J. V. BECK
5/92

DERIVATION OF THE EQUATIONS FOR THE SOLUTION OF A NONLINEAR INVERSE HEAT CONDUCTION PROBLEM USING ITERATIVE REGULARIZATION

INTRODUCTION

The problem of solving for the surface heat flux, q, as a function of time, t, is solved for the nonlinear inverse heat conduction problem. The iterative regularization method of Alifanov [ ] is used. The solution requires adjoint and sensitivity problems as well as the direct problem. The adjoint boundary value problem can be derived by different ways [,]. The approach based on the analysis of Lagrangian functional stationary conditions [ ] is used. This functional is written for the problem of constraint minimization of the residual functional, S(q) with respect to q where q(t) is the desired surface heat flux. The residual functional is the integral of the square deviation between the measured and calculated temperatures at the thermosensor positions. Note that the measurements are first assumed to be continuous and that the desired heat flux is also continuous. Therefore, equations of the analyzed mathematical model play the role of constraints for calculated values of temperature.

Three problems must be solved. The first is the direct problem, the second problem is the sensitivity problem and the third problem is the adjoint problem. The direct problem involves solution of the nonlinear heat conduction equation

$$\rho c(T)\frac{\partial T}{\partial t} = \frac{\partial}{\partial x}\left(k(T)\frac{\partial T}{\partial x}\right),\ 0<x<L,\ 0<t\le t_f \tag{1}$$

$$T(x,0) = T_o(x),\ 0\le x\le L \tag{2}$$

$$-k(T(0,t))\frac{\partial T(0,t)}{\partial x} = q(t) = ? \tag{3}$$

$$\beta_1 k(T(L,t))\frac{\partial T(L,t)}{\partial x} + \beta_2 T(L,t) = q_L(t) \tag{4}$$

By assigning the different values to the parameters, β_1 and β_2, it is possible to analyze the boundary condition of the first, second and third kinds on the boundary $x=L$. The heat flux $q_L(t)$ is known. The thermal conductivity k is a function of temperature, T, and the specific heat c is also. The density ρ is assumed to be constant with T. The thickness of the body is L.

In the inverse heat conduction problem, the heat flux q(t) is unknown, but there is the additional information about the state variable T in the form of temperature history measured at a point inside of the [0,L] interval,

$$T_{meas}(d,t) = Y(t) \tag{5}$$

where d is the coordinate of thermosensor location and Y(t) is the measured temperature. The temperature could be measured at many locations inside the body but for simplicity only one is considered herein. The main equation to change will be the adjoint equation and the change to accomodate multiple interior temperatures will be given.

The q(t) function is to be estimated by minimizing the residual functional

$$S(q) = \int_0^{t_f} [Y(t) - T(d,t)]^2 dt + \alpha \int_0^{t_f} [q_{est}(t) - q(t)]^2 dt \tag{6}$$

with respect to this function. The constant α is a regularizing constant; for the iterative regularizing method it could be zero. The difficulty in minimizing Eq. (6) is that it is an integral and that q(t) is a function. The adjoint method is used to overcome these problems.

DIRECTIONAL DERIVATIVE

For the finite dimensional problem (finite number of heat flux components) the gradient of S, $\nabla S(q)$, is determined by using standard differential calculus. For the infinite dimensional problem (q(t), t is continuous), it is necessary to develop an adjoint problem to compute the gradient $\nabla S(q)$, which is needed in the minimization process.

Definition of $\nabla S(q)$

The gradient of the functional S(q), at q(t), denoted $\nabla S(q)$, is related to the variation of S at q(t) by the equation

$$S(q+\epsilon\Delta q) - S(q) = \int_0^{t_f} \nabla S(t;q(t))\epsilon\Delta q(t)dt + \textit{higher order terms} \tag{7a}$$

where ϵ is a real number and $\Delta q(t)$ is some time-variable deviation from $q(t)$.

The <u>directional</u> <u>derivative</u> of S at q(t) in the direction $\Delta q(t)$, denoted $D_{\Delta q}S(q)$, is defined by

$$D_{\Delta q}S(q) = \lim_{\epsilon \to 0} \frac{S(q+\epsilon q) - S(q)}{\epsilon} \tag{7b}$$

and is related to the gradient $\nabla S(q)$ by

$$D_{\Delta q}S(q) = \int_0^{t_f} \nabla S(t;q(t)) \Delta q(t) dt \tag{7c}$$

The units of $D_{\Delta q}$ S(q) are the same as those of S, namely, K^2-s. The units of $\nabla S(t;q(t))$ are K^2-m^2/W. In the following sections, an explicit expression for $\nabla S(t;q)$ is derived; it utilizes the solution of the sensitivity and adjoint problems.

DEFINITION OF SENSITIVITY FUNCTION

Let $\Delta T_{\epsilon \Delta q}$ be the time-and space-varying increment of temperature resulting from the change of the unknown function q(t) in the amount $\epsilon \Delta q$; that is,

$$\Delta T_{\epsilon \Delta q} = T(x,t;q+\epsilon \Delta q) - T(x,t;q) \tag{8a}$$

The directional derivative of T, $D_{\Delta q}T(q)$, evaluated at (x,t) in the direction Δq, is defined as above in connection with Eq. (7b) so that

$$D_{\Delta q}T(x,t;q(t)) = \lim_{\epsilon \to 0} \frac{T(x,t;q+\epsilon \Delta q) - T(x,t;q)}{\epsilon} \tag{8b}$$

This is also called a sensitivity function which will have the notation $\theta(x,t)$, or

$$\theta(x,t) \triangleq D_{\Delta q}T(x,t;q) \tag{8c}$$

which has the units of K. The problem defining the sensitivity function is found using the direct problem for $q + \epsilon \Delta q$ and then for q; the corresponding equations are subtracted and the limiting process defined by Eq. (8b) is applied. This is discussed further below.

DIRECT PROBLEM AS TWO LAYERS

This problem is to be solved using the Lagrange multiplier method. Before using this method for this case, it aids our thinking to divide the body into two regions, from x = 0 to d and then from x = d to L. One can imagine a fictitious internal boundary passing the measurement point at x = d. Then the heat conduction model, Eqs. (1) - (4), can be written as a heat conduction problem for a two-layer system with ideal thermal contact between layers and both of them having the same temperature-dependent thermal properties. The describing equations are,

$$\rho c(T_1)\frac{\partial T_1}{\partial t} = \frac{\partial}{\partial x}\left(k(T_1)\frac{\partial T_1}{\partial x}\right),\ 0<x<d,\ 0<t\leq t_f \tag{9a}$$

$$\rho c(T_2)\frac{\partial T_2}{\partial t} = \frac{\partial}{\partial x}\left(k(T_2)\frac{\partial T_2}{\partial x}\right),\ d<x<L,\ 0<t<\leq t_f \tag{9b}$$

$$T_1(x,0) = T_o(x), \quad 0\leq x\leq d, \tag{10a}$$

$$T_2(x,0) = T_o(x), \quad d\leq x\leq L, \tag{10b}$$

$$-k\big(T_1(L,t)\big)\frac{\partial T_1(0,t)}{\partial x} = q(t) \tag{11}$$

$$\frac{\partial T_1(d,t)}{\partial x} = \frac{\partial T_2(d,t)}{\partial x}, \tag{12}$$

$$T_1(d,t) = T_2(d,t), \tag{13}$$

$$\beta_1 k\big(T_2(L,t)\big)\frac{\partial T_2(L,t)}{\partial x} + \beta_2 T_2(L,t) = q_L(t) \tag{14}$$

The above equations (9) -(14) are another statement of the direct problem when q(t) is known.

SENSITIVITY PROBLEM

The sensitivity problem is now found for the direct problem just given. The directional derivatives are found using the above formalism. The direct equations given by Eqs. (9) -(14) are formed with q(t) replaced q(t) + $\epsilon\Delta q$ which gives $T(x,t;q+\epsilon\Delta q)$. The equations are again used for q(t) to get T(x,t;q). Consider now the left hand side of Eq. (9a) and notice that there is a 1 subscript which is omitted for the moment. The q(t) in Eq. (11) is to be replaced by $q(t) + \epsilon\Delta q(t)$. The left hand side of Eq. (9a) with $\rho c(T(x,t;q+\epsilon\Delta q)$ expanded in a Taylor series about T(x,t;q) is

$$\rho c(T(q+\epsilon\Delta q))\frac{\partial T(q+\epsilon\Delta q)}{\partial t} \approx \left[\rho c(T(q)) + \rho\frac{dc(T(q))}{dT}\Delta T\right]\frac{\partial T(q+\epsilon\Delta q)}{\partial t} \qquad \textbf{(15a)}$$

where $\Delta T = T(q + \epsilon\Delta q) - T(q)$ and the dependence on x and t is also omitted for convenience. Now the expression for the left side of Eq. (9) with T(x,t;q) is subtracted from this equation to get after taking the limit of $\epsilon \to 0$

$$\lim_{\epsilon\to 0}\left[\frac{1}{\epsilon}\left(\rho c(T(q+\epsilon\Delta q))\frac{\partial T(q+\epsilon\Delta q)}{\partial t} - \rho c(T(q))\frac{\partial T(q)}{\partial t}\right)\right]$$

$$= \rho c(T(q))\frac{\partial\Theta}{\partial t} + \rho\frac{dc(T(q))}{dT}\frac{\partial T(q)}{\partial t}\Theta \qquad \textbf{(15b)}$$

where Eq. (8) is used. This result can be used for evaluating the right side for Eq. (9a). We can write

$$\frac{\partial}{\partial x}\left(k(T(q+\epsilon\Delta q))\frac{\partial T(q+\epsilon\Delta q)}{\partial x}\right) - \frac{\partial}{\partial x}\left(k(T(q))\frac{\partial T(q)}{\partial x}\right) =$$

$$\frac{\partial}{\partial x}\left(k(T(q+\epsilon\Delta q))\frac{\partial T(q+\epsilon\Delta q)}{\partial x} - k(T(q))\frac{\partial T(q)}{\partial x}\right) \qquad \textbf{(15c)}$$

Now use Eq. (15b) with $\rho c \to k$ and $t \to x$ to get

$$\lim_{\epsilon\to 0}\frac{1}{\epsilon}\left[\frac{\partial}{\partial x}\left(k(T(q+\epsilon\Delta q))\frac{\partial T(q+\epsilon\Delta q)}{\partial x}\right) - \frac{\partial}{\partial x}\left(k(T(q))\frac{\partial T(q)}{\partial x}\right)\right] \approx$$

$$\frac{\partial}{\partial x}\left(k(T(q))\frac{\partial\Theta}{\partial x} + \frac{dk(T(q))}{dT}\frac{\partial T(q)}{\partial x}\Theta\right) =$$

$$\frac{\partial}{\partial x}\left(k\frac{\partial\Theta}{\partial x}\right) + \frac{d^2k}{dT^2}\left(\frac{\partial T}{\partial x}\right)^2\Theta + \frac{dk}{dT}\frac{\partial^2 T}{\partial x^2}\Theta + \frac{dk}{dT}\frac{\partial T}{\partial x}\frac{\partial\Theta}{\partial x} \qquad \textbf{(15d)}$$

Using the results given by Equs. (15b) and (15d) and following the same procedure for the other equations gives

$$\rho c(T_1)\frac{\partial \Theta_1}{\partial t} = \frac{\partial}{\partial x}\left(k(T_1)\frac{\partial \Theta_1}{\partial x}\right) + \frac{dk}{dT_1}\,\frac{\partial T_1}{\partial x}\,\frac{\partial \Theta_1}{\partial x} +$$

$$\left[\frac{dk}{dT_1}\,\frac{\partial^2 T_1}{\partial x^2} + \frac{d^2k}{dT_1^2}\left(\frac{\partial T_1}{\partial x}\right)^2 - \rho\frac{dc}{dT_1}\frac{\partial T_1}{\partial t}\right]\Theta_1,$$

$$0 < x < d,\ 0 < t \le t_p \tag{16}$$

$$\rho c(T_2)\frac{\partial \Theta_2}{\partial t} = \frac{\partial}{\partial x}\left(k(T_2)\frac{\partial \Theta_2}{\partial x}\right) + \frac{dk}{dT_2}\frac{\partial T_2}{\partial x}\frac{\partial \Theta_2}{\partial x} +$$

$$\left[\frac{dk}{dT_2}\frac{\partial^2 T_2}{\partial x^2} + \frac{d^2k}{dT_2^2}\left(\frac{\partial T_2}{\partial x}\right)^2 - \rho\frac{dc}{dT_2}\frac{\partial T_2}{\partial t}\right]\Theta_2,$$

$$d < x < L,\ 0 < t \le t_p c \tag{17}$$

$$\Theta_1(x,0) = 0,\ 0 \le x \le d, \tag{18}$$

$$\Theta_2(x,0) = 0,\ d \le x \le L, \tag{19}$$

$$-k(T_1(0,t))\frac{\partial \Theta_1(0,t)}{\partial x} - \frac{dk(T_1(0,t))}{dT}\frac{\partial T_1(0,t)}{\partial x}\Theta_1(0,t) = \Delta q(t) \tag{20}$$

$$\frac{\partial \Theta_1(d,t)}{\partial x} = \frac{\partial \Theta_2(d,t)}{\partial x}, \tag{21}$$

$$\Theta_1(d,t) = \Theta_2(d,t) \tag{22}$$

$$\beta_2 k(T_2(L,t))\frac{\partial\Theta_2(L,t)}{\partial x} + \left[\beta_1\frac{\partial T_1(L,t)}{\partial x}\frac{dk(T_2(L,t))}{dT_2} + \beta_2\right]\Theta_2(L,t) = 0 \tag{23}$$

Equations (16)-(23) form the sensitivity problem. Notice that it is a linear problem for the dependent variables of $\Theta_1(x,t)$ and $\Theta_2(x,t)$ even though the direct problem is nonlinear. Also note that the nonlinearity of the direct problem (caused by temperature-dependence of the thermal conductivity and volumetric specific heat) results in additional terms being introduced into the sensitivity partial differential equations, Eqs. (16) and (17). If these properties are independent of temperature, Eqs. (16) and (17) reduce to exactly the same form as those for the direct problem. In any case the $\Delta q(t)$ term is the only nonhomogeneous term and is the driving "force" or energy term in the set of equations; if it were always zero, the solution for the sensitivity problem would be also zero.

The directional derivative of S in the direction Δq is related to the sensitivity problem by

$$D_{\Delta q}S(q) = 2\int_0^{t_f}[Y(t)-T(d,t)]\,[-\Theta(d,t)]dt + 2\alpha\int_0^{t_f}[q_{est}(t)-q(t)]\,[-\Delta q(t)]dt \tag{24}$$

LAGRANGE FUNCTIONAL

The task is now to find q(t). This is to be accomplished by minimizing the sum of squares functional, Eq. (6), by employing the Lagrange multipliers. A Lagrange multiplier is defined for each equation from Eq. (9) through Eq. (14). Each of these equations is rearranged to equal zero, multiplied by a Lagrange multiplier, integrated over the appropriate domain, and added to Eq. (24). The resulting Lagrangian is

$$L = S(q) + \int_0^{t_f}\int_0^{d}\psi_1(x,t)\left[\frac{\partial}{\partial x}\left(k(T_1)\frac{\partial T_1}{\partial x}\right) - \rho c(T_1)\frac{\partial T_1}{\partial t}\right]dxdt +$$

$$\int_0^{t_f}\int_d^{L}\psi_2(x,t)\left[\frac{\partial}{\partial x}\left(k(T_2)\frac{\partial T_2}{\partial x}\right) - \rho c(T_2)\frac{\partial T_2}{\partial t}\right]dxdt +$$

$$\int_0^{d}\eta_1(x,0)[T_1(x,0)-T_0(x)]dx + \int_d^{L}\eta_2(x,0)[T_2(x,0)-T_0(x)]dx +$$

$$\int_0^{t_f}\eta(0,t)\left[k(T_1(0,t))\frac{\partial T_1(0,t)}{\partial x} + q(t)\right]dt +$$

$$\int_0^{t_f}\eta(d,t)\left[\frac{\partial T_1(d,t)}{\partial x} - \frac{\partial T_2(d,t)}{\partial x}\right]dt +$$

$$\int_0^{t_f}\mu(d,t)\left[T_1(d,t) - T_2(d,t)\right]dt +$$

$$\int_L^{t_f}\eta(L,t)\left[\beta_1 k(T_2(L,t))\frac{\partial T_2(L,t)}{\partial x} + \beta_2 T_2(L,t) - q_L(t)\right]dt \tag{25}$$

where

$$\psi_i(x,t),\ i = 1,2;\ \eta_i(x,0),\ i = 1,2;\ \eta(0,t);\ \eta(d,t);\ \mu(d,t)\ and\ \eta(L,t),$$

are Lagrange multipliers for corresponding constraints (9) - (14).

DIRECTIONAL DERIVATIVE OF THE LAGRANGIAN

Now the objective is to derive the adjoint equations. The directional derivative of the Lagrangian functional can be derived using the definitions given above, such as Eq. (7b). Symbolically one can write

$$D_{\Delta q}L = D_{\Delta q}S(q) + D_{\Delta q}I_{pde} + D_{\Delta q}I_{ic} + D_{\Delta q}I_{bc0} + D_{\Delta q}I_{int} + D_{\Delta q}I_{bcL} \tag{26}$$

where the subscript pde denoted partial differential equation and is related to Equs. (9a,b) for T and (16) and (17) for Θ; ic is for initial condition (Equs. (10a,b), (18) and (19); bc0 is for the x = 0 boundary condition (Equs. (11) and (20)); int is for the interface conditions (Equs. (12), (13), (21) and (22)); and bcL is for the boundary condition at x = L (Equs. (14) and (23)). $D_{\Delta q}S(q)$ is given by Eq. (24). Note that the adjoint variables are not functions of the unknown q(t). Then using the sensitivity equations, the various terms in Eq. (26) are

$$D_{\Delta q}I_{pde} = \int_0^{t_f}\int_0^d \psi_1(x,t)\left\{\frac{\partial}{\partial x}\left(k(T_1)\frac{\partial\Theta_1}{\partial x}\right) + \frac{dk}{dT_1}\frac{\partial T_1}{\partial x}\frac{\partial\Theta_1}{\partial x} +\right.$$

$$\left[\frac{dk}{dT_1}\frac{\partial^2 T_1}{\partial x^2} + \frac{d^2k}{dT_1^2}\left(\frac{\partial T_1}{\partial x}\right)^2 - \rho\frac{dc}{dT_1}\frac{\partial T_1}{\partial t}\right]\Theta_1 - \rho c(T_1)\frac{\partial \Theta_1}{\partial t}\Bigg\} dxdt +$$

$$\int_0^{t_f}\int_d^L \psi_2(x,t)\Bigg\{\frac{\partial}{\partial x}\left(k(T_2)\frac{\partial \Theta_2}{\partial x}\right) + \frac{dk}{dT_2}\frac{\partial T_2}{\partial x}\frac{\partial \Theta_2}{\partial x} +$$

$$\left[\frac{dk}{dT_2}\frac{\partial^2 T_2}{\partial x^2} + \frac{d^2k}{dT_2^2}\left(\frac{\partial T_2}{\partial x}\right)^2 - \rho\frac{dc}{dT_2}\frac{\partial T_2}{\partial t}\right]\Theta_2 - \rho c(T_2)\frac{\partial \Theta_2}{\partial x}\Bigg\} dxdt \qquad (27)$$

$$D_{\Delta q}I_{ic} = \int_0^d \eta_1(x,0)\Theta_1(x,0)dx + \int_d^L \eta_2(x,0)\Theta_2(x,0)dx \qquad (28)$$

$$D_{\Delta q}I_{bc0} = \int_0^{t_f}\eta(0,t)\left[k(T_1(0,t))\frac{\partial \Theta_1(0,t)}{\partial x} + \frac{dk(T_1(0,t))}{dT_1}\frac{\partial T_1(0,t)}{\partial x}\Theta_1(0,t) + \Delta q(t)\right]dt \qquad (29)$$

$$D_{\Delta q}I_{int} = \int_0^{t_f}\eta(d,t)\left[\frac{\partial \Theta_1(d,t)}{\partial x} - \frac{\partial \Theta_2(d,t)}{\partial x}\right]dt + \int_0^{t_f}\mu(d,t)\left[\Theta_1(d,t) - \Theta_2(d,t)\right]dt \qquad (30)$$

$$D_{\Delta q}I_{bcL} = \int_0^{t_f}\eta(L,t)\left\{\beta_1 k(T_2(L,t))\frac{\partial \Theta_2(L,t)}{\partial x} + \left[\beta_1\frac{dk(T_2(L,t))}{dT_2}\frac{\partial T_2(L,t)}{\partial x} + \beta_2\right]\Theta_2(L,t)\right\}dt \qquad (31)$$

There are two almost identical parts in Eq. (27), one for $0 < x < d$ and the other for $d < x < L$. Since the same procedure is followed for both, only the first part is considered in detail. There are six basic components to the integral denoted $D_{\Delta q}\, I_{pde}$; each is considered separately. The goal is to use integration by parts so that the derivative will be on $\psi_1(x,t)$ $(or\ \psi_2(x,t))$ rather than on $\Theta_1(x,t)$ $(or\ \Theta_2(x,t))$. This procedure ultimately yields the adjoint equations. First, let us consider the first term in Eq. (27),

$$D_{\Delta q}I_{pde,1} = \int_0^{t_f}\int_0^d \psi_1(x,t)\frac{\partial}{\partial x}\left(k(T_1)\frac{\partial \Theta_1}{\partial x}\right)dxdt \qquad (32)$$

By using integration by parts, one can get

$$D_{\Delta q}I_{pde,1} = \int_0^{t_f}\left(k\psi_1\frac{\partial\Theta_1}{\partial x} - k\frac{\partial\psi_1}{\partial x}\Theta_1\right)\Big|_0^d dt + \int_0^{t_f}\int_0^d \left[k\frac{\partial^2\psi_1}{\partial x^2} + \frac{dk}{dT_1}\frac{\partial T_1}{\partial x}\frac{\partial\psi_1}{\partial x}\right]\Theta_1 dxdt \quad (33)$$

In a similar manner one can get for the second and sixth terms,

$$D_{\Delta q}I_{pde,2} = \int_0^{t_f}\int_0^d \psi_1\frac{dk}{dT_1}\frac{\partial T_1}{\partial x}\frac{\partial\Theta_1}{\partial x}\,dxdt = \int_0^{t_f}\left(\frac{dk}{dT_1}\frac{\partial T_1}{\partial x}\psi_1\Theta_1\right)\Big|_0^d dt -$$

$$\int_0^{t_f}\int_0^d \left[\frac{dk}{dT_1}\frac{\partial^2 T_1}{\partial x^2}\psi_1 + \frac{d^2k}{dT_1^2}\left(\frac{\partial T_1}{\partial x}\right)^2\psi_1 + \frac{dk}{dT_1}\frac{\partial T_1}{\partial x}\frac{\partial\psi_1}{\partial x}\right]\Theta_1\,dxdt \quad (34)$$

$$D_{\Delta q}I_{pde,6} = \int_0^d\int_0^{t_f}\rho c\psi_1\frac{\partial\Theta_1}{\partial t}\,dtdx = \int_0^d(\rho c\psi_1\Theta_1)\big|_0^{t_f}dx - \int_0^d\int_0^{t_f}\left[\rho c\frac{\partial\psi_1}{\partial t} + \rho\frac{dc}{dT_1}\frac{\partial T_1}{\partial t}\psi_1\right]\Theta_1 dtdx \quad (35)$$

The third, fourth and fifth terms of I_{pde} do not contain derivatives of Θ_1.

Substituting expressions (33) - (35) in (27) and using similar relations for the second region, one can get after cancellations

$$D_{\Delta q}I_{pde} = \int_0^{t_f}\int_0^d \left[\rho c\frac{\partial\psi_1}{\partial t} + k\frac{\partial^2\psi_1}{\partial x^2}\right]\Theta_1\,dxdt +$$

$$+ \int_0^{t_f}\int_d^L \left[\rho c\frac{\partial\psi_2}{\partial t} + k\frac{\partial^2\psi_2}{\partial x^2}\right]\Theta_2\,dxdt +$$

$$+ \int_0^{t_f}\left[k\psi_1\frac{\partial\Theta_1}{\partial x} - k\frac{\partial\psi_1}{\partial x}\Theta_1 + \frac{dk}{dT_1}\frac{\partial T_1}{\partial x}\psi_1\Theta_1\right]\Big|_0^d dt +$$

$$+ \int_0^{t_f} \left[k\psi_2 \frac{\partial \Theta_2}{\partial x} - k \frac{\partial \psi_2}{\partial x} \Theta_2 + \frac{dk}{dT_2} \frac{\partial T_2}{\partial x} \psi_2 \Theta_2 \right] \Big|_d^L dt -$$

$$- \int_0^d \left[\rho c \psi_1 \Theta_1 \right] \Big|_0^{t_f} dx - \int_d^L \left[\rho c \psi_2 \Theta_2 \right] \Big|_0^{t_f} dx \tag{36}$$

For more details, see Appendix A.

Integration by parts cannot be used for the other directional derivatives, $D_{\Delta q} I_{ic}$ through $D_{\Delta q} I_{bcL}$. The sum of expressions (24), (28), (29) and (37) is the directional derivative of the Lagrangian functional.

Now let us consider the stationary conditions of the Lagrangian functional $D_{\Delta q} L=0$. For these purposes, it is necessary to make independent coefficients in the Lagrangian functional variation equal to zero for the corresponding sensitivity functions, $\Theta_1(x,t)$, $\Theta_2(x,t)$, $\Theta_1(0,t)$, $\partial\Theta_1(0,t)/\partial x$, $\partial\Theta_2(L,t)/\partial x$, $\partial\Theta_1(d,t)/\partial x$, $\partial\Theta_2(d,t)/\partial x$, $\Theta_1(d,t)$, $\Theta_2(d,t)$, $\Theta_2(L,t)$, $\partial\Theta_2(L,t)/\partial x$, $\Theta_1(x,0)$, $\Theta_1(x,t_f)$, $\Theta_2(x,0)$ *and* $\Theta_2(x,t_f)$.
One can get after equating the coefficients equal to zero, (see Appendix B)

$$- \rho c(T_1) \frac{\partial \psi_1}{\partial t} = \frac{\partial}{\partial x} \left(k(T_1) \frac{\partial \psi_1}{\partial x} \right) - \frac{dk}{dT_1} \frac{\partial T_1}{\partial x} \frac{\partial \psi_1}{\partial x}, \quad 0<x<d, \; 0<t<t_f \tag{37}$$

$$-\rho c(T_2) \frac{\partial \psi_2}{\partial t} = \frac{\partial}{\partial x} \left(k(T_2) \frac{\partial \psi_2}{\partial x} \right) - \frac{dk}{dT_2} \frac{\partial T_2}{\partial x} \frac{\partial \psi_2}{\partial x}, \quad d<x<L, \; 0<t<t_f, \tag{38}$$

$$\psi_1(x,t_f)=0, \tag{39}$$

$$\psi_2(x,t_f)=0 \tag{40}$$

$$-k(T_1(0,t)) \frac{\partial \psi_1(0,t)}{\partial x} = 0 \tag{41}$$

$$k(T_1(d,t))\left[\frac{\partial\psi_1(d,t)}{\partial x} - \frac{\partial\psi_2(d,t)}{\partial x}\right] = -2[Y(t)-T_1(d,t)] \tag{42}$$

$$\psi_1(d,t) = \psi_2(d,t) \tag{43}$$

$$\beta_1 k(T_2(L,t))\frac{\partial\psi_2(L,t)}{\partial x} + \beta_2\psi_2(L,t) = 0 \tag{44}$$

At the interface $T_1(d,t)$ in Eq. (42) is also equal to $T_2(d,t)$. Eqs. (37) - (44) provide the adjoint problem.

This problem is also linear. Notice that the nonhomogeneous terms are only in the interface condition, Eq. (42). A very important point is that these equations for the complete adjoint problem must be solved backward in time; the initial conditions, given by Eqs. (39) and (40) are at the final time, t_f. If t is replaced by $t_f - t$, the problem becomes the usual forward one.

Another observation relates to the nonlinearity of the direct problem. Though both the sensitivity and adjoint equations are linear even if the direct problem is nonlinear, the forms of the equations are different from each other and the original direct problem. If the problem were linear, each of these would be the same. It is interesting to note that the form of the adjoint partial differential equations is included in the sensitivity problem, although the interface equations are different.

The nonhomogeneous term in Eq. (42) can be introduced into the differential equation. The effect of this term, which is caused by the difference between the calculated and measured temperatures, can be simulated by plane volume source. Then instead of solving the problem in two parts, it can be solved in one part and have one ψ in the solution. The resulting adjoint problem is then equivalently written as

$$-\rho c(T)\frac{\partial\psi}{\partial t} = \frac{\partial}{\partial x}\left(k(T)\frac{\partial\psi}{\partial x}\right) - \frac{\partial k}{\partial T}\frac{\partial T}{\partial x}\frac{\partial\psi}{\partial x} + 2(T(x,t)-Y(t))\delta(x-d) \tag{45}$$

$$\psi(x,t_f) = 0, \tag{46}$$

$$-k(T(0,t))\frac{\partial\psi(0,t)}{\partial x} = 0 \tag{47}$$

$$\beta_1 k(T(L,t))\frac{\partial\psi(L,t)}{\partial x} + \beta_2\psi(L,t) = 0 \tag{48}$$

The term $2(T(x,t)-Y(t))\delta(x-d)$ acts like a plane source (or sink) at x = d. As convergence proceeds, the term tends to become smaller. If this term were equal to zero, then the adjoint variable $\psi(x,t)$ goes to zero.

MULTIPLE MEASURED TEMPERATURES

For the case of multiple measured temperatures, the sum of squares functional becomes

$$S(q)=\sum_{j=1}^{m}\int_0^{t_f}\left[Y_j(t)-T(d_j,t)\right]^2 dt + \alpha\int_0^{t_f}\left[q_{est}(t)-q(t)\right]^2 dt \tag{49}$$

for the case of m sensors. This equation is a generalization of Eq. (6) which is for a single sensor. Few changes are needed to accommodate multiple sensors. The direct model given by Eqs. (1) to (4) remain the same.

The sensitivity problem can be written as

$$\rho c(T)\frac{\partial \Theta}{\partial t} = \frac{\partial}{\partial x}\left(k(T)\frac{\partial \Theta}{\partial x}\right)+\frac{dk}{dT}\frac{\partial T}{\partial x}\frac{\partial \Theta}{\partial x} +$$

$$\left[\frac{dk}{dT}\frac{\partial^2 T}{\partial x^2} + \frac{d^2k}{dT^2}\left(\frac{\partial T}{\partial x}\right)^2 - \rho\frac{dc}{dT}\frac{\partial T}{\partial t}\right]\Theta$$

$$0 < x < L,\ 0 < t \le t_f \tag{50}$$

with boundary conditions

$$-k(T(0,t))\frac{\partial \Theta(0,t)}{\partial x} - \frac{dk(T(0,t))}{dT}\frac{\partial T(0,t)}{\partial x}\Theta(0,t) = \Delta q(t) \tag{51a}$$

$$\beta_2 k(T(L,t))\frac{\partial \Theta(L,t)}{\partial x} + \left[\beta_1\frac{\partial T(L,t)}{\partial x}\frac{dk(T(L,t))}{dT}+\beta_2\right]\Theta(L,t) = 0$$

The initial condition is

$$\Theta(x,0) = 0 \tag{52}$$

The adjoint equation is the only one that is really changed. Figs (45) - (48) remain the same except the last term in Eq. (45) is replaced by

$$2\sum_{j=1}^{m}\left[T(x,t)-Y(x,t)\right]\delta\left(x-d_j\right)$$

APPENDIX A. DIRECTIONAL DERIVATIVE OF I_{pde} FOR REGION 1

The parts of the directional derivative of I_{pde}, region 1, are:

$$D_{\Delta q}I_{pde,1} = \int_0^{t_f}\int_0^d\left[k\frac{\partial^2\psi}{\partial x^2} + \frac{dk}{dT_1}\frac{\partial T_1}{\partial x}\frac{\partial \psi_1}{\partial x}\right]\Theta_1 dxdt + \int_0^{t_f}\left(k\psi_1\frac{\partial \Theta_1}{\partial x} - k\frac{\partial \psi_1}{\partial x}\Theta_1\right|_0^d dt \qquad \textbf{(A.1)}$$

$$D_{\Delta q}I_{pde,2} = -\int_0^{t_f}\int_0^d\left[\frac{dk}{dT_1}\frac{\partial^2 T_1}{\partial x^2}\psi_1 + \frac{d^2k}{dT_1^2}\left(\frac{\partial T_1}{\partial x}\right)^2\psi_1 + \frac{dk}{dT_1}\frac{\partial T_1}{\partial x}\frac{\partial \psi_1}{\partial x}\right]\Theta_1 dxdt + \int_0^{t_f}\left(\frac{dk}{dT_1}\frac{\partial T_1}{\partial x}\psi_1\Theta_1\right)\Big|_0^d dt \qquad \textbf{(A.2)}$$

$$D_{\Delta q}I_{pde,3,4,5} = \int_0^{t_f}\int_0^d\left[\frac{dk}{dT_1}\frac{\partial^2 T_1}{\partial x^2} + \frac{d^2k}{dT_1^2}\left(\frac{\partial T_1}{\partial x}\right)^2 - \rho\frac{dc}{dT_1}\frac{\partial T_1}{\partial t}\right]\psi_1\Theta_1 dxdt \qquad \textbf{(A.3)}$$

$$D_{\Delta q}I_{pde,6} = +\int_0^{t_f}\int_0^d\left[\rho c\frac{\partial \psi_1}{\partial t} + \rho\frac{dc}{dT_1}\frac{\partial T_1}{\partial t}\psi_1\right]\Theta_1 dxdt - \int_0^d(\rho c\psi_1\Theta_1)\big|_0^{t_f}dx \qquad \textbf{(A.4)}$$

These expressions are added to get $D_{\Delta q}\, I_{pde}$. A number of cancellations occur. The second term of the *pde*,1 equation cancels with the third term of the *pde*,2 equation. The first term of the *pde*,2 equation cancels with *pde*,3. The second term of the *pde*,2 equation cancels with *pde*,4. Finally, the *pde*,5 term cancels with the second term in the *pde*,6 equation. The result of adding the above *pde* components is

$$D_{\Delta q}I_{pde,1} = \int_0^{t_f}\int_0^d\left[k\frac{\partial^2\psi_1}{\partial x^2} + \rho c\frac{\partial \psi_1}{\partial t}\right]\Theta_1 dxdt$$

$$+\int_0^{t_f}\left[k\psi_1\frac{\partial \Theta_1}{\partial x} - k\frac{\partial \psi_1}{\partial x}\Theta_1 + \frac{dk}{dT_1}\frac{\partial T_1}{\partial x}\psi_1\Theta_1\right]\Big|_0^d dt$$

$$-\int_0^d \rho c\psi_1\Theta_1\big|_0^{t_f}dx \qquad \textbf{(A.5)}$$

Recall that this is just for the first region $0 < x < d$. A similar expression is found for the second region.

APPENDIX B. DIRECTIONAL DERIVATIVE OF L

The various terms of the directional derivative of the Lagrangian L are now combined to obtain

$$D_{\Delta q}L = -2\int_0^{t_f} [Y(t) - T(d,t)]\Theta_1(d,t)dt - 2\alpha\int_0^{t_f} [q_{est}(t) - q(t)]\Delta q(t)dt$$

$$+ D_{\Delta q}I_{pde} + D_{\Delta q}I_{ic} + D_{\Delta q}I_{bc0} + D_{\Delta q}I_{int} + D_{\Delta q}I_{bcL} \qquad \textbf{(B.1)}$$

where $D_{\Delta q}I_{pde}$ is given by Eq. (36); $D_{\Delta q}I_{ic}$ is given by Eq. (28); $D_{\Delta q}I_{bc0}$ is given by Eq. (29); $D_{\Delta q}I_{int}$ is given by Eq. (30); and $D_{\Delta q}I_{bcL}$ is given by Eq. (31). At the minimum of $D_{\Delta q}L$, it is equal to zero. Let us then collect the various terms as coefficients of the various sensitivity functions, Θ_1 *and* Θ_2, and derivatives arranged in the following order: $\Theta_1(x,t)$, $\Theta_2(x,t)$, $\Theta_1(0,t)$, $\partial\Theta_1(0,t)/\partial x$, $\partial\Theta_2(L,t)/\partial x$, $\partial\Theta_1(d,t)/\partial x$, $\partial\Theta_2(d,t)/\partial x$, $\Theta_1(d,t)$, $\Theta_2(d,t)$, $\Theta_2(L,t)$, $\partial\Theta_2(L,t)/\partial x$, $\Theta_1(x,0)$, $\Theta_1(x,t_f)$, $\Theta_2(x,0)$ *and* $\Theta_2(x,t_f)$.

Then $D_{\Delta q}L$ is given by

$$D_{\Delta q}L = \int_0^{t_f}\int_0^{d}\left[k\frac{\partial^2\psi_1}{\partial x^2} + \rho c\frac{\partial\psi_1}{\partial t}\right]\Theta_1(x,t)dxdt$$

$$+ \int_0^{t_f}\int_d^{L}\left[k\frac{\partial^2\psi_2}{\partial x^2} + \rho c\frac{\partial\psi_2}{\partial t}\right]\Theta_2(x,t)dxdt$$

$$+ \int_0^{t_f}\left[+k(T_1(0,t))\frac{\partial\psi_1(0,t)}{\partial x} - \frac{dk(T_1(0,t))}{dT_1}\,\frac{\partial T_1(0,t)}{\partial x}\psi_1(0,t) + \eta(0,t)\frac{dk(T_1(0,t))}{dT_1}\,\frac{\partial T_1(0,t)}{\partial x}\right]\Theta_1(0,t)dt$$

$$+ \int_0^{t_f}\left[-k(T_1(0,t))\psi_1(0,t) + \eta(0,t)k(T_1(0,t))\right]\frac{\partial\Theta_1(0,t)}{\partial x}dt$$

$$+ \int_0^{t_f}\left[k(T_2(L,t))\psi_2(L,t) + \eta(L,t)\beta_1 k(T_2(L,t))\right]\frac{\partial\Theta_2(L,t)}{\partial x}dt$$

$$\int_0^{t_f} \left[k(T_1(d,t))\psi_1(d,t) + \eta(d,t)\right] \frac{\partial\Theta_1(d,t)}{\partial x} dt$$

$$+ \int_0^{t_f} \left[-k(T_2(d,t))\psi_2(d,t) - \eta(d,t)\right] \frac{\partial\Theta_2(d,t)}{\partial x} dt$$

$$+ \int_0^{t_f} \left[-k(T_1(d,t))\frac{\partial\psi_1(d,t)}{\partial x} + \frac{dk(T_1(d,t))}{dT_1} \frac{\partial T_1(d,t)}{\partial x}\psi_1(d,t) + \mu(d,t)-2(Y(t)-T(d,t))\right]\Theta_1(d,t)dt$$

$$+ \int_0^{t_f} \left[+k(T_2(d,t)) \frac{\partial\psi_2(d,t)}{\partial x} - \frac{dk(T_2(d,t))}{dT_2} \frac{\partial T_2(d,t)}{\partial x}\psi_2(d,t) - \mu(d,t)\right]\Theta_2(d,t)dt +$$

$$\int_0^{t_f}\left\{-k(T_2(L,t))\frac{\partial\psi_2(L,t)}{\partial x} + \frac{dk(T_2(L,t))}{dT_2}\frac{\partial T_2(L,t)}{\partial x}\psi_2(L,t) + \eta(L,t)\left[\beta_1\frac{dk(T_2(L,t))}{dT_2}\frac{\partial T_2(L,t)}{\partial x} + \beta_2\right]\right\}\Theta_2(L,t)d$$

$$+ \int_0^{t_f} \left\{k(T_2(L,t))\psi_2(L,t) + \eta(L,t)\beta_1 k(T_2(L,t))\right\}\frac{\partial\Theta_2(L,t)}{\partial x} dt$$

$$+ \int_0^{d} \left[\rho c(T_1(x,0))\psi_1(x,0) + \eta(x,0)\right]\Theta_1(x,0)dx$$

$$+ \int_0^{d} \left[-\rho c(T_1(x,t_f))\psi_1(x,t_f)\right]\Theta_1(x,t_f)dx$$

$$+ \int_d^{L} \left[\rho c(T_2(x,0))\psi_2(T_2(x,0)) + \eta_2(x,0)\right]\Theta_2(x,0)dx$$

$$+ \int_d^{L} \left[-\rho c(T_2(x,t_f))\psi_2(x,t_f)\right]\Theta_2(x,t_f)dx$$

$$+ \int_0^{t_f} \left[-2\alpha\left[q_{est}(t)-q(t)\right] + \eta(0,t)\right]\Delta q(t)dt \qquad \text{(B.2)}$$

Each of above integrals is now considered separately with two exceptions. These exceptions are the sixth and seventh integrals (related derivatives through Eq. (21)) and integrals 8 and 9 (related by continuity of Θ). Recall that the directional derivative is equal to zero. Also each integral is independent of the others except 6 and 7, and 8 and 9; hence, each integral (except 6th and 7th, and 8th and 9th) must be equal to zero. From the first integral which is for $\Theta_1(x,t)$, we obtain the partial differential equation,

$$k\,\frac{\partial^2\psi_1}{\partial x^2} + \rho c\frac{\partial\psi_1}{\partial t} = 0,\ 0 < x < d,\ 0 < t < t_f \tag{B.3}$$

This is a partial differential equation because there is a double integration, one on each independent variable. The same reasoning for the second integral yields

$$k\,\frac{\partial^2\psi_2}{\partial x^2} + \rho c\frac{\partial\psi_2}{\partial t},\ d < x < L,\ 0 < t < t_f \tag{B.4}$$

Consider next the third integral in Eq. (B.2), the one for $\Theta_1(0,t)$, which involves integration only over t. This integral can be used to find the ψ_1 boundary condition. Let us choose

$$k\,\big(T_1(0,t)\big)\,\frac{\partial\psi_1(0,t)}{\partial x} = 0 \tag{B.5a}$$

$$\psi_1(0,t) = \eta(0,t) \tag{B.5b}$$

The fourth integral is made equal to zero by using Eq. (B.5b).
The fifth integral is satisfied by the condition

$$\beta_1\eta(L,t) = -\psi_2(L,t) \tag{B.6}$$

The sixth and seventh integrals are considered together. These equations can be satisfied by having continuity conditions on ψ

$$\psi_1(d,t) = \psi_2(d,t) \tag{B.7a}$$

since Eq. (21) gives

$$\frac{\partial\Theta_1(d,t)}{\partial x} = \frac{\partial\Theta_2(d,t)}{\partial x} \tag{B.7b}$$

The eighth and ninth integrals in Eq. (B.2) are considered together. Eq. (B.7a) and the sensitivity relation given by Eq. (22),

$$\Theta_1(d,t) = \Theta_2(d,t) \tag{B.8a}$$

then yield

$$-k(T_1(d,t))\,\frac{\partial\psi_1(d,t)}{\partial x} + k(T_2(d,t))\frac{\partial\psi_2(d,t)}{\partial x}$$

$$-2\,[Y(t)-T(d,t)] = 0 \tag{B.8b}$$

The derivatives dk/dT and $\partial T/\partial x$ are also continuous at x = d. Eqs. (B.7a) and (B.8b) are interface conditions for $\psi(x,t)$.

Before considering integral 10, use the eleventh integral to get

$$\psi_2(L,t) = -\beta_1\eta(L,t) \tag{B.9}$$

en this reltaion is used in the integrand of integral ten, and after a cancellation, one obtains

$$\beta_1 k(T_2(L,t))\frac{\partial\psi_2(L,t)}{\partial x} + \beta_2\psi_2(L,t) = 0 \tag{B.10}$$

At t = 0, the sensitivity functions $\Theta_1(x,t)$ and $\Theta_2(x,t)$ are equal to zero. (See Equs. (18) and (19). Consequently, integrals twelve and fourteen are satisfied (that is, equal to zero).

The thirteenth and fifteenth integrals (the ones involving $\Theta_1(x,t_f)$ and $\Theta_2(x,t_f)$) are satisfied by using the zero initial conditions on ψ, given by Equs. (39) and (40).

This now leads to the last integral in Eq. (B.2). We do not set this coefficient equal to zero. Instead, notice that Eq. (5b) permits Eq. (B.2) to be written as (using Eq. (B.5b))

$$D_{\Delta q}L(q) = \int_0^{t_f}\left[-2\alpha\left(q_{est}(t)-q(t)\right)+\psi_1(0,t)\right]\Delta q(t)dt \tag{B.11}$$

which is also equal to $D_{\Delta q}\,S(q)$. Then comparing Eq. (B.11) with Eq. (7c), the gradient of S is

$$\nabla S(t;q(t)) = \psi_1(0,t) - 2\alpha\left(q_{est}(t)-q(t)\right) \tag{B.12}$$