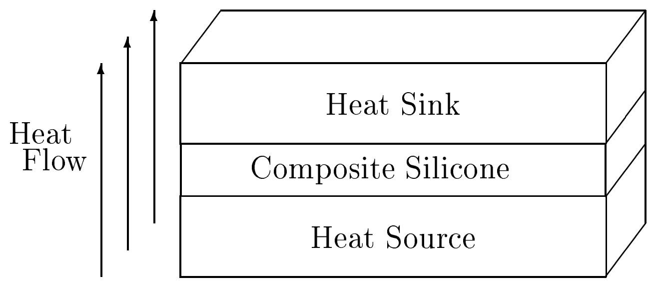

Figure 1: Three dimensional heat transfer model

of the heat flow) of the three dimensional model as depicted in Figure 2. We assume the composite silicone is significantly thicker in the direction normal to the slice compared to the slice itself, so all heat will flow directly through the composite silicone with negligible lateral dissipation. For our experimental test pieces, the diameters of the pieces were much greater than the thickness of the piece, so our assumption is reasonable. Furthermore we assume the geometry of the composite silicone is uniform normal to the slice, provided we are in the center of the composite silicone away from lateral edges. Thus the two dimensional model heat transport properties should closely resemble that of the three dimensional model.

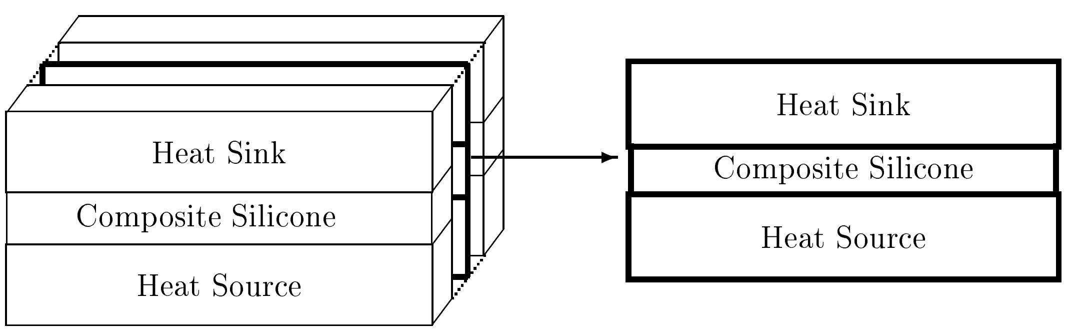

Figure 2: Two dimensional heat transfer model

We will continue to assume the sides of the composite silicone are insulated. The boundary at the heat source will be a Neumann boundary condition given by the heat flux due to the laser and the boundary at the heat sink will still be described by Newton cooling.

It is clear that the filler particles will not be uniform in size, and will most likely be randomly dispersed throughout the base silicone polymer. However, it will be necessary to know the size of each particle and the arrangement of the particles in order to determine the value of k, ρ, and c_p at a particular point in the composite silicone. To facilitate our modeling, we will assume the filler particles are fixed and comprise the appropriate volume percent of the composite silicone and that there is a known particle arrangement.

We will denote the ambient temperature by T_∞ and the initial temperature of the composite silicone by u_0. We denote the Newton cooling constant by h, and define $S_0(t)$ to be the flux due to the heat source. Thus if $u(t, \bar{z})$ is the composite silicone temperature at a given time t and coordinate $\bar{z}$, we have the following system describing the temperature in the sample:

$$\begin{cases} \rho(z)c_p(z)\dot{u}(t,z) = \nabla \cdot (k(z)\nabla u(t,z)), \quad z \in \Omega & \\ k(z)\frac{\partial u}{\partial n}(t,z)|_{\gamma_4} = S_0(t) & (source) \\ k(z)\frac{\partial u}{\partial n}(t,z)|_{\gamma_2} = h(T_\infty - u(t,z))|_{\gamma_2} & (sink) \\ k(z)\frac{\partial u}{\partial n}(t,z)|_{\gamma_1} = 0 & \\ k(z)\frac{\partial u}{\partial n}(t,z)|_{\gamma_3} = 0 & \\ u(0,z) = \Upsilon(z), \quad z \in \Omega & \end{cases} \tag{1}$$

where $\Omega = [-\frac{c_1}{2}, \frac{c_1}{2}] \times [-\frac{c_2}{2}, \frac{c_2}{2}]$ and $t \in [0, T]$, and $\dot{u} = \frac{\partial u}{\partial t}$, with c_1, c_2, and T assumed finite, positive constants. Let $\partial\Omega = \gamma_1 \cup \gamma_2 \cup \gamma_3 \cup \gamma_4$ where

$$\begin{aligned} \gamma_1(s) &= \{(\frac{c_1}{2}, s) : s \in [-\frac{c_2}{2}, \frac{c_2}{2}]\}, \\ \gamma_2(s) &= \{(s, \frac{c_2}{2}) : s \in [-\frac{c_1}{2}, \frac{c_1}{2}]\}, \\ \gamma_3(s) &= \{(-\frac{c_1}{2}, s) : s \in [-\frac{c_2}{2}, \frac{c_2}{2}]\}, \text{ and} \\ \gamma_4(s) &= \{(s, -\frac{c_2}{2}) : s \in [-\frac{c_1}{2}, \frac{c_1}{2}]\}, \end{aligned}$$

as depicted in Figure 3. We define $\Omega_s \subset \Omega$ to be the region occupied by the silicone and $\Omega_p \subset \Omega$ to be the region occupied by the filler particles. Note $\Omega_s \cap \Omega_p = \emptyset$ and $\Omega_s \cup \Omega_p = \Omega$.

It is important to note that ρ, c_p and k are all spatially dependent. They will have one

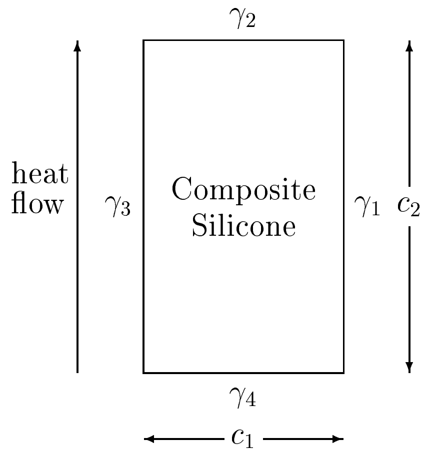

Figure 3: Two dimensional composite silicone slice

value in the silicone polymer and another value in the filler particles. For the two dimensional case investigated computationally below and in [8], we assumed all particles were circles in a known, although not necessarily uniform, particle arrangement.

2.2 Matlab PDE Toolbox Solutions

The major benefit of using the two dimensional model is that we can use Matlab's Partial Differential Equation Toolbox (PDE Toolbox) to solve (1). Matlab's PDE Toolbox can solve two dimensional parabolic partial differential equations. In order to solve (1) using the PDE Toolbox we must provide the boundary conditions, the PDE coefficients and the composite silicone geometry. The PDE Toolbox generates a triangular mesh using the Delaunay triangulation algorithm and numerically solves the PDE using the finite element method with linear elements (the only type of elements the PDE Toolbox employs). The PDE Toolbox automatically defines the mesh, although the user has the option to refine the mesh. See [14] for further information about Matlab's Partial Differential Equation Toolbox.

Matlab's PDE Toolbox allowed us to carry out simulations for many different geometry configurations. For example, geometries with uniform, shifted and random geometries can be considered. We can (and did) also consider geometries of both same sized and varying sized particles. A summary of our numerical simulations for different geometries (random, fixed, etc.) and different distributions of particle size is given in [8].

For the numerical results we present in *this* paper, we assume all aluminum filler particles in the two dimensional model are circles of uniform diameter arranged in a uniform geometry, i.e., the particles are uniformly spaced and aligned in rows. Since our sample composite silicone contains Grade 6 aluminum particles we will use the mean diameter of the volume distribution provided by the aluminum supplier, 24.14 μ (microns), as the diameter of each particle. We will concentrate on the 25% by volume composite silicone, but all ideas presented here extend in a natural way to composite silicones with different compositions.

The silicone polymer used as the base for the composite silicone wets well, meaning it forms a thin film around each of the particles. The film formed around each particle is estimated to be approximately 50 angstroms. Hence, we assume each particle is separated by a minimum distance of 0.01 microns and that no particles touch the boundary of the composite silicone slice which is 321.5 μ wide and 1638 μ high, i.e., $c_1 = 321.5$ and $c_2 = 1638$ in the two dimensional model of the previous section. The composite silicone slice we use in computations reported on below contains 288 circles of diameter 24.14 μ in a uniform arrangement representing the 25% by area aluminum particles used by the PDE Toolbox as the geometry for our composite silicone.

We note that k, ρ and c_p are all spatially dependent. In order to differentiate between the value of each parameter in the silicone versus the aluminum particle we will quantify this variability as follows: for $z \in \Omega$, the value for each parameter is given by:

$$k(z) = \begin{cases} k_s & z \in \Omega_s \\ k_p & z \in \Omega_p \end{cases}$$

$$\rho(z) = \begin{cases} \rho_s & z \in \Omega_s \\ \rho_p & z \in \Omega_p \end{cases}$$

and

$$c_p(z) = \begin{cases} c_{p_s} & z \in \Omega_s \\ c_{p_p} & z \in \Omega_p, \end{cases}$$

where k_s, k_p, ρ_s, ρ_p, c_{p_s}, and c_{p_p} are all finite constants. Observe that k, ρ, and c_p are each functions from Ω to $\mathbb{R}$ and each is piecewise constant.

We assume the composite silicone was initially at the ambient temperature and the temperature was uniform throughout the sample. Thus we set $\Upsilon(z) = T_\infty$. We choose the Newton constant to represent air cooling as we have in our model. The exact model parameters used in the simulations reported here are in Table 1. In the table, g/cm^3 is grams per cubic centimeter and J/gK is Joules per gram-Kelvin.

k_s	0.12 W/mK
k_p	217 W/mK
ρ_s	1 g/cm^3
ρ_p	2.7 g/cm^3
c_{p_s}	1.55 J/gK
c_{p_p}	0.90 J/gK
T_∞	296.15 K
h	350
S_ℓ	4.32×10^7 W/m^2

Table 1: Model parameters

The source flux will approximate the energy in the laser pulse. The laser energy as configured in the Microflash is approximately 7 J. For our testing there is a 20% filter screen, so the actual laser energy is approximately 1.4 J. In addition, since the pieces are graphite coated, technicians at Holometrix estimate there is an additional 20% energy loss. Given that the length of the laser pulse is 330 microseconds and the diameter of the laser is 10 mm, we calculate the flux due to the laser pulse to be $S_\ell = 4.32 \times 10^7$ W/m^2 (Watts per meter squared). Thus the source flux is given by

$$S_0(t) = \begin{cases} S_\ell & 0 \leq t \leq t_p \\ 0 & t_p < t, \end{cases}$$

where $t_p = 0.000330$ seconds. While we believe this is a high estimate, it is sufficient for our purposes here and in [8].

3 Well-Posedness

3.1 Problem in Variational Form

In this section we investigate theoretical issues relating to the two dimensional model formulated in Section 2. We define a class of abstract parabolic equations and establish that this class of equations is well-posed. Furthermore, we verify that our two dimensional heat transfer model fits this class of equations for a large number of examples with different particle shapes, size distributions and geometry. These results guarantee the existence and uniqueness of weak solutions to our model as well as continuous dependence on the initial data, forcing function and model parameters for most examples of interest. *We note here that these theoretical results (and those of Sections 4 and 5) are easily extended to three dimensions*, but we choose to concentrate on the two dimensional problem since it relates to our use of Matlab's PDE Toolbox.

3.1.1 Preliminaries

We begin with the two dimensional model (1) from Section 2 with rather general but fixed particle shapes, sizes and geometry of location. We define for simplicity of notation $g(z) = \rho(z)c_p(z)$ throughout and assume there exists constants R_L and R_U such that

$$0 < R_L \leq g(z) \leq R_U < \infty \tag{2}$$

and constants K_L and K_U such that

$$0 < K_L \leq k(z) \leq K_U < \infty \tag{3}$$

for all $z \in \Omega$. Furthermore we assume h is a finite, positive constant.

Define $H = L^2(\Omega)$ with the usual L^2 inner product, $\langle \cdot, \cdot \rangle_{L^2}$, and define $\mathcal{H} = L^2(\Omega)$ with the weighted inner product $\langle \cdot, \cdot \rangle_{\mathcal{H}} = \langle g\ \cdot, \cdot \rangle_{L^2}$. Note the norms generated by the $\mathcal{H}$-inner product and the L^2-inner product are equivalent. Let $V = H^1(\Omega)$ with inner product

$$\langle \phi, \psi \rangle_V = \langle \nabla\phi, \nabla\psi \rangle_{L^2} + \langle \phi, \psi \rangle_{L^2}$$

for $\phi, \psi \in V$ and let $\mathcal{V} = H^1(\Omega)$ with inner product

$$\langle \phi, \psi \rangle_{\mathcal{V}} = \langle \nabla\phi, \nabla\psi \rangle_{\mathcal{H}} + \langle \phi, \psi \rangle_{L^2} \tag{4}$$

for $\phi, \psi \in \mathcal{V}$. We will want to use the following equivalent representation of the inner product in $\mathcal{V}$:

$$\langle \phi, \psi \rangle_{\mathcal{F}} \equiv \langle \nabla\phi, \nabla\psi \rangle_{\mathcal{H}} + \int_{\gamma_2} (Tr_2\ \phi)(z)(Tr_2\ \psi)(z)\ dS_2 \tag{5}$$

where $Tr_j\ : H^1(\Omega) \rightarrow H^{\frac{1}{2}}(\gamma_j)$ is the continuous trace operator mapping $f \in H^1(\Omega) \rightarrow H^{\frac{1}{2}}(\gamma_j) \subset H^0(\gamma_j) = L^2(\gamma_j)$, on γ_j, $j = 1, 2, 3, 4$, with $(Tr_j\ f)(z) = f(z)|_{\gamma_j}$. The following theorem from Maz'ja [16, p. 27] shows the norms generated by these inner products are equivalent:

Theorem 3.1 (Maz'ja) *Let Ω be a bounded domain in $\mathbb{R}^n$ such that $L_p^\ell(\Omega) \subset L_p(\Omega)$. Let $\mathcal{F}(u)$ be a continuous functional in $W_p^\ell(\Omega)$, $\mathcal{F}(\Pi_{\ell-1}) \neq 0$ for any nonzero polynomial $\Pi_{\ell-1}$ of degree not higher than $\ell - 1$. Then the norm*

$$||\nabla_\ell\, u||_{L_p(\Omega)} + \mathcal{F}(u)$$

is equivalent to the norm in $W_p^\ell(\Omega)$.

Here $L_p^\ell(\Omega)$ is the space of distributions on Ω with derivatives of order ℓ in $L_p(\Omega)$, and $W_p^\ell(\Omega) = L_p^\ell(\Omega) \cap L_p(\Omega)$. Also $\nabla_\ell = \{D^\alpha\}$, where $|\alpha| = \ell$ for α a multi-index $(\alpha_1, \cdots, \alpha_n)$ with $D^\alpha = D_{x_1}^{\alpha_1} \cdots D_{x_n}^{\alpha_n}$. (Note for our problem $W_p^\ell(\Omega) = W_2^1(\Omega) = H^1(\Omega)$, i.e., $p = 2$ and $\ell = 1$ and $n = 2$.) If we define

$$\mathcal{F}(u) = \int_\Gamma |tr(u)|^2 dx$$

where $\Gamma \subset \partial\Omega$ and tr is the continuous trace operator mapping $u \in H^1(\Omega) \to H^{\frac{1}{2}}(\partial\Omega) \subset H^0(\partial\Omega) = L^2(\partial\Omega)$, then we have

$$\begin{aligned} |\mathcal{F}(u)| &= \int_\Gamma |tr(u)|^2 dx \\ &\leq \int_{\partial\Omega} |tr(u)|^2 dx \\ &\leq K||u||^2_{H^1(\Omega)} \end{aligned}$$

and hence $\mathcal{F}$ is a continuous functional on $H^1(\Omega)$. Also note that taking $\ell = 1$, $\Pi_{\ell-1} = c$, where c is any non-zero constant, and

$$\mathcal{F}(c) = \int_\Gamma |tr(c)|^2 dx$$

is non-zero if and only if the measure of Γ is non-zero. Thus the norms generated by the inner products (4), (5) are equivalent by Theorem 3.1 and there are finite, positive constants M_L, M_U such that

$$M_L||\phi||^2_{\mathcal{F}} \leq ||\phi||^2_{\mathcal{V}} \leq M_U||\phi||^2_{\mathcal{F}} \tag{6}$$

for all $\phi \in \mathcal{V}$ where

$$||\phi||^2_{\mathcal{F}} = ||\nabla\phi||^2_{\mathcal{H}} + \int_{\gamma_2} |Tr_2\ \phi|^2\ dS_2, \tag{7}$$

is the norm generated by (5).

Define a sesquilinear form $\sigma : \mathcal{V} \times \mathcal{V} \to \mathbb{R}$ by

$$\sigma(\phi, \psi) = \langle \frac{1}{g} k\nabla\phi, \nabla\psi\rangle_{\mathcal{H}} + h\int_{\gamma_2} (Tr_2\ \phi)(z)(Tr_2\ \psi)(z)\ dS_2. \tag{8}$$

Note σ defines an operator $A \in \mathscr{L}(\mathcal{V}, \mathcal{V}^*)$ where $\langle A\phi, \psi\rangle_{\mathcal{V}^*,\mathcal{V}} = \sigma(\phi, \psi)$ and $\mathscr{L}(\mathcal{V}, \mathcal{V}^*)$ is the set of all bounded, linear functionals from $\mathcal{V}$ to $\mathcal{V}^*$. This follows due to the continuity of σ on $\mathcal{V} \times \mathcal{V}$ guaranteed by (6) (see (12) below).

Define $F : [0, T] \to \mathcal{V}^*$ by

$$[F(t)](\psi) = hT_\infty \int_{\gamma_2} (Tr_2\ \psi)(z)\ dS_2 + S_0(t) \int_{\gamma_4} (Tr_4\ \psi)(z)\ dS_4 \tag{9}$$

for $\psi \in \mathcal{V}$.

3.1.2 Weak Solution

Suppose u solves

$$\dot{u} + Au = F \qquad \text{in } \mathcal{V}^*, \tag{10}$$

i.e., for all $\psi \in \mathcal{V}$,

$$\langle \dot{u} + Au - F, \psi \rangle_{\mathcal{V}^*,\mathcal{V}} = 0.$$

By definition we have

$$\begin{aligned}
\langle \dot{u}(t), \psi \rangle_{\mathcal{V}^*,\mathcal{V}} &= \langle -Au(t), \psi \rangle_{\mathcal{V}^*,\mathcal{V}} + \langle F, \psi \rangle_{\mathcal{V}^*,\mathcal{V}} \\
&= \langle -\frac{1}{g} k \nabla u(t), \nabla \psi \rangle_{\mathcal{H}} - h \int_{\gamma_2} (Tr_2\ u(t))(z)(Tr_2\ \psi)(z)\ dS_2 \\
&\qquad + hT_\infty \int_{\gamma_2} (Tr_2\ \psi)(z)\ dS_2 + S_0(t) \int_{\gamma_4} (Tr_4\ \psi)(z)\ dS_4 \\
&= \langle -k \nabla u(t), \nabla \psi \rangle_{L^2} - h \int_{\gamma_2} ((Tr_2\ u(t))(z) - T_\infty)(Tr_2\ \psi)(z)\ dS_2 \\
&\qquad + S_0(t) \int_{\gamma_4} (Tr_4\ \psi)(z)\ dS_4.
\end{aligned}$$

Now, if $u \in V$ and $k\nabla u \in V$, using the Divergence Theorem and the vector identity

$$\nabla \cdot (k(z)\nabla s(t,z)\psi(z)) = (\nabla \cdot (k(z)\nabla s(t,z))\psi(z) + k(z)(\nabla s(t,z) \cdot \nabla \psi(z))$$

one can argue that a solution u of (10) (if it exists) is a weak solution of (1). That is, (10) is the weak form of (1).

3.2 Well-Posedness (Existence, Uniqueness, Continuous Dependence on Data)

We establish existence of solutions to parabolic systems of the form

$$\begin{cases} \dot{u} + Au = F & \text{in } \mathcal{V}^* \\ u(0) = u_0. \end{cases} \tag{11}$$

We will use the Gelfand triple $\mathcal{V} \hookrightarrow \mathcal{H} \cong \mathcal{H}^* \hookrightarrow \mathcal{V}^*$ where the embedding $\mathcal{V} \hookrightarrow \mathcal{H}$ is dense and continuous with $||\phi||_{\mathcal{H}} \leq c||\phi||_{\mathcal{V}}$ for all $\phi \in \mathcal{V}$ and some finite constant $c > 0$. Note the desired inequality holds:

$$\begin{aligned} ||\phi||_{\mathcal{V}}^2 &= \langle \nabla\phi, \nabla\phi \rangle_{\mathcal{H}} + \langle \phi, \phi \rangle_{L^2} \\ &\geq \langle \phi, \phi \rangle_{L^2} \\ &= \langle \frac{1}{g}\phi, \phi \rangle_{\mathcal{H}} \\ &\geq R_U^{-1}||\phi||_{\mathcal{H}}^2 \end{aligned}$$

so in fact $||\phi||_{\mathcal{H}} \leq \sqrt{R_U}\ ||\phi||_{\mathcal{V}}$.

We shall argue and then use two standard conditions on σ defined by (8):

(1) The form σ is $\mathcal{V}$-bounded: for all $\phi, \psi \in \mathcal{V}$, there exists a $B < \infty$ such that

$$|\sigma(\phi, \psi)| \leq B||\phi||_{\mathcal{V}}||\psi||_{\mathcal{V}}. \tag{12}$$

(2) The form σ is $\mathcal{V}$-coercive: for all $\phi \in \mathcal{V}$, there exists a $C > 0$ such that

$$|\sigma(\phi, \phi)| \geq C||\phi||_{\mathcal{V}}^2. \tag{13}$$

We also find that if the source S_0 is in $L^2(0,T)$, then the forcing term F defined by (9) satisfies

$$F \in L^2(0, T; \mathcal{V}^*). \tag{14}$$

To show that σ of (8) satisfies (12), we use (2), (3), and (7):

$$\begin{aligned} |\sigma(\phi, \psi)| &= |\langle \frac{1}{g}k\nabla\phi, \nabla\psi \rangle_{\mathcal{H}} + h\int_{\gamma_2} (Tr_2\ \phi)(z)(Tr_2\ \psi)(z)\ dS_2| \\ &\leq \max\{R_L^{-1}K_U, h\}(||\nabla\phi||_{\mathcal{H}}||\nabla\psi||_{\mathcal{H}} + ||Tr_2\ \phi||_{\gamma_2}||Tr_2\ \psi||_{\gamma_2}) \\ &\leq \max\{R_L^{-1}K_U, h\}(||\nabla\phi||_{\mathcal{H}} + ||Tr_2\ \phi||_{\gamma_2})(||\nabla\psi||_{\mathcal{H}} + ||Tr_2\ \psi||_{\gamma_2}) \\ &\leq \max\{R_L^{-1}K_U, h\}(2||\phi||_{\mathcal{F}})(2||\psi||_{\mathcal{F}}) \end{aligned}$$

$$\leq 4M_L^{-1} \max\{R_L^{-1}K_U, h\}||\phi||_{\mathcal{V}}||\psi||_{\mathcal{V}}$$

where $||f||_{\gamma_2}^2 = \displaystyle\int_{\gamma_2} |f(z)|^2 \, dS_2$ for any $f \in H^{\frac{1}{2}}(\gamma_2)$. Thus σ is $\mathcal{V}$-bounded.

Similarly, for (13) we have the following:

$$\sigma(\phi, \phi) = \langle \frac{1}{g} k \nabla\phi, \nabla\phi\rangle_{\mathcal{H}} + h \int_{\gamma_2} (Tr_2 \ \phi)(z)(Tr_2 \ \phi)(z) \, dS_2$$

$$\geq \min\{R_U^{-1}K_L, h\}(||\nabla\phi||_{\mathcal{H}}^2 + \int_{\gamma_2} |(Tr_2 \ \phi)(z)|^2 \, dS_2)$$

$$\geq \min\{R_U^{-1}K_L, h\}M_U^{-1}||\phi||_{\mathcal{V}}^2$$

so σ is $\mathcal{V}$-coercive.

In order to see that (14) holds, recall $Tr_2 \ : \mathcal{V} = H^1(\Omega) \to H^{\frac{1}{2}}(\gamma_2)$. So, for any $\psi \in \mathcal{V}$, $Tr_2 \ \psi \in H^{\frac{1}{2}}(\gamma_2) \subset L^2(\gamma_2)$, and hence $\displaystyle\int_{\gamma_2} Tr_2 \ \psi \ dS_2 \in \mathbb{R}$. Thus $\psi \to \int_{\gamma_2} Tr_2 \ \psi \ dS_2$ is a continuous mapping from $\mathcal{V} \to \mathbb{R}$, i.e., it is in $\mathcal{V}^*$. If $S_0 \in L^2(0,T)$ (which we assume throughout), then $F \in L^2(0,T;\mathcal{V}^*)$.

Given the above hypothesis, the system (11) is equivalently written

$$\begin{cases} \langle \dot{u}(t), \psi\rangle + \sigma(u(t), \psi) = \langle F(t), \psi\rangle \\ u(0) = u_0 \end{cases} \tag{15}$$

for $\psi \in \mathcal{V}$ where the duality product $\langle \cdot, \cdot\rangle$ is $\langle \cdot, \cdot\rangle_{\mathcal{V}^*,\mathcal{V}}$.

Assume for the moment that (15) has a solution u. We derive an *a priori* bound. Let $\psi = u(t)$ for a fixed t. Substituting into (15) we obtain

$$\langle \dot{u}(t), u(t)\rangle_{\mathcal{V}^*,\mathcal{V}} + \sigma(u(t), u(t)) = \langle F(t), u(t)\rangle_{\mathcal{V}^*,\mathcal{V}}$$

and since $\langle \dot{u}(t), u(t)\rangle_{\mathcal{V}^*,\mathcal{V}} = \frac{1}{2}\frac{d}{dt}\{||u(t)||_{\mathcal{H}}^2\}$ we see

$$\frac{1}{2}\frac{d}{dt}\{||u(t)||_{\mathcal{H}}^2\} + \sigma(u(t), u(t)) = \langle F(t), u(t)\rangle_{\mathcal{V}^*,\mathcal{V}}$$

for any t in a given interval $[0,T]$. Integrating from 0 to t we have

$$\int_0^t \{\frac{1}{2}\frac{d}{d\xi}\{||u(\xi)||_{\mathcal{H}}^2\} + \sigma(u(\xi), u(\xi))\} \, d\xi = \int_0^t \langle F(\xi), u(\xi)\rangle_{\mathcal{V}^*,\mathcal{V}} \, d\xi$$

and thus

$$\frac{1}{2}||u(t)||^2_{\mathcal{H}} - \frac{1}{2}||u(0)||^2_{\mathcal{H}} + \int_0^t \sigma(u(\xi), u(\xi))\ d\xi = \int_0^t \langle F(\xi), u(\xi)\rangle_{\mathcal{V}^*,\mathcal{V}}\ d\xi.$$

Using (13), the Cauchy Schwartz inequality and the fact $2ab \leq a^2 + b^2$, we have

$$\begin{aligned} ||u(t)||^2_{\mathcal{H}} + 2C\int_0^t ||u(\xi)||^2_{\mathcal{V}}\ d\xi &\leq ||u_0||^2_{\mathcal{H}} + 2\left|\int_0^t \langle F(\xi), u(\xi)\rangle_{\mathcal{V}^*,\mathcal{V}}\ d\xi\right| \\ &\leq ||u_0||^2_{\mathcal{H}} + 2\int_0^t ||F(\xi)||_{\mathcal{V}^*}||u(\xi)||_{\mathcal{V}}\ d\xi \\ &\leq ||u_0||^2_{\mathcal{H}} + \frac{1}{C}\int_0^t ||F(\xi)||^2_{\mathcal{V}^*}\ d\xi + C\int_0^t ||u(\xi)||^2_{\mathcal{V}}\ d\xi \end{aligned}$$

and hence

$$||u(t)||^2_{\mathcal{H}} + C\int_0^t ||u(\xi)||^2_{\mathcal{V}}\ d\xi \leq ||u_0||^2_{\mathcal{H}} + \frac{1}{C}\int_0^t ||F(\xi)||^2_{\mathcal{V}^*}\ d\xi. \tag{16}$$

Thus

$$||u(t)||^2_{\mathcal{H}} + C\int_0^t ||u(\xi)||^2_{\mathcal{V}}\ d\xi \leq \hat{C}$$

where $\hat{C} = \hat{C}(||u_0||_{\mathcal{H}}, C, ||F||_{L^2(0,T;\mathcal{V}^*)})$.

The *a priori* bound arguments are the basis of existence as well as continuous dependence. Using them along with quite standard arguments (see Chapter III of [13], §26 of [23]), we can establish the desired existence and uniqueness (detailed arguments are given in [8]).

Theorem 3.2 *Under assumptions (12), (13), and (14), for $u_0 \in V$, there exists a solution of (11) (and hence a weak solution of (1)) with $u \in L^2(0,T;\mathcal{V})$ and $\dot{u} \in L^2(0,T;\mathcal{V}^*)$. Furthermore, this solution is unique.*

In a similar standard approach (again see [8, 13, 23]) one can establish continuous dependence of solutions on initial data and forcing function. We only recall the ideas here.

Suppose $u = u(\,\cdot\,; u_0, F)$ is a weak solution of

$$\begin{cases} \dot{u} + Au = F \\ u(0) = u_0 \end{cases} \tag{17}$$

and suppose $u_n = u_n(\,\cdot\,; u_{n0}, F_n)$ is a weak solution of

$$\begin{cases} \dot{u}_n + Au_n = F_n \\ u_n(0) = u_{n0} \end{cases} \tag{18}$$

with $u_{n0} \to u_0$ in $\mathcal{H}$ and $F_n \to F$ in $L^2(0,T;\mathcal{V}^*)$. Given systems (17) and (18) we see

$$\begin{cases} \langle \dot{u} - \dot{u}_n, \psi \rangle + \sigma(u - u_n, \psi) = \langle F(t) - F_n(t), \psi \rangle \\ u(0) - u_n(0) = u_0 - u_{n0} \end{cases} \tag{19}$$

for all $\psi \in \mathcal{V}$. If we let $\psi = u(t) - u_n(t)$ in (19) and use the same arguments as in establishing (16), we see

$$||u(t) - u_n(t)||^2_{\mathcal{H}} + C\int_0^t ||u(\xi) - u_n(\xi)||^2_{\mathcal{V}}\, d\xi \leq ||u_0 - u_{n0}||^2_{\mathcal{H}} + \frac{1}{C}\int_0^t ||F(\xi) - F_n(\xi)||^2_{\mathcal{V}^*}\, d\xi$$

and thus

$$||u(t) - u_n(t)||^2_{\mathcal{H}} + C\int_0^t ||(\xi) - u_n(\xi)||^2_{\mathcal{V}}\, d\xi \leq ||u_0 - u_{n0}||^2_{\mathcal{H}} + \frac{1}{C}||F - F_n||_{L^2(0,T;\mathcal{V}^*)}.$$

Thus given that $u_{n0} \to u_0$ in $\mathcal{H}$ and $F_n \to F$ in $L^2(0,T;\mathcal{V}^*)$, we see $u \to u_n$ in $C(0,T;\mathcal{H})$ and also in $L^2(0,T;\mathcal{V})$. Indeed we have

Theorem 3.3 *The mapping $(u_0, F) \to u(\,\cdot\,; u_0, F)$, where $u(\,\cdot\,; u_0, F)$ is a solution to (11) is continuous from $\mathcal{H} \times L^2(0,T;\mathcal{V}^*)$ to $C(0,T;\mathcal{H}) \cap L^2(0,T;\mathcal{V})$.*

We remark that one can actually establish the somewhat stronger continuity from $\mathcal{H} \times L^2(0,T;\mathcal{V}^*)$ to $\mathcal{U} = L^2(0,T;\mathcal{V}) \cap H^1(0,T;\mathcal{V}^*)$, see [13, 23] for details.

3.3 Continuous Dependence on Parameters

3.3.1 Continuous Dependence on k and h

Suppose $u(\,\cdot\,; k, h)$ is a weak solution of

$$\begin{cases} \dot{u} + Au = F \\ u(0) = u_0 \end{cases} \tag{20}$$

and let $u_n(\,\cdot\,; k_n, h_n)$ be a weak solution of

$$\begin{cases} \dot{u}_n + A_n u_n = F_n \\ u_n(0) = u_0 \end{cases} \tag{21}$$

where

$$\langle A_n\phi, \psi\rangle_{\mathcal{V}^*,\mathcal{V}} \equiv \sigma_n(\phi,\psi) = \langle \frac{1}{g} k_n \nabla\phi, \nabla\psi\rangle_{\mathcal{H}} + h_n \int_{\gamma_2} (Tr_2\ \phi)(z)(Tr_2\ \psi)(z)\ dS_2 \tag{22}$$

and

$$\langle F_n(t), \psi\rangle_{\mathcal{V}^*,\mathcal{V}} = h_n T_\infty \int_{\gamma_2} (Tr_2\ \psi)(z)\ dS_2 + S_0(t) \int_{\gamma_4} (Tr_4\ \psi)(z)\ dS_4.$$

Let $\{h_n\}$ be a sequence such that $h_n \to h$ and let $\{k_n\}$ be a sequence such that $k_n \to k$ uniformly in z, i.e., $k_n \to k$ in $C(\Omega)$. Since we know $h_n \to h$, this implies $F_n \to F$ in $L^2(0,T;\mathcal{V}^*)$. From the previous section we know solutions depend continuously on the forcing function when $F_n \to F$ in $L^2(0,T;\mathcal{V}^*)$. Thus without loss of generality we can suppress the dependence of F on h_n and take F for F_n in (21) with $u_n(\,\cdot\,; k_n, h_n)$ a weak solution of

$$\begin{cases} \dot{u}_n + A_n u_n = F \\ u_n(0) = u_0 \end{cases} \tag{23}$$

where A_n is defined as in (22). By (3) we know for N_1 sufficiently large there exist constants $\bar{K}_L > 0$ and $\bar{K}_U < \infty$ such that $k_n(z) \in [\bar{K}_L, \bar{K}_U]$, $k(z) \in [\bar{K}_L, \bar{K}_U]$ for all $z \in \Omega$ and all $n \geq N_1$. Since $h_n \to h$, for N_2 sufficiently large there exist constants $\bar{h}_L > 0$ and $\bar{h}_U < \infty$ such that $h_n \in [\bar{h}_L, \bar{h}_U]$, $h \in [\bar{h}_L, \bar{h}_U]$ for all $n \geq N_2$. Without loss of generality, hereafter we assume all n will satisfy $n \geq N = \max\{N_1, N_2\}$.

Note σ_n is uniformly (in n) $\mathcal{V}$-coercive satisfying $\sigma_n(\phi,\phi) \geq C_1||\phi||^2_{\mathcal{V}}$, where

$$C_1 = \min\{R_U^{-1}\bar{K}_L, \bar{h}_L\}M_U^{-1}$$

and C_1 is independent of n.

Subtracting the weak form of (23) from (20) we obtain

$$\langle \dot{u}(t) - \dot{u}_n(t), \psi\rangle_{\mathcal{V}^*,\mathcal{V}} + \sigma(u(t),\psi) - \sigma_n(u_n(t),\psi) = 0$$

for all $\psi \in \mathcal{V}$. Thus

$$\langle \dot{u}(t) - \dot{u}_n(t), \psi \rangle_{\mathcal{V}^*,\mathcal{V}} + \langle \frac{1}{g}(k \nabla u(t) - k_n \nabla u_n(t)), \nabla \psi \rangle_{\mathcal{H}} + \int_{\gamma_2} (h(Tr_2\ u(t))(z) - h_n(Tr_2\ u_n(t))(z))(Tr_2\ \psi)(z)\ dS_2 = 0$$

for all $\psi \in \mathcal{V}$.

Adding and subtracting terms we see

$$\langle \dot{u}(t) - \dot{u}_n(t), \psi \rangle_{\mathcal{V}^*,\mathcal{V}} + \langle \frac{1}{g}(k - k_n) \nabla u(t), \nabla \psi \rangle_{\mathcal{H}} + \langle \frac{1}{g} k_n (\nabla u(t) - \nabla u_n(t)), \psi \rangle_{\mathcal{H}} + (h - h_n) \int_{\gamma_2} (Tr_2\ u(t))(z)(Tr_2\ \psi)(z)\ dS_2 + h_n \int_{\gamma_2} (Tr_2\ (u(t) - u_n(t)))(z)(Tr_2\ \psi)(z)\ dS_2 = 0$$

for all $\psi \in \mathcal{V}$.

Fix $t \in [0, T]$ and let $\psi = u(t) - u_n(t)$ in the previous equation. Thus

$$\begin{aligned} \frac{1}{2}\frac{d}{dt}\{||u(t) - u_n(t)||^2_{\mathcal{H}}\} &+ \langle \frac{1}{g} k_n (\nabla u(t) - \nabla u_n(t)), \nabla u(t) - \nabla u_n(t) \rangle_{\mathcal{H}} \\ &+ h_n \int_{\gamma_2} (Tr_2\ (u(t) - u_n(t)))(z)(Tr_2\ (u(t) - u_n(t)))(z)\ dS_2 \\ &= \langle \frac{1}{g}(k_n - k) \nabla u(t), \nabla u(t) - \nabla u_n(t) \rangle_{\mathcal{H}} \\ &+ (h_n - h) \int_{\gamma_2} (Tr_2\ u(t))(z)(Tr_2\ (u(t) - u_n(t)))(z)\ dS_2 \end{aligned}$$

and hence using the definition of σ_n and integrating from 0 to t, for $t \in [0, T]$ we obtain

$$\begin{aligned} ||u(t) - u_n(t)||^2_{\mathcal{H}} &+ 2 \int_0^t \sigma_n(u(\xi) - u_n(\xi), u(\xi) - u_n(\xi))\ d\xi \\ &= 2 \int_0^t \langle \frac{1}{g}(k_n - k) \nabla u(\xi), \nabla u(\xi) - \nabla u_n(\xi) \rangle_{\mathcal{H}}\ d\xi \\ &+ 2 \int_0^t (h_n - h) \int_{\gamma_2} (Tr_2\ u(\xi))(z)(Tr_2\ (u(\xi) - u_n(\xi)))(z)\ dS_2\ d\xi. \end{aligned}$$

Using the fact σ_n is $\mathcal{V}$-coercive on the left side of the equation, and the Cauchy-Schwartz inequality, the relation $2ab \leq a^2 + b^2$, and the equivalent form of the $\mathcal{V}$-norm generated by

(5) on the right side, we see

$$
\begin{aligned}
&||u(t) - u_n(t)||_{\mathcal{H}}^2 + 2C_1 \int_0^t ||u(\xi) - u_n(\xi)||_{\mathcal{V}}^2 \, d\xi \\
&\quad \leq 2 \int_0^t ||\frac{1}{g}(k_n - k)\nabla u(\xi)||_{\mathcal{H}} ||\nabla u(\xi) - \nabla u_n(\xi)||_{\mathcal{H}} \, d\xi \\
&\qquad + 2 \int_0^t |(h_n - h) \int_{\gamma_2} (Tr_2 \; u(\xi))(z)(Tr_2 \; (u(\xi) - u_n(\xi)))(z) \; dS_2| \; d\xi \\
&\quad \leq \frac{2}{C_1} \int_0^t R_L^{-2} ||k_n - k||_\infty^2 ||\nabla u(\xi)||_{\mathcal{H}}^2 \, d\xi + \frac{C_1}{2} \int_0^t ||\nabla u(\xi) - \nabla u_n(\xi)||_{\mathcal{H}}^2 \, d\xi \\
&\qquad + \frac{2M_L^{-1}}{C_1} \int_0^t |h_n - h|^2 \int_{\gamma_2} |(Tr_2 \; u(\xi))(z)|^2 \; dS_2 \; d\xi \\
&\qquad + \frac{C_1}{2M_L^{-1}} \int_0^t \int_{\gamma_2} |(Tr_2 \; (u(\xi) - u_n(\xi)))(z)|^2 \; dS_2 \; d\xi \\
&\quad \leq \frac{2}{C_1 R_L^2} ||k_n - k||_\infty^2 \int_0^t ||u(\xi)||_{\mathcal{V}}^2 \, d\xi + \frac{C_1}{2} \int_0^t ||u(\xi) - u_n(\xi)||_{\mathcal{V}}^2 \, d\xi \\
&\qquad + \frac{2}{C_1 M_L^2} |h_n - h|^2 \int_0^t ||u(\xi)||_{\mathcal{V}}^2 \, d\xi + \frac{C_1}{2} \int_0^t ||u(\xi) - u_n(\xi)||_{\mathcal{V}}^2 \, d\xi
\end{aligned}
$$

where $||\cdot||_\infty$ is the $C(\Omega)$ norm. Combining like terms we see

$$
\begin{aligned}
&||u(t) - u_n(t)||_{\mathcal{H}}^2 + C_1 \int_0^t ||u(\xi) - u_n(\xi)||_{\mathcal{V}}^2 \, d\xi \\
&\qquad \leq \left(\frac{2}{C_1 R_L^2} ||k_n - k||_\infty^2 + \frac{2}{C_1 M_L^2} |h_n - h|^2\right) \int_0^t ||u(\xi)||_{\mathcal{V}}^2 \, d\xi.
\end{aligned}
$$

If we define $G_n(T)$ by

$$
G_n(T) = \left(\frac{2}{C_1 R_L^2} ||k_n - k||_\infty^2 + \frac{2}{C_1 M_L^2} |h_n - h|^2\right) ||u||_{L^2(0,T;\mathcal{V})}
$$

and recall $k_n \to k$ in $C(\Omega)$, $h_n \to h$ and $u \in L^2(0, T; \mathcal{V})$, we see $G_n(T) \to 0$. Thus

$$
||u(t) - u_n(t)||_{\mathcal{H}}^2 + \frac{C_1}{2} \int_0^t ||u(\xi) - u_n(\xi)||_{\mathcal{V}}^2 \, d\xi \leq G_n(T) \tag{24}
$$

and so as $n \to \infty$, $u \to u_n$ in $C(0, T; \mathcal{H})$ and in $L^2(0, T; \mathcal{V})$. Thus the solution depends continuously on the parameters k and h. We actually have proved the somewhat stronger result:

Theorem 3.4 *The mapping $(k,h) \to u(\,\cdot\,;k,h)$, where $u(\,\cdot\,;k,h)$ is a weak solution to (20) is Lipschitz continuous from $C(\Omega) \times \mathbb{R}_1^+$ to $C(0,T;\mathcal{H}) \cap L^2(0,T;\mathcal{V})$.*

3.3.2 Continuous Dependence on ρ and c_p

As before, let $g = \rho c_p$ and define a sequence $\{g_n\}$ such that $g_n \to g$ uniformly in z, i.e., in $C(\Omega)$. Thus we know by (2) for N sufficiently large, there exist constants $\bar{R}_L > 0$ and $\bar{R}_U < \infty$ such that for N sufficiently large, $g_n(z) \in [\bar{R}_L, \bar{R}_U]$, $g(z) \in [\bar{R}_L, \bar{R}_U]$ holds for all $n \geq N$ and all $z \in \Omega$. Without loss of generality, from hereafter we assume all n will satisfy $n \geq N$.

Let $\mathcal{H}_n = H^1(\Omega)$ with the weighted inner product $\langle \cdot, \cdot \rangle_{\mathcal{H}_n} = \langle g_n \cdot, \cdot \rangle_{L^2}$. Note the $\mathcal{H}_n$ norm is equivalent to the $\mathcal{H}$ norm uniformly in n and there are finite, positive constants J_L, J_U such that

$$J_L ||\phi||_{\mathcal{H}}^2 \leq ||\phi||_{\mathcal{H}_n}^2 \leq J_U ||\phi||_{\mathcal{H}}^2 \tag{25}$$

for all n. Define $\mathcal{V}_n = H^1(\Omega)$ with inner product

$$\langle \phi, \psi \rangle_{\mathcal{V}_n} = \langle \nabla\phi, \nabla\psi \rangle_{\mathcal{H}_n} + \langle \phi, \psi \rangle_{L^2}$$

which has equivalent representation

$$\langle \phi, \psi \rangle_{\mathcal{V}_n} \cong \langle \nabla\phi, \nabla\psi \rangle_{\mathcal{H}_n} + \int_{\gamma_2} h(Tr_2\ \phi)(z)(Tr_2\ \psi)(z)\ dS_2$$

by Theorem 3.1.

Suppose $u(\,\cdot\,;g)$ is a solution of

$$\begin{cases} \dot{u} + Au = F \\ u(0) = u_0 \end{cases} \tag{26}$$

in $\mathcal{V}^*$ and suppose $u_n(\,\cdot\,;g_n)$ is a solution of

$$\begin{cases} \dot{u}_n + A_n u_n = F_n \\ u_n(0) = u_0 \end{cases} \tag{27}$$

in $\mathcal{V}_n^*$ where

$$\langle A_n\phi, \psi\rangle_{\mathcal{V}_n^*,\mathcal{V}_n} = \sigma_n(\phi,\psi) = \langle \frac{1}{g_n} k\nabla\phi, \nabla\psi\rangle_{\mathcal{H}_n} + h\int_{\gamma_2} (Tr_2\ \phi)(z)(Tr_2\ \psi)(z)\ dS_2$$

and

$$\langle F_n(t)\phi, \psi\rangle_{\mathcal{V}_n^*,\mathcal{V}_n} = \langle F(t)\phi, \psi\rangle_{\mathcal{V}^*,\mathcal{V}}.$$

for all $\psi \in \mathcal{V}_n \cong \mathcal{V}$.

Subtracting the weak form of (27) from (26) we obtain

$$\begin{aligned}\langle \dot{u}(t), \psi\rangle_{\mathcal{V}^*,\mathcal{V}} - &\langle \dot{u}_n(t), \psi\rangle_{\mathcal{V}_n^*,\mathcal{V}_n} + \sigma(u(t),\psi) - \sigma_n(u_n(t),\psi)\\ &= \langle F(t), \psi\rangle_{\mathcal{V}^*,\mathcal{V}} - \langle F_n(t),\psi\rangle_{\mathcal{V}_n^*,\mathcal{V}_n}\end{aligned}$$

for all $\psi \in \mathcal{V}$. Thus

$$\begin{aligned}\langle \dot{u}(t),\psi\rangle_{\mathcal{V}^*,\mathcal{V}} &- \langle \dot{u}_n(t), \psi\rangle_{\mathcal{V}_n^*,\mathcal{V}_n} + \langle \frac{1}{g} k\nabla u(t), \nabla\psi\rangle_{\mathcal{H}}\\ &+ h\int_{\gamma_2} (Tr_2\ u(t))(z)(Tr_2\ \psi)(z)\ dS_2 - \langle \frac{1}{g_n} k\nabla u_n(t), \nabla\psi\rangle_{\mathcal{H}_n}\\ &- h\int_{\gamma_2} (Tr_2\ u_n(t))(z)(Tr_2\ \psi)(z)\ dS_2 = 0\end{aligned}$$

and hence

$$\begin{aligned}\langle \dot{u}(t),\psi\rangle_{\mathcal{V}^*,\mathcal{V}} &- \langle \dot{u}_n(t), \psi\rangle_{\mathcal{V}_n^*,\mathcal{V}_n} + \langle k\nabla u(t), \nabla\psi\rangle_{L^2}\\ &+ h\int_{\gamma_2} (Tr_2\ u(t))(z)(Tr_2\ \psi)(z)\ dS_2 - \langle k\nabla u_n(t), \nabla\psi\rangle_{L^2}\\ &- h\int_{\gamma_2} (Tr_2\ u_n(t))(z)(Tr_2\ \psi)(z)\ dS_2 = 0\end{aligned}$$

for all $\psi \in \mathcal{V}$. Define $\tilde{\sigma}$ by

$$\tilde{\sigma}(\phi,\psi) = \langle k\nabla\phi, \nabla\psi\rangle_{L^2} + h\int_{\gamma_2} (Tr_2\ \phi)(z)(Tr_2\ \psi)(z)\ dS_2$$

and note $\tilde{\sigma}$ is $\mathcal{V}$-coercive satisfying $\tilde{\sigma}(\phi,\phi) \geq C_2||\phi||_{\mathcal{V}}$ where

$$C_2 = \min\{R_U^{-1}K_L, h\}M_U^{-1}.$$

Adding and subtracting terms we see

$$\langle \dot{u}(t), \psi\rangle_{\mathcal{V}^*,\mathcal{V}} - \langle \dot{u}(t), \psi\rangle_{\mathcal{V}_n^*,\mathcal{V}_n} + \langle \dot{u}(t) - \dot{u}_n(t), \psi\rangle_{\mathcal{V}_n^*,\mathcal{V}_n} + \tilde{\sigma}(u(t) - u_n(t), \psi) = 0.$$

Fix $t \in [0, T]$ and let $\psi = u(t) - u_n(t)$ in the previous equation. Thus

$$\frac{1}{2}\frac{d}{dt}\{||u(t) - u_n(t)||^2_{\mathcal{H}_n}\} + \tilde{\sigma}(u(t) - u_n(t), u(t) - u_n(t))$$
$$= \langle \frac{g_n}{g}\dot{u}(t) - \dot{u}(t), u(t) - u_n(t)\rangle_{\mathcal{V}^*,\mathcal{V}}$$

and hence integrating from 0 to t we obtain

$$||u(t) - u_n(t)||^2_{\mathcal{H}_n} + 2\int_0^t \tilde{\sigma}(u(\xi) - u_n(\xi), u(\xi) - u_n(\xi))\ d\xi$$
$$= 2\int_0^t \langle(\frac{g_n}{g} - 1)\dot{u}(\xi), u(t) - u_n(t)\rangle_{\mathcal{V}^*,\mathcal{V}}\ d\xi.$$

Since the $\mathcal{H}_n$ norm is equivalent to the $\mathcal{H}$ norm uniformly in n, using (25) we can rewrite this equation as

$$J_L||u(t) - u_n(t)||^2_{\mathcal{H}} + 2\int_0^t \tilde{\sigma}(u(\xi) - u_n(\xi), u(\xi) - u_n(\xi))\ d\xi$$
$$\leq 2\int_0^t |\langle(\frac{g_n}{g} - 1)\dot{u}(\xi), u(t) - u_n(t)\rangle_{\mathcal{V}^*,\mathcal{V}}|\ d\xi.$$

Using the fact that $\tilde{\sigma}$ is $\mathcal{V}$-coercive on the left side of the equation, and the Cauchy Schwartz inequality and the relation $2ab \leq a^2 + b^2$ on the right side, we see

$$J_L||u(t) - u_n(t)||^2_{\mathcal{H}} + 2C_2\int_0^t ||u(\xi) - u_n(\xi)||^2_{\mathcal{V}}\ d\xi$$

$$\leq 2\int_0^t ||(\frac{g_n}{g} - 1)\dot{u}(\xi)||_{\mathcal{V}^*}||u(\xi) - u_n(\xi)||_{\mathcal{V}}\ d\xi$$

$$\leq \frac{1}{C_2}\int_0^t ||(\frac{g_n}{g} - 1)\dot{u}(\xi)||^2_{\mathcal{V}^*}\ d\xi + C_2\int_0^t ||u(\xi) - u_n(\xi)||^2_{\mathcal{V}}\ d\xi.$$

Combining like terms we see

$$J_L||u(t) - u_n(t)||^2_{\mathcal{H}} + C_2\int_0^t ||u(\xi) - u_n(\xi)||^2_{\mathcal{V}}\ d\xi \leq \frac{1}{C_2}\int_0^t ||\frac{g_n}{g} - 1||^2_{\infty}||\dot{u}(\xi)||^2_{\mathcal{V}^*}\ d\xi.$$

Let $G_n(T)$ be defined by

$$G_n(T) = \frac{1}{C_2}||\frac{g_n - g}{g}||^2_\infty ||\dot{u}||_{L^2(0,T;\mathcal{V}^*)}$$

and note $G_n(T) \to 0$ since $g_n \to g$ in $C(\Omega)$ and $\dot{u} \in L^2(0,T;\mathcal{V}^*)$. Hence we have

$$J_L||u(t) - u_n(t)||^2_{\mathcal{H}} + C_2 \int_0^t ||u(\xi) - u_n(\xi)||^2_{\mathcal{V}}\, d\xi \leq G_n(T)$$

and so $u_n \to u$ in $C(0,T;\mathcal{H})$ and in $L^2(0,T;\mathcal{V})$. Thus the solution depends Lipschitz continuously on the parameters ρ and c_p. We have proved the following theorem:

Theorem 3.5 *The mapping $g \to u(\,\cdot\,; g)$, where $u(\,\cdot\,; g)$ is a solution to (26) is Lipschitz continuous from $C(\Omega)$ to $C(0,T;\mathcal{H}) \cap L^2(0,T;\mathcal{V})$.*

4 Formulation of the Inverse Problem

4.1 Preliminaries

For $\{t_i\}_{i=1}^n \subset [0,T]$, $T < \infty$, we can find (weak) solutions $u(t_i)$ to (1) for $1 \leq i \leq n < \infty$. From the solutions $\{u(t_i, z)\}_{i=1}^n$ we can compute the average temperature change between consecutive time steps at the heat sink interface (boundary γ_2). We define the average temperature change from t_{i-1} to t_i by

$$T_i = \frac{1}{|\gamma_2|}\int_{\gamma_2} Tr_2\ (u(t_i) - u(t_{i-1}))(z)\, dS_2 \tag{28}$$

for $i = 2, \ldots, n$. Recall Tr_2 is the continuous trace operator from $H^1(\Omega) \to H^{\frac{1}{2}}(\gamma_2)$ defined by $(Tr_2\ f)(z) = f(z)|_{\gamma_2}$. We choose to look at the data this way in order to relate our model data to our experimental data.

Before using the experimental data we have collected in our parameter estimation problem, we first used generated data for proof of concept. We generated data by solving (1) at the eight times corresponding to our data with the parameter values from Table 1. We call these solutions $\hat{u}(t_1, z),\ \hat{u}(t_2, z),\ \ldots,\ \hat{u}(t_8, z)$. We define the vector of average temperature changes $\hat{T} = [\hat{T}_2\ \hat{T}_3\ \cdots\ \hat{T}_8]$ where

$$\hat{T}_j = \frac{1}{|\gamma_2|}\int_{\gamma_2} Tr_2\ (\hat{u}(t_j) - \hat{u}(t_{j-1}))(z)\ dS_2$$

for $2 \leq j \leq 8$. Furthermore, we define $T(q)$ to be the vector generated by the solution using the specified parameter (or parameters) q, which we will denote $u(t, z; q)$, and (28), i.e.,

$$T_j(q) = \frac{1}{|\gamma_2|}\int_{\gamma_2} Tr_2\ (u(t_j; q) - u(t_{j-1}; q))(z)\ dS_2$$

for $2 \leq j \leq 8$ and $T(q) = [T_2(q)\ T_3(q)\ \cdots\ T_8(q)]$. We will assume any unspecified parameters are given by the values in Table 1.

We first tried to estimate a constant value for the thermal conductivity of the aluminum particles (for examples with uniformly distributed particles of equal size) that best matched our generated data. This parameter estimation problem was unsuccessful even in this simplest of cases. In comparison, we were successful in estimating the constant value for the thermal conductivity of the silicone polymer that best matched our generated data. These results were not surprising, however, when the graphs of the cost functions for the parameter identification were plotted as a function of the parameter. The cost function for the particle parameter was jagged with no clear minimum, whereas the cost function for the silicone parameter was smooth with a clearly defined minimum. For further information on our constant parameter estimation problem see [8] and for general inverse problems see [3, 4, 5].

4.2 Estimating the Thermal Conductivity Parameters as Random Variables

The theoretical basis of this approach can be found in [1] (see also [9, 12]). While this formulation allows us to estimate the distributions for both of the thermal conductivity parameters, k_p and k_s, at the same time, we will estimate them individually here. We first assume the parameter k_p is a realization for a normally distributed random variable with mean μ_p and variance σ_p^2 and attempt to estimate its distribution. For now, we will hold all other parameters constant. In order to ensure all values in the distribution for k_p are positive we will use a truncated Gaussian distribution and require $\mu_p - 3\sigma_p > 0$. Thus the probability density function for the random variable is given by

$$f(x) = \frac{1}{0.9974\,\sigma_p\sqrt{2\pi}}\, e^{-(x-\mu_p)^2/2\sigma_p^2} \tag{29}$$

for $x \in [\mu_p - 3\sigma_p, \mu_p + 3\sigma_p]$. If we define $q_p = (\mu_p, \sigma_p)$, we can define the expected value of T by

$$\mathcal{E}[T(t_i; q_p)|P_p] = \int_{\mu_p-3\sigma_p}^{\mu_p+3\sigma_p} T(t_i; x)\frac{1}{0.9974\,\sigma_p\sqrt{2\pi}}\, e^{-(x-\mu_p)^2/2\sigma_p^2}\, dx$$

where P_p is the probability distribution function arising from (29) with mean μ_p and variance σ_p^2. Thus the "best fit" parameter q_p^* is the solution to the least squares problem

$$\min_{q_p\in Q} J(P_p, \hat{T}) \equiv \min_{q_p\in Q} J(P_p) \equiv \min_{q_p\in Q} \sum_{i=1}^{n} |\mathcal{E}[T(t_i; q_p)|P_p] - \hat{T}_i|^2 \tag{30}$$

where $Q = \mathbb{R}^+ \times \mathbb{R}^+$ with the additional restriction $\mu_p - 3\sigma_p > 0$.

For proof of concept, we used the same generated data described in Section 4.1. While we realize the data was not generated with k_p normally distributed, we would consider a successful parameter estimation to have the mean of the distribution near the true value for k_p and small standard deviation. We carried out numerous estimation trials and in Table 2 we present values for two of these minimizations of (30). We used Matlab's constrained minimization routine `fmincon`. The function `fmincon` uses a Sequential Quadratic Programming method. The three main steps of this algorithm are the solving of a Quadratic Programming subproblem, the updating of the Hessian matrix of the Lagrangian solution, and the calculation of a merit function and line search. A complete description of this method can be found in [15].

The initial guess is denoted by $q_{p_0} = (\mu_{p_0}, \sigma_{p_0})$ and the best parameter fit found by Matlab is denoted by $q_p^* = (\mu_p^*, \sigma_p^*)$. For all of these minimizations, $n = 5$ in (30).

In all our tests, the mean of the "best fit" distribution did not closely resemble the actual parameter value, $k_p = 217$ and the standard deviation was not small. In all cases, the optimal parameters are not far from the initial guesses. While we used a relatively small number

μ_{p_0}	σ_{p_0}	$J(q_{p_0})$	μ_p^*	σ_p^*	$J(q_p^*)$
1000	100	0.0197193	1242.66	297.228	0.0153633
250	50	0.0391095	250.001	50.0005	0.0391080

Table 2: Estimating distribution of k_p

for n and a constant distribution, we would still expect better results if the inverse problem were well behaved.

In contrast, suppose we instead view k_s as a realization for a normally distributed random variable and estimate μ_s and σ_s for the distribution. As before we used a truncated Gaussian to ensure all possible values are positive, with probability density function

$$f(x) = \frac{1}{0.9974\,\sigma_s\sqrt{2\pi}}\, e^{-(x-\mu_s)^2/2\sigma_s^2} \tag{31}$$

for $x \in [\mu_s - 3\sigma_s, \mu_s + 3\sigma_s]$, $\mu_s - 3\sigma_s > 0$. If we define $q_s = (\mu_s, \sigma_s)$, we can define

$$\mathcal{E}[T(t_i; q_s)|P_s] = \int_{\mu_s - 3\sigma_s}^{\mu_s + 3\sigma_s} T(t_i; x) \tfrac{1}{0.9974\,\sigma_s\sqrt{2\pi}}\, e^{-(x-\mu_s)^2/2\sigma_s^2}\, dx$$

where P_s is the probability distribution function arising from (31) with mean μ_s and variance σ_s^2. Thus the "best fit" parameter q_s^* is the solution to the least squares problem

$$\min_{q_s \in Q} J(P_s, \hat{T}) \equiv \min_{q_s \in Q} J(P_s) \equiv \min_{q_s \in Q} \sum_{i=1}^{n} |\mathcal{E}[T(t_i; q_s)|P_s] - \hat{T}_i|^2 \tag{32}$$

where $Q = \mathbb{R}^+ \times \mathbb{R}^+$ with the additional restriction $\mu_p - 3\sigma_p > 0$.

In Table 3 we see values for one minimization of (32) (again we carried out multiple tests, obtaining similar results). We used Matlab and the generated data as before. The initial guess is denoted by $q_{s_0} = (\mu_{s_0}, \sigma_{s_0})$ and the best parameter fit found by Matlab by $q_s^* = (\mu_s^*, \sigma_s^*)$. For all of these minimizations, $n = 5$ in (32).

In this example, note the mean μ_s^* of the distribution is very close to the actual value of $k_s = 0.12$ W/mK used to generate the data and the standard deviation is small. This indicates that despite the fact we are using a small number for n, the parameter estimation algorithm performs well when estimating k_s (or its distribution).

μ_{s_0}	σ_{s_0}	$J(q_{s_0})$	μ_s^*	σ_s^*	$J(q_S^*)$
1	0.25	19.294	0.12036	2.5087e-05	1.4140e-02

Table 3: Estimating distribution of k_s

5 Sensitivity Equations

In the previous section we found that small changes in the parameter for the thermal conductivity of the particles, k_p, seem to have little impact on the solution $u(t, z)$. In contrast, small changes in the thermal conductivity of the silicone, k_s, appear to significantly change the solution $u(t, z)$. Sensitivity equations allow us to anticipate and quantify how changes in the parameters affect changes in the solutions. Thus, we turn to sensitivity equations to investigate whether k_p and k_s are, in fact, influencing the solutions as we suspect. Readers are referred [19, 20, 21, 22] for more information on sensitivity equation methods and their use in inverse problem methodology.

5.1 An Abstract Derivation in Terms of Fréchet Derivatives

In order to derive the sensitivity equations, we must formally differentiate our system of equations, including the boundary conditions, and then interchange the order of differentiation. Before explicitly following this procedure, we first present a framework that rigorously justifies the derivation. This derivation relies on the Implicit Function Theorem and a corollary to the Implicit Function Theorem, both of which we state here.

Theorem 5.1 (Implicit Function Theorem) *[7, Theorem 3.1.10, p.115] Let X, Y, and Z be Banach spaces. Suppose $f(x, y)$ is a continuous mapping of a neighborhood U of (x_0, y_0) in $X \times Y$ into Z, $f(x_0, y_0) = 0$ and $f_y(x_0, y_0)$ exists, is continuous in x, and is a linear homeomorphism of Y onto Z. Then there is a unique continuous mapping g defined in a neighborhood U_1 of x_0, $g : U_1 \to Y$, such that $g(x_0) = y_0$ and $f(x, g(x)) = 0$ for $x \in U_1$.*

Corollary 5.2 *[7, Corollary 3.1.11, p.115] If, in addition to the hypothesis of the Implicit Function Theorem, $f_x(x, y)$ exists and is continuous for (x, y) near (x_0, y_0), then the function*

$g(x)$ is continuously differentiable for $x \in U_1$ and

$$g'(x) = -[f_y(x, g(x))]^{-1} f_x(x, g(x)). \tag{33}$$

A proof of Theorem 5.1 and Corollary 5.2 can be found in [7].

In Section 3.2 we found there exists a unique weak solution to

$$\begin{cases} \dot{u} + Au = F \\ u(0) = u_0 \end{cases} \tag{34}$$

where F is defined in (9) and A is given by (8). Without loss of generality, we assume $u(0) = 0$. (If not use a simple change of variables, $\hat{u} = u - u(0)$.) We are interested in examining the sensitivity of these solutions with respect to the thermal conductivity parameter k, or, more specifically, with respect to parameters q in a parameterization $k(q)$ of the thermal conductivity. Let Q be the space of all possible parameter values, $\mathcal{Y} = L^2(0, T; \mathcal{V}^*)$ and $\mathcal{U} = L^2(0, T; \mathcal{V}) \cap H^1(0, T; \mathcal{V}^*)$. The norm on $\mathcal{U}$ is given by

$$||v||^2_{\mathcal{U}} = ||v||^2_{L^2(0,T;\mathcal{V})} + ||v||^2_{H^1(0,T;\mathcal{V}^*)}$$

for $v \in \mathcal{U}$ (see [13, p. 102]).

Note F as defined in (9) does not depend on q. The thermal conductivity does depend on q, $k = k(q) : Q \to \mathbb{R}$ and so by (8) we have $A = A(q) : Q \to \mathscr{L}(\mathcal{V}, \mathcal{V}^*)$, with

$$\langle A(q)\phi, \psi\rangle_{\mathcal{V}^*,\mathcal{V}} = \langle \frac{1}{g} k(q) \nabla\phi, \nabla\psi\rangle_{\mathcal{H}} + h \int_{\gamma_2} (Tr_2\ \phi)(z)(Tr_2\ \psi)(z)\ dS_2$$

for $\phi, \psi \in \mathcal{V}$. Thus for each $q \in Q$ there is an associated weak solution $u(\,\cdot\,; q) \in \mathcal{U}$.

Define $M : Q \to \mathscr{L}(\mathcal{U}, \mathcal{Y})$ by

$$[M(q)]v = \dot{v} + A(q)v.$$

Since (34) possesses a unique solution for each $F \in L^2(0, T; \mathcal{V}^*)$, we see that $M(q)$ is invertible for each $q \in Q$. Note also $M(q)$ is linear in v, i.e., $[M(q)](v_1 + v_2) = [M(q)]v_1 + [M(q)]v_2$. Define $N : Q \to \mathcal{Y}$ by

$$N(q) = F.$$

Finally, define $G : \mathcal{U} \times Q \to \mathcal{Y}$ by

$$G(u, q) = ([M(q)]u) - [N(q)],$$

and associate $u(\,\cdot\,; q)$ with the pair $(u(\,\cdot\,; q), q)$ satisfying $G(u(\,\cdot\,; q), q) = 0$ in the $\mathcal{Y} = L^2(0, T; \mathcal{V}^*)$ sense. Note G induces a natural mapping from Q to $\mathcal{U}$ given by $q \mapsto u(\,\cdot\,; q)$. Also, $u \mapsto G(u(\cdot, q), q)$ is an affine map from $\mathcal{U}$ to $\mathcal{Y}$.

Fix $q_0 \in Q$ and let $u_0 \equiv u_0(\,\cdot\,; q_0) \in \mathcal{U}$. In order to characterize the sensitivity at q_0 we need the operator $D_q u(q_0) \in \mathscr{L}(Q, \mathcal{U})$. We assume $(u_0, q_0) \equiv (u_0(\,\cdot\,; q_0), q_0)$ satisfies $G(u_0, q_0) = 0$ in the $\mathcal{Y} = L^2(0, T; \mathcal{V}^*)$ sense.

Lemma 5.3 *The partial Fréchet derivative $\partial_u G(u_0, q_0) : \mathcal{U} \to \mathcal{Y}$ exists and is given by $\partial_u G(u_0, q_0) = M(q_0) \in \mathscr{L}(\mathcal{U}, \mathcal{Y})$.*

Proof: For $h \neq 0 \in \mathcal{U}$,

$$\begin{aligned}
&||G(u_0 + h, q_0) - G(u_0, q_0) - M(q_0)h||_{\mathcal{Y}} \\
&\qquad = ||[M(q_0)](u_0 + h) - [N(q_0)] - ([M(q_0)]u_0 - [N(q_0)]) - [M(q_0)]h||_{\mathcal{Y}} \\
&\qquad = ||[M(q_0)]h - [M(q_0)]h||_{\mathcal{Y}} \\
&\qquad = 0.
\end{aligned}$$

We assume the function $k : Q \to \mathbb{R}$ is Fréchet differentiable at q_0 and so we define $\mathscr{M} : Q \to \mathscr{L}(Q, \mathscr{L}(\mathcal{U}, \mathcal{Y}))$ by

$$[\mathscr{M}(q_0)u] = \mathscr{A}(q_0)u$$

where $\mathscr{A} : Q \to \mathscr{L}(Q, \mathscr{L}(\mathcal{V}, \mathcal{V}^*))$ is given by

$$\langle \mathscr{A}(q_0)\phi, \psi \rangle_{\mathcal{V}^*, \mathcal{V}} = \langle \frac{1}{g} D_q k(q_0) \nabla \phi, \nabla \psi \rangle_{\mathcal{H}}$$

for $\phi, \psi \in \mathcal{V}$. Note that $k : Q \to \mathbb{R}$ and so $D_q k(q_0) \in \mathscr{L}(Q, \mathbb{R})$.

Let $\mathscr{X} = \mathscr{L}(\mathcal{U}, \mathcal{Y})$. Since $\mathcal{Y}$ and $\mathcal{U}$ are Banach spaces, $\mathscr{X}$ is a Banach space as well. Thus we can define a norm on $\mathscr{X}$ by

$$||T||_{\mathscr{X}} = \sup_{||v||_{\mathcal{U}} = 1} ||Tv||_{\mathcal{Y}}$$

for $T \in \mathscr{X}$. Recall for $\zeta \in \mathcal{V}^*$

$$||\zeta||_{\mathcal{V}^*} = \sup_{||\psi||_{\mathcal{V}}=1} \langle \zeta, \psi \rangle_{\mathcal{V}^*,\mathcal{V}}$$

and for $\phi \in \mathcal{V}$

$$||\phi||_{\mathcal{V}}^2 = ||\nabla\phi||_{\mathcal{H}}^2 + ||\phi||_{L^2}^2.$$

Recall from (2) that g is positive and finite and note that for any $\phi \in \mathcal{V}$,

$$\begin{aligned} ||\nabla\phi||_{L^2(\Omega)}^2 &= \langle \nabla\phi, \nabla\phi \rangle_{L^2(\Omega)} \\ &= \langle \frac{1}{g} \cdot g\nabla\phi, \nabla\phi \rangle_{L^2(\Omega)} \\ &= \langle \frac{1}{g}\nabla\phi, \nabla\phi \rangle_{\mathcal{H}} \\ &\leq R_L^{-1} ||\nabla\phi||_{\mathcal{H}}^2 \\ &\leq R_L^{-1} ||\phi||_{\mathcal{V}}^2 \end{aligned}$$

and so $||\nabla\phi||_{L^2(\Omega)} \leq \sqrt{R_L^{-1}}\, ||\phi||_{\mathcal{V}}$.

Lemma 5.4 *M is Fréchet differentiable at q_0, with $[\mathscr{M}(q_0)u]h = [D_q M(q_0)h]u$. Furthermore, $\mathscr{M}(q_0)$ is a bounded linear operator.*

Proof: For $h \neq 0 \in Q$ we want to show

$$\lim_{h\to 0} \frac{1}{||h||_Q} ||M(q_0+h) - M(q_0) - [\mathscr{M}(q_0)]h||_{\mathscr{X}} = 0.$$

By definition of the norm in $\mathscr{X}$,

$$||M(q_0+h) - M(q_0) - [\mathscr{M}(q_0)]h||_{\mathscr{X}} = \sup_{||u||_{\mathcal{U}}=1} ||[M(q_0+h)u - M(q_0)u - [\mathscr{M}(q_0)u]h]||_{\mathcal{Y}}.$$

For any $u \in \mathcal{U}$ with $||u||_{\mathcal{U}} = 1$,

$$||[M(q_0+h)u - M(q_0)u - [\mathscr{M}(q_0)u]h]||_{\mathcal{Y}}^2$$

$$= \int_0^T ||([M(q_0+h)]u)(t) - ([M(q_0)]u)(t) - ([\mathscr{M}(q_0)u]h)(t)||_{\mathcal{V}^*}^2 \, dt$$

$$= \int_0^T ||\dot{u}(t) + A(q_0+h)u(t) - [\dot{u}(t) + A(q_0)u(t)] - \mathscr{A}(q_0)u(t)h||_{\mathcal{V}^*}^2 \, dt$$

$$= \int_0^T \sup_{||\psi||_{\mathcal{V}}=1} \langle A(q_0+h)u(t) - A(q_0)u(t) - \mathscr{A}(q_0)u(t)h, \psi\rangle_{\mathcal{V}^*,\mathcal{V}}^2 \, dt$$

$$= \int_0^T \sup_{||\psi||_{\mathcal{V}}=1} \langle \frac{1}{g}k(q_0+h)\nabla u(t) - \frac{1}{g}k(q_0)\nabla u(t) - \frac{1}{g}D_q k(q_0)h\nabla u(t), \nabla\psi\rangle_{\mathcal{H}}^2 \, dt$$

$$\leq \int_0^T \sup_{||\psi||_{\mathcal{V}}=1} ||k(q_0+h) - k(q_0) - D_q k(q_0)h||_\infty^2 \, \langle \nabla u(t), \nabla\psi\rangle_{L^2(\Omega)}^2 \, dt$$

$$\leq \sup_{||\psi||_{\mathcal{V}}=1} ||k(q_0+h) - k(q_0) - D_q k(q_0)h||_\infty^2 \, ||\nabla\psi||_{L^2(\Omega)}^2 \int_0^T ||\nabla u(t)||_{L^2(\Omega)}^2 \, dt$$

$$\leq \sup_{||\psi||_{\mathcal{V}}=1} ||k(q_0+h) - k(q_0) - D_q k(q_0)h||_\infty^2 \, R_L^{-1} \, ||\psi||_{\mathcal{V}}^2 \int_0^T R_L^{-1}||u(t)||_{\mathcal{V}}^2 \, dt$$

$$= ||k(q_0+h) - k(q_0) - D_q k(q_0)h||_\infty^2 \, R_L^{-2} \, ||u||_{L^2(0,T;\mathcal{V})}^2$$

$$\leq ||k(q_0+h) - k(q_0) - D_q k(q_0)h||_\infty^2 \, R_L^{-2} \, ||u||_{\mathcal{U}}^2$$

Thus

$$||M(q_0+h) - M(q_0) - [\mathscr{M}(q_0)]h||_{\mathscr{X}} \leq ||k(q_0+h) - k(q_0) - D_q k(q_0)h||_\infty \, R_L^{-1}.$$

We know

$$\lim_{h\to 0} \frac{1}{||h||_Q} ||k(q_0+h) - k(q_0) - D_q k(q_0)h||_\infty = 0$$

since we assume k is Fréchet differentiable. Thus

$$\lim_{h\to 0} \frac{1}{||h||_Q} ||M(q_0+h) - M(q_0) - [\mathscr{M}(q_0)]h||_{\mathscr{X}} = 0$$

and so M is Fréchet differentiable with $D_q M = \mathscr{M}$ and $\mathscr{M}(q_0) \in \mathscr{L}(Q, \mathscr{L}(\mathcal{U},\mathcal{Y})) = \mathscr{L}(Q,\mathscr{X})$.

Lemma 5.5 *If $D_q N(q_0) : Q \to \mathcal{Y}$ and $D_q M(q_0) : Q \to \mathscr{L}(\mathcal{U}, \mathcal{Y})$ exist in the Fréchet sense, then the partial derivative of G with respect to Q at (u_0, q_0) exists and $[\partial_q G(u_0, q_0)] \in \mathscr{L}(Q, \mathcal{Y})$ is given by*

$$[\partial_q G(u_0, q_0)] = \mathscr{M}(q_0)u_0 - D_q N(q_0).$$

Proof: By Lemma 5.4, $D_q M(q_0) = \mathscr{M}(q_0) \in \mathscr{L}(Q, \mathscr{L}(\mathcal{U}, \mathcal{Y}))$. Since $N(q_0)$ has no dependence on q, $D_q N(q_0)$ is the zero operator and so $D_q N(q_0) \in \mathscr{L}(Q, \mathcal{Y})$. Thus $\mathscr{M}(q_0)u_0 - D_q N(q_0) \in \mathscr{L}(Q, \mathcal{Y})$.

For $h \neq 0 \in Q$,

$$\begin{aligned} ||G(u_0, q_0 + h) - &G(u_0, q_0) - [\mathscr{M}(q_0)u_0 - D_q N(q_0)]h||_{\mathcal{Y}} \\ &= ||[M(q_0 + h)]u_0 - N(q_0 + h) - ([M(q_0)]u_0 - N(q_0)]) \\ &\qquad - ([D_q M(q_0)h]u_0 - D_q N(q_0)h||_{\mathcal{Y}} \\ &\leq ||M(q_0 + h) - M(q_0) - D_q M(q_0)h||_{\mathscr{X}} ||u_0||_{\mathcal{U}} \\ &\qquad + ||N(q_0 + h) - N(q_0) - D_q N(q_0)h||_{\mathcal{Y}} \end{aligned}$$

Since $D_q M(q_0)$ exists in the Fréchet sense,

$$\lim_{h \to 0} \frac{1}{||h||_Q} ||M(q_0 + h) - M(q_0) - D_q M(q_0)h||_{\mathscr{X}} = 0.$$

Moreover, since N has no dependence on q,

$$N(q_0 + h) - N(q_0) - D_q N(q_0)h \equiv 0.$$

Thus

$$\lim_{h \to 0} \frac{1}{||h||_Q} ||G(u_0, q_0 + h) - G(u_0, q_0) - [\mathscr{M}(q_0)u_0 - D_q N(q_0)]h||_{\mathcal{Y}} = 0$$

and so $[\partial_q G(u_0, q_0)] = \mathscr{M}(q_0)u_0 - D_q N(q_0)$.

Theorem 5.6 *Let Q_0 be a subset of the interior of Q and let $\mathcal{U}_0$ be a subset of the interior of $\mathcal{U}$. Fix $q_0 \in Q_0 \subset Q$. Suppose there exists a unique $u_0(\,\cdot\,; q_0) \in \mathcal{U}_0 \subset \mathcal{U}$ such that $G(u_0(\,\cdot\,; q_0), q_0) = 0$. If $[M(q_0)]^{-1}$ exists in $\mathscr{L}(\mathcal{Y}, \mathcal{U})$ and if $D_q M(q_0) = \mathscr{M}(q_0)$ and $D_q N(q_0)$*

exist in the Fréchet sense in $\mathscr{L}(Q,\mathscr{X})$ *and* $\mathscr{L}(Q,\mathcal{Y})$ *respectively, then the sensitivity operator,* $s \equiv D_q u(\,\cdot\,; q_0) \in \mathscr{L}(Q,\mathcal{U})$*, exists and satisfies*

$$M(q_0)s = -\mathscr{M}(q_0)u_0 + D_q N(q_0)$$

<u>Proof</u>: In the Implicit Function Theorem 5.1, we set $X = Q$, $Y = \mathcal{U}$, and $Z = \mathcal{Y}$. The function $f(x,y)$ in Theorem 5.1 is our $G(u,q)$, and by assumption $G(u_0,q_0) = 0$. By Lemma 5.3, we know $\partial_u G(u_0,q_0) \in \mathscr{L}(\mathcal{U},\mathcal{Y})$. Since $M(q)$ is invertible for each $q \in Q$, $[M(q_0)]^{-1} \in \mathscr{L}(\mathcal{Y},\mathcal{U})$. Thus $u(\,\cdot\,,q)$ satisfies $G(u(\,\cdot\,,q),q) = 0$ for $q \in Q_0$.

By Lemma 5.5, we know $\partial_q G(u_0,q_0) \in \mathscr{L}(Q,\mathcal{Y})$. Furthermore, by Lemma 5.4 we know $D_q M(q_0) = \mathscr{M}(q_0)$ and so by Corollary 5.2, $M(q_0)s = -\mathscr{M}(q_0)u_0 + D_q N(q_0)$. In fact, since $D_q N(q_0)$ is the zero operator, $M(q_0)s = -\mathscr{M}(q_0)u_0$.

5.2 Sensitivity to the Particle Thermal Conductivity

5.2.1 Derivation of Sensitivity Equations

In Section 3.1 we established the system (1) has a weak solution $u(t,z)$. If we assume the thermal conductivity is dependent on the parameter q, then $q \mapsto k(z;q)$ is given by

$$k(z;q) = \begin{cases} \bar{q}_s & z \in \Omega_s \\ q_p & z \in \Omega_p. \end{cases} \tag{35}$$

We want to consider the thermal properties of the composite silicone as we hold the constant $\bar{q}_s$ fixed and let the constant q_p vary over a range of admissible material values. Thus any weak solution of (1) will have the form $u(t,z;q)$. By studying the sensitivity of the solution u to changes in q_p, we can study the sensitivity of the system to the thermal conductivity of the particles.

In order to derive the sensitivity equations, we will formally differentiate (1) with respect to q_p, interchange the order of differentiation and define the sensitivity. Our analysis in Section 5.1 guarantees the existence of these derivatives and that the resulting sensitivity equation can be rigorously interpreted in terms of an associated weak or variational system.

First, formally differentiating $g(z)\dot{u}(t,z) = \nabla \cdot (k(z)\nabla u(t,z))$ with respect to q_p yields

$$g(z)\frac{\partial}{\partial q_p}(\dot{u}(t,z;q)) = \frac{\partial}{\partial q_p}(\nabla \cdot (k(z;q)\nabla u(t,z;q))).$$

Switching the order of differentiation we see

$$g(z)\frac{\partial}{\partial t}(\frac{\partial u}{\partial q_p}(t,z;q)) = \nabla \cdot (\frac{\partial k}{\partial q_p}(z;q)\nabla u(t,z;q)) + \nabla \cdot (k(z;q)\nabla \frac{\partial u}{\partial q_p}(t,z;q)).$$

If we then define the *sensitivity to* q_p as $s(t,z;q) = \frac{\partial u}{\partial q_p}(t,z;q)$ and substitute into the previous equation we have

$$g(z)\dot{s}(t,z;q) = \nabla \cdot (\frac{\partial k}{\partial q_p}(z;q)\nabla u(t,z;q)) + \nabla \cdot (k(z;q)\nabla s(t,z;q)).$$

It is also necessary to differentiate the boundary conditions with respect to q_p. To do this, note

$$\begin{aligned}\frac{\partial}{\partial q_p}(k(z;q)\frac{\partial u}{\partial n}(t,z;q)) &= \frac{\partial k}{\partial q_p}(z;q)\frac{\partial u}{\partial n}(t,z;q) + k(z;q)\frac{\partial}{\partial n}(\frac{\partial u}{\partial q_p}(t,z;q)) \\ &= k(z;q)\frac{\partial s}{\partial n}(t,z;q) + \frac{\partial k}{\partial q_p}(z;q)\frac{\partial u}{\partial n}(t,z;q).\end{aligned}$$

We will assume the source flux S_0 and the initial condition Υ are independent of q_p.

It is important to note that

$$\frac{\partial k}{\partial q_p}(z;q) = \begin{cases} 0 & z \in \Omega_s \\ 1 & z \in \Omega_p \end{cases}$$

and so $\frac{\partial k}{\partial q_p}(z;q) \in L^\infty(\Omega)$. Furthermore, $\frac{\partial k}{\partial q_s}(z;q) = 0$ since we are holding $q_s = \bar{q}_s$ fixed. Since $q = (q_p, q_s)$, $D_q k(q) = (\frac{\partial k}{\partial q_p}, \frac{\partial k}{\partial q_s}) = (\frac{\partial k}{\partial q_p}, 0)$. Also, since $u \in L^2(0,T;\mathcal{V})$, we know $\nabla u \in L^2(0,T;L^2(\Omega)^2)$. Then if we define

$$f(t,z;q) = \frac{\partial k}{\partial q_p}(z;q)\nabla u(t,z;q), \tag{36}$$

we have $f(\cdot,\cdot;q) \in L^2(0,T;L^2(\Omega)^2)$.

Thus we formally have the following system for our sensitivity equation:

$$\begin{cases} g(z)\dot{s}(t,z;q) = \nabla\cdot(k(z;q)\nabla s(t,z;q)) + \nabla\cdot f(t,z;q) \\ k(z;q)\frac{\partial s}{\partial n}(t,z;q)|_{\gamma_4} = -\frac{\partial k}{\partial q_p}(z;q)\frac{\partial u}{\partial n}(t,z;q)|_{\gamma_4} \\ k(z;q)\frac{\partial s}{\partial n}(t,z;q)|_{\gamma_2} = -(\frac{\partial k}{\partial q_p}(z;q)\frac{\partial u}{\partial n}(t,z;q) + hs(t,z;q))|_{\gamma_2} \\ k(z;q)\frac{\partial s}{\partial n}(t,z;q)|_{\gamma_1} = -\frac{\partial k}{\partial q_p}(z;q)\frac{\partial u}{\partial n}(t,z;q)|_{\gamma_1} \\ k(z;q)\frac{\partial s}{\partial n}(t,z;q)|_{\gamma_3} = -\frac{\partial k}{\partial q_p}(z;q)\frac{\partial u}{\partial n}(t,z;q)|_{\gamma_3} \\ s(0,z;q) = 0 \end{cases} \tag{37}$$

Note the solution $u(t,z;q)$ to (1) acts as part of the forcing term f on the solution to (37).

5.2.2 Weak Solution to Sensitivity Equation

We refer to the spaces H, V, $\mathcal{H}$, and $\mathcal{V}$ defined in Section 3.1.1. Define a sesquilinear form $\beta : \mathcal{V}\times\mathcal{V}\to\mathbb{R}$ by

$$\beta(\phi,\psi) = \langle\frac{1}{g}k\nabla\phi,\nabla\psi\rangle_{\mathcal{H}} + h\int_{\gamma_2}(Tr_2\ \phi)(z)(Tr_2\ \psi)(z)\ dS_2 \tag{38}$$

and note β defines an operator $\mathcal{A}\in\mathscr{L}(\mathcal{V},\mathcal{V}^*)$ where $\langle\mathcal{A}\phi,\psi\rangle_{\mathcal{V}^*,\mathcal{V}} = \beta(\phi,\psi)$. We observe that $\beta = \beta(q)$ is just the parameter dependent sesquilinear form σ of (8) and $\mathcal{A} = \mathcal{A}(q)$ is the analog of A generated by σ.

Define $\mathcal{F} : [0,T]\to\mathcal{V}^*$ by

$$[\mathcal{F}(t)](\psi) = \langle -\frac{1}{g}f,\nabla\psi\rangle_{\mathcal{H}} \tag{39}$$

where f is given in (36). We shall see shortly that $\mathcal{A}$ and $\mathcal{F}$ are the operators we need to find the weak or variational form of (37).

Suppose s solves

$$\dot{s} + \mathcal{A}s = \mathcal{F} \qquad \text{in } \mathcal{V}^*,$$

i.e., for all $\psi\in\mathcal{V}$,

$$\langle\dot{s}(t) + \mathcal{A}s(t) - \mathcal{F}(t),\psi\rangle_{\mathcal{V}^*,\mathcal{V}} = 0.$$

By definition

$$\langle \dot{s}(t) + \mathcal{A}s(t), \psi \rangle_{\mathcal{V}^*,\mathcal{V}} = \langle \mathcal{F}(t), \psi \rangle_{\mathcal{V}^*,\mathcal{V}}$$

and thus

$$\begin{aligned}\langle \dot{s}(t), \psi \rangle_{\mathcal{V}^*,\mathcal{V}} =& \langle -\frac{1}{g} k \nabla s(t), \nabla \psi \rangle_{\mathcal{H}} - h \int_{\gamma_2} (Tr_2\ s(t))(z)(Tr_2\ \psi)(z)\ dS_2 \\ &+ \langle -\frac{1}{g} f(t), \nabla \psi \rangle_{\mathcal{H}}.\end{aligned} \tag{40}$$

Note that the result in Theorem 5.6 says the sensitivity operator, s, satisfies $M(q)s = -\mathscr{M}(q)u$, i.e.,

$$\dot{s}(t) + A(q)s(t) = -\mathscr{A}(q)u,$$

which by definition is

$$\begin{aligned}\langle \dot{s}(t), \psi \rangle_{\mathcal{V}^*,\mathcal{V}} + & \langle \frac{1}{g} k \nabla s(t), \nabla \psi \rangle_{\mathcal{H}} + h \int_{\gamma_2} (Tr_2\ s(t))(z)(Tr_2\ \psi)(z)\ dS_2 \\ &= \langle -\frac{1}{g} D_q k(q) \nabla u(t), \nabla \psi \rangle_{\mathcal{H}}.\end{aligned}$$

Clearly this is equivalent to (40) and hence our formal and rigorous derivations result in the same system.

Returning to equation (40), we see it is equivalent to

$$\begin{aligned}\langle \dot{s}(t), \psi \rangle_{\mathcal{V}^*,\mathcal{V}} =& \langle -k \nabla s(t), \nabla \psi \rangle_{L^2} - h \int_{\gamma_2} (Tr_2\ s(t))(z)(Tr_2\ \psi)(z)\ dS_2 \\ &+ \langle -f(t), \nabla \psi \rangle_{L^2}\end{aligned}$$

by the definition of the $\mathcal{H}$-norm.

Now, if $s \in L^2(0,T;V)$, $k\nabla s \in L^2(0,T;V)$, and $f \in L^2(0,T;V)$, using the Divergence Theorem and the identity

$$\nabla \cdot (k(z) \nabla s(t,z) \psi(z)) = (\nabla \cdot (k(z) \nabla s(t,z)) \psi(z) + k(z)(\nabla s(t,z) \cdot \nabla \psi(z))$$

in the previous equation, we see

$$\langle \dot{s}(t), \psi \rangle_{\mathcal{V}^*,\mathcal{V}} = \langle \nabla \cdot (k \nabla s(t)), \psi \rangle_{L^2} - \int_{\partial\Omega} (Tr_\Omega\ (n \cdot k \nabla s(t)))(z)(Tr_\Omega\ \psi)(z)\ dS$$

$$- h \int_{\gamma_2} (Tr_2\ s(t))(z)(Tr_2\ \psi)(z)\ dS_2$$
$$- \int_{\partial\Omega} (Tr_\Omega\ (n \cdot f(t)))(z)(Tr_\Omega\ \psi)(z)\ dS + \langle \nabla \cdot f(t), \psi \rangle_{L^2}$$

where Tr_Ω is the continuous trace operator mapping $f \in H^1(\Omega) \to H^{\frac{1}{2}}(\partial\Omega)$ with $(Tr_\Omega\ f)(z) = f(z)|_{\partial\Omega}$.

If we have enough smoothness on s with respect to the time derivative (i.e., $\dot{s} \in L^2(0, T; \mathcal{H})$) then

$$\langle \dot{s}(t), \psi \rangle_{\mathcal{V}^*, \mathcal{V}} = \langle \dot{s}(t), \psi \rangle_{\mathcal{H}} = \langle g\dot{s}(t), \psi \rangle_{L^2}$$

and so

$$\begin{aligned} \langle g\dot{s}(t) - &\nabla \cdot (k\nabla u(t)) - \nabla \cdot f(t), \psi \rangle_{L^2} = \\ &- \int_{\partial\Omega} (Tr_\Omega\ n \cdot (k\nabla s(t) - \frac{\partial k}{\partial q_p} \nabla u(t)))(z)(Tr_\Omega\ \psi)(z)\ dS \\ &\qquad - h \int_{\gamma_2} (Tr_2\ s(t))(z)(Tr_2\ \psi)(z)\ dS_2 \end{aligned} \tag{41}$$

for all $\psi \in \mathcal{V}$. We know (41) holds for all $\psi \in \mathcal{V} = H^1(\Omega)$, thus for all $\psi \in H_0^1(\Omega)$,

$$\langle g\dot{s}(t) - \nabla \cdot (k\nabla u(t)) - \nabla \cdot f(t), \psi \rangle_{L^2} = 0.$$

Since $H_0^1(\Omega)$ is a dense subset of $L^2(\Omega)$, we know

$$g\dot{s}(t) - \nabla \cdot (k\nabla u(t)) - \nabla \cdot f(t) = 0$$

in the L^2 sense. Thus we can rewrite (41) as

$$\begin{aligned} &- \int_{\partial\Omega} (Tr_\Omega\ n \cdot (k\nabla s(t) - \frac{\partial k}{\partial q_p} \nabla u(t)))(z)(Tr_\Omega\ \psi)(z)\ dS \\ &\qquad - h \int_{\gamma_2} (Tr_2\ s(t))(z)(Tr_2\ \psi)(z)\ dS_2 = 0. \end{aligned} \tag{42}$$

We know $\partial\Omega = \gamma_1 \cup \gamma_2 \cup \gamma_3 \cup \gamma_4$. Thus for $\psi \in H_{\gamma_1} \equiv \{\phi \in H^1(\Omega) : \phi|_{\gamma_2,\gamma_3,\gamma_4} = 0\} \subset H^1(\Omega)$, by (42) we see

$$- \int_{\gamma_1} (Tr_1\ n \cdot (k\nabla s(t) + \frac{\partial k}{\partial q_p} \nabla u))(z)(Tr_1\ \psi)(z)\ dS_1 = 0$$

and so $k(z)\frac{\partial s}{\partial n}(t,z)|_{\gamma_1} = -\frac{\partial k}{\partial q_p}(z)\frac{\partial u}{\partial n}(t,z)|_{\gamma_1}$. A similar argument shows $k(z)\frac{\partial s}{\partial n}(t,z)|_{\gamma_3} = -\frac{\partial k}{\partial q_p}(z)\frac{\partial u}{\partial n}(t,z)|_{\gamma_3}$ and $k(z)\frac{\partial s}{\partial n}(t,z)|_{\gamma_4} = -\frac{\partial k}{\partial q_p}(z)\frac{\partial u}{\partial n}(t,z)|_{\gamma_4}$.

For $\psi \in H_{\gamma_2} \equiv \{\phi \in H^1(\Omega) : \phi|_{\gamma_1,\gamma_3,\gamma_4} = 0\} \subset H^1(\Omega)$, using (42) we see

$$-\int_{\gamma_2} (Tr_2\ n \cdot (k\nabla s(t) + \frac{\partial k}{\partial q_p}\nabla u))(z)(Tr_2\ \psi)(z)\ dS_2 \\ - h\int_{\gamma_2} (Tr_2\ s(t))(z)(Tr_2\ \psi)(z)\ dS_2 = 0$$

and thus $k(z)\frac{\partial s}{\partial n}(t,z)|_{\gamma_2} = -(\frac{\partial k}{\partial q_p}(t,z)\frac{\partial u}{\partial n}(t,x) + hs(t,z))|_{\gamma_2}$. Thus if s satisfies (40), and f and s have sufficient additional regularity, s provides a strong solution to (37).

Thus (40) is the weak or variational form of (37), and hence any solution s of (40) (if it exists) is a weak solution of (37).

5.2.3 Well-Posedness

We next establish existence of solutions to parabolic systems of the form

$$\begin{cases} \dot{s} + \mathcal{A}s = \mathcal{F} \quad \text{in } \mathcal{V}^* \\ s(0) = s_0. \end{cases} \tag{43}$$

We use the Gelfand triple $\mathcal{V} \hookrightarrow \mathcal{H} \cong \mathcal{H}^* \hookrightarrow \mathcal{V}^*$ as in Section 3.2. Since β defined in (38) is equivalent to σ defined in (8), we know β is $\mathcal{V}$-bounded and $\mathcal{V}$-coercive uniformly in $q \in Q$. We also observe that the forcing term $\mathcal{F}$ defined in (39) satisfies

$$\mathcal{F} \in L^2(0,T;\mathcal{V}^*). \tag{44}$$

In order to see that (44) holds, recall $f \in L^2(0,T;L^2(\Omega)^2)$. Thus $\mathcal{F}(t) : \mathcal{V} \to \mathbb{R}$ and is linear, i.e., $\mathcal{F}(t) \in \mathcal{V}^*$ and so $\mathcal{F} \in L^2(0,T;\mathcal{V}^*)$.

Given the above hypothesis, the weak or variational form of the system (43) is

$$\begin{cases} \langle \dot{s}(t), \psi\rangle + \beta(s(t),\psi) = \langle \mathcal{F}(t),\psi\rangle \\ u(0) = u_0 \end{cases} \tag{45}$$

for $\psi \in \mathcal{V}$ and $\langle\,\cdot\,,\,\cdot\,\rangle$ is $\langle\,\cdot\,,\,\cdot\,\rangle_{\mathcal{V}^*,\mathcal{V}}$. Note the system (43) is the same as (45).

At this point, existence, uniqueness, and continuous dependence on the forcing function follow using an argument analogous to the arguments in Section 3.2. Thus the sensitivity system is well-posed.

5.2.4 Matlab Solutions

Using Matlab's PDE Toolbox, we are able to numerically solve the sensitivity equation system. Since we are interested in the temperature of the composite silicone at the heat sink interface, i.e., the γ_2 boundary, we are interested in the sensitivity at the heat sink interface as a function of q_p. Recall that in our model we assume the particles never touch any boundary of the composite silicone. (A reasonable assumption based on the properties of the silicone polymer.) Thus $\frac{\partial k}{\partial q_p}(z;q)|_{\gamma_j} = 0$ for $j = 1, 2, 3, 4$ and we can reduce (37) to

$$\begin{cases} g(z)\dot{s}(t,z;q) = \nabla \cdot (k(z;q)\nabla s(t,z;q)) + \nabla \cdot f(t,z;q) \\ k(z;q)\frac{\partial s}{\partial n}(t,z;q)|_{\gamma_4} = 0 \\ k(z;q)\frac{\partial s}{\partial n}(t,z;q)|_{\gamma_2} = -hs(t,z;q)|_{\gamma_2} \\ k(z;q)\frac{\partial s}{\partial n}(t,z;q)|_{\gamma_1} = 0 \\ k(z;q)\frac{\partial s}{\partial n}(t,z;q)|_{\gamma_3} = 0 \\ s(0,z;q) = 0 \end{cases} \tag{46}$$

To solve (46), we first fix a value for q_p and solve (1). Then with that solution we can solve (46) with the same fixed value of q_p. We will define the average sensitivity at the boundary γ_2 for a fixed q_p at time t_i by

$$s_2(t_i;q_p) = \frac{1}{|\gamma_2|}\int_{\gamma_2} Tr_2 \; s(t_i;q_p)(z) \; dS_2 \tag{47}$$

where Tr_2 is again the continuous trace operator from $H^1(\Omega) \to H^{\frac{1}{2}}(\gamma_2)$ defined by $(Tr_2 \; f)(z) = f(z)|_{\gamma_2}$. Repeating this process for different values of $q_p \in Q$, we can then define the relative average sensitivity to the thermal conductivity of the particles by

$$s_{2r}(t_i;q_p) = \frac{s_2(t_i;q_p)}{\max_{q_p\in Q}(s_2(t_i;q_p))}.$$

We fix $k_s = \bar{q}_s = 0.12$ W/mK. The remainder of the parameters are given in Table 1.

In Figure 4 we depict the plots of $s_{2r}(t_i; q_p)$ as a function of q_p. We let $q_p = 100, 110, \ldots, 1100$ and solve at each of the times t_2, t_3, t_4, and t_5 (similar graphs for t_6, t_7, and t_8 are found in [8]). Note that as a function of q_p, there is little variation in the relative average sensitivity along the heat sink interface at each time step. In contrast, in Section 5.3.2 we present plots of the relative average sensitivity with respect to the thermal conductivity of the silicone, and find that there is a substantial variation in the sensitivity as a function of q_s. Thus, based on our results in this section and in Section 5.3.2, we conclude the solution u to (1) is not very sensitive to the thermal conductivity of the particles.

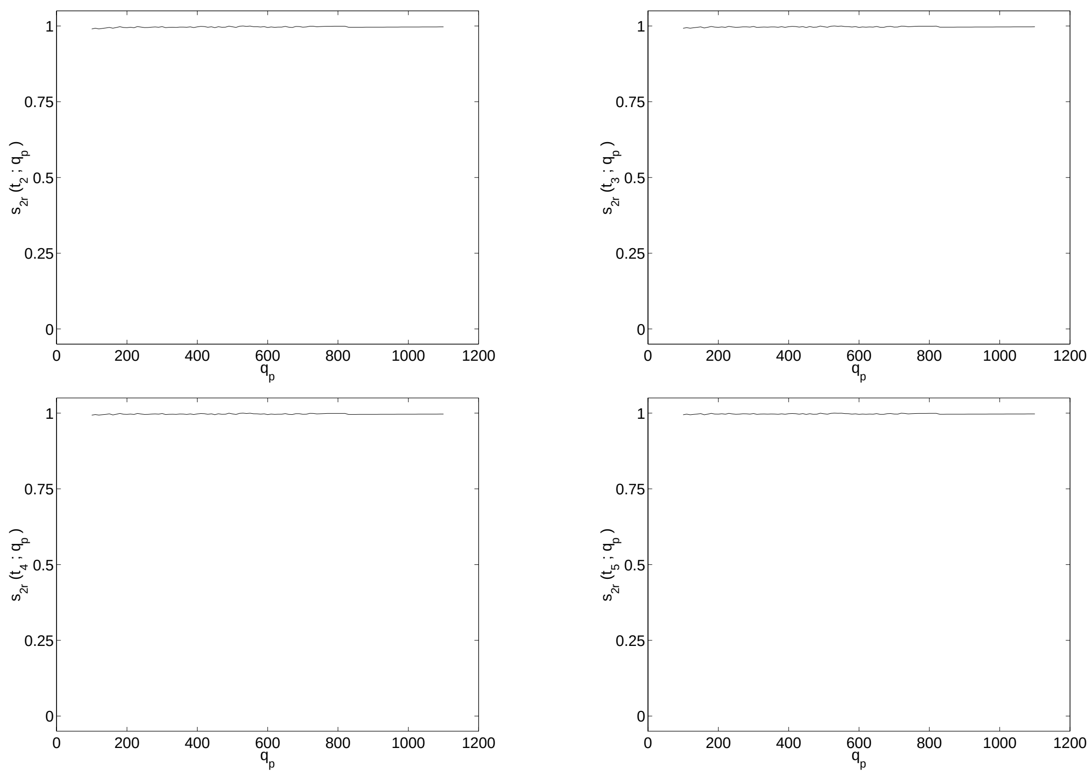

Figure 4: Relative average sensitivity at γ_2 at times t_2, t_3, t_4, and t_5 as a function of q_p

5.3 Sensitivity to the Silicone Polymer Thermal Conductivity

5.3.1 Derivation of Sensitivity Equations

We again begin with (1), and now we assume the thermal conductivity $k(z)$ is given by

$$k(z;q) = \begin{cases} q_s & z \in \Omega_s \\ \bar{q}_p & z \in \Omega_p \end{cases}$$

where $\bar{q}_p$ is a constant, and q_s is varied in a range of admissible values. Any weak solution of (1) will again have the form $u(t,z;q)$. In order to derive the sensitivity equations we will differentiate (1) with respect to q_s.

The differentiation follows in a manner similar to the differentiation in Section 5.2.1. We will define the *sensitivity to* q_s as $w(t,z;q) = \frac{\partial u}{\partial q_s}(t,z;q)$. We will again assume the source flux S_0 and the initial condition Υ are independent of q_s.

It is important to note that

$$\frac{\partial k}{\partial q_s}(z;q) = \begin{cases} 1 & z \in \Omega_s \\ 0 & z \in \Omega_p \end{cases}$$

and hence $\frac{\partial k}{\partial q_s}(z;q) \in L^\infty(\Omega)$. Furthermore, $\frac{\partial k}{\partial q_p}(z;q) = 0$ since we are holding $q_p = \bar{q}_p$ fixed. Thus, since $q = (q_p, q_s)$, $D_q k(q) = (\frac{\partial k}{\partial q_p}, \frac{\partial k}{\partial q_s}) = (0, \frac{\partial k}{\partial q_s})$. Recall $u \in L^2(0,T;\mathcal{V})$, and hence $\nabla u \in L^2(0,T;L^2(\Omega)^2)$. Then if we define

$$f_s(t,z;q) = \frac{\partial k}{\partial q_s}(z;q)\nabla u(t,z;q)$$

we have $f_s(\cdot,\cdot;q) \in L^2(0,T;L^2(\Omega)^2)$.

Thus we formally have the following system for our sensitivity equation:

$$\begin{cases} g(z)\dot{w}(t,z;q) = \nabla \cdot (k(z;q)\nabla w(t,z;q)) + \nabla \cdot f_s(t,z;q) \\ k(z;q)\frac{\partial w}{\partial n}(t,z;q)|_{\gamma_4} = -\frac{\partial k}{\partial q_s}(z;q)\frac{\partial u}{\partial n}(t,z;q)|_{\gamma_4} \\ k(z;q)\frac{\partial w}{\partial n}(t,z;q)|_{\gamma_2} = -(\frac{\partial k}{\partial q_s}(z;q)\frac{\partial u}{\partial n}(t,z;q) + hw(t,z;q))|_{\gamma_2} \\ k(z;q)\frac{\partial w}{\partial n}(t,z;q)|_{\gamma_1} = -\frac{\partial k}{\partial q_s}(z;q)\frac{\partial u}{\partial n}(t,z;q)|_{\gamma_1} \\ k(z;q)\frac{\partial w}{\partial n}(t,z;q)|_{\gamma_3} = -\frac{\partial k}{\partial q_s}(z;q)\frac{\partial u}{\partial n}(t,z;q)|_{\gamma_3} \\ w(0,z;q) = 0. \end{cases} \tag{48}$$

Using an argument analogous to the arguments in Section 5.2.2 and Section 5.2.3 it can be shown there exists a unique weak solution w to (48) and that the problem is well-posed.

5.3.2 Matlab Solutions

As in Section 5.2.4 we can use Matlab to solve the sensitivity equation (48) for different values of q_s. Since we assume the particles never touch any boundary of the composite silicone, $\frac{\partial k}{\partial q_s}|_{\gamma_j} = 1$ for $j = 1, 2, 3, 4$ and therefore we can reduce (48) to

$$\begin{cases} g(z)\dot{w}(t,z;q) = \nabla \cdot (k(z;q)\nabla w(t,z;q)) + \nabla \cdot f_s(t,z;q) \\ k(z;q)\frac{\partial w}{\partial n}(t,z;q)|_{\gamma_4} = -S_0(t) \\ k(z;q)\frac{\partial w}{\partial n}(t,z;q)|_{\gamma_2} = -(h(T_\infty - u(t,z;q)) + hw(t,z;q))|_{\gamma_2} \\ k(z;q)\frac{\partial w}{\partial n}(t,z;q)|_{\gamma_1} = 0 \\ k(z;q)\frac{\partial w}{\partial n}(t,z;q)|_{\gamma_3} = 0 \\ w(0,z;q) = 0. \end{cases} \tag{49}$$

We fix $k_p = \bar{q}_p = 217$ W/mK. The remaining parameters are given in Table 1. In order to implement the boundary condition for γ_2 in the PDE Toolbox, we will use the average value of $u(t,z;q)$ on γ_2 for $u(t,z;q)$ in $k(z;q)\frac{\partial w}{\partial n}(t,z;q)|_{\gamma_2} = -(h(T_\infty - u(t,z;q)) + hw(t,z;q))|_{\gamma_2}$.

As in Section 5.2.4, we define the average sensitivity at the boundary γ_2 for a fixed q_s at time t_i by

$$w_2(t_i;q_s) = \frac{1}{|\gamma_2|}\int_{\gamma_2} Tr_2\ w(t_i;q_s)(z)\ dS_2 \tag{50}$$

where $w(t_i;q_s)$ is the solution to (49) at t_i for a given q_s and fixed q_p. Repeating this process for different values of $q_s \in Q$, we can then define the relative average sensitivity to the thermal conductivity of the silicone by

$$w_{2r}(t_i;q_s) = \frac{w_2(t_i;q_s)}{\max_{q_s\in Q}(w_2(t_i;q_s))}.$$

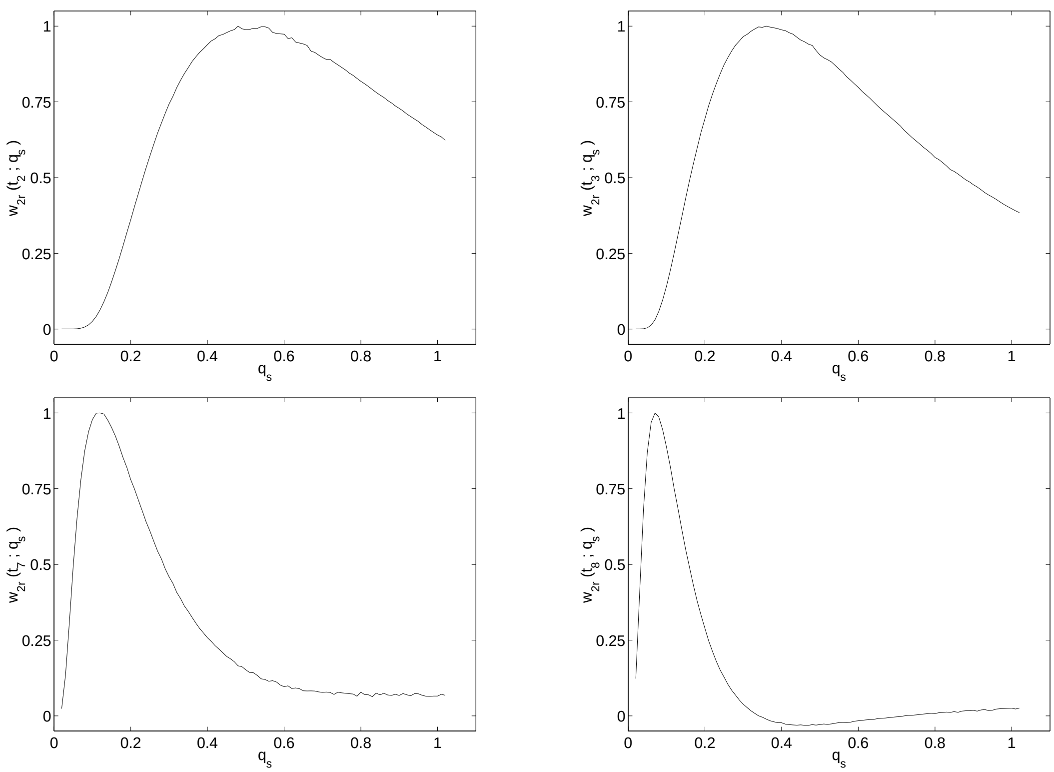

Figure 5: Relative average sensitivity at γ_2 at times t_2, t_3, t_7, and t_8 as a function of q_s

In Figure 5 we present several plots of $w_{2r}(t_i;q_s)$ as a function of q_s. We solved (49) with $q_s = 0.02, 0.02, \ldots, 1.02$ at each of the times $t_2, t_3, \ldots, t_8$. In each these graphs it clear that as a function of q_s there is significant variation along the heat sink interface. Thus we conclude the solution u to (1) exhibits significant sensitivity to changes in the thermal conductivity of the silicone. Also, we note the significant difference between the graphs presented here and those in Section 5.2.4. Based on these results, increasing the thermal conductivity of the particles should not result in much improvement of the overall thermal conductivity of the composite. (We remark that this agrees with initial experimental findings.) Clearly the composite is more sensitive to the thermal conductivity of the base material. Thus a better means of improving the overall thermal conductivity of the composite is to increase the thermal conductivity of the base polymer used in the composite.

6 Conclusions

We have presented analysis of a two dimensional model based on the composite silicone and the data collection process. We summarized numerical findings using Matlab's PDE Toolbox for our two dimensional model. Matlab's PDE Toolbox allowed us to accommodate the oscillatory coefficients in a variety of particle geometries. (In [8] results for various particle geometries, including random and uniform geometries, were presented in some detail.) It was found that the geometry of the composite silicone has a significant impact on the heat flux at the interface between the heat sink and the composite. In this paper we have given theoretical results for general geometries and some numerical findings for the special case of a uniform geometry.

We have given existence and uniqueness theorems based on our two dimensional model, and have shown the model depends continuously on parameters, as well as the initial data and forcing function. We have presented a formulation and numerical results for two different parameter estimation problems: estimating parameters as constants and estimating parameters as realizations of random variables. Estimating parameters as realizations of random variables used a probability based approach, and we have provided a careful theoretical framework for this approach in a separate reference [1]. All of these results readily hold for the corresponding three dimensional model.

We carried out several numerical experiments. In each of our parameter estimation formulations (using simulated data for proof of concept) in two dimensions, with a uniform geometry, we were able to accurately estimate the thermal conductivity of the silicone, but not the thermal conductivity of the aluminum filler particles.

After deriving the sensitivity equations, we studied the sensitivity of model solutions to both the thermal conductivity of the particles and the thermal conductivity of the silicone. Our numerical results clearly indicated the solution is significantly more sensitive to the thermal conductivity of the silicone than to the thermal conductivity of the particles. This supported our results from the parameter estimation and experimental findings to date. Thus, in order to significantly increase the thermal conductivity of the composite silicone (or any composite adhesive), we suggest it is best to work at increasing the thermal conductivity of the base silicone (or base adhesive). However, we believe there is still a great deal to learn about thermally conductive adhesives using the methodology in this paper with variable particle geometries.

While we have not presented the results in this paper, we note that as an alternative to using Matlab's PDE Toolbox one could use the mathematical theory of homogenization. Homogenization [2, 6, 10, 17, 18, 24] combines the oscillatory coefficients into an "average" or "effective" thermal conductivity. See [8] and the above cited references for further information on this approach.

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