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UTILIZATION OF SENSITIVITY COEFFICIENTS TO GUIDE THE DESIGN OF A THERMAL BATTERY

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ABSTRACT

Equations are presented to describe the sensitivity of the temperature field in a heat-conducting body to changes in the volumetric heat source and volumetric heat capacity. These sensitivity equations, along with others not presented, are applied to a thermal battery problem to compute the sensitivity of the temperature field to 19 model input parameters. Sensitivity coefficients, along with assumed standard deviation in these parameters, are used to estimate the uncertainty in the temperature prediction. From the 19 parameters investigated, the battery cell heat source and volumetric heat capacity were clearly identified as being the major contributors to the overall uncertainty in the temperature predictions. The operational life of the thermal battery was shown to be very sensitive to uncertainty in these parameters.

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NOMENCLATURE

$\mathcal{A}$	area, m^2
C	$= \rho c_p$, volumetric heat capacity, $\text{J}/\text{m}^3\text{-K}$
c_p	specific heat, $\text{J}/\text{kg-K}$
$\dot{e}'''$	energy source, W/m^3
h	convective heat transfer coefficient, $\text{W}/\text{m}^2\text{-K}$
k	thermal conductivity, $\text{W}/\text{m-K}$
k_{ii}	principal component of thermal conductivity tensor, $\text{W}/\text{m-K}$
$\tilde{\mathbf{k}}$	thermal conductivity tensor, $\text{W}/\text{m-K}$
$\hat{n}$	unit normal vector
p_i	i th parameter
$\dot{q}''$	heat flux, W/m^2
r	radial coordinate, m
S_i	source term for Region i , W/m^3
T	temperature, K
T_o	initial temperature, K
T_{p_i}	temperature sensitivity coefficient for parameter p_i , K
T_r	ambient temperature for radiation, K
T_∞	ambient temperature for convection, K
t	time, s
t_o	time when source is turned off, s
V_i	relative variance, Eq (21)
$\mathcal{V}$	volume, m^3
$\hat{\mathbf{x}}_b$	position vector along boundary
z	axial coordinate, m
Greek	
ε	emittance
ρ	density, kg/m^3
σ	Stefan-Boltzmann constant

INTRODUCTION

Sensitivity coefficients are useful for a wide variety of engineering problems. These applications include estimation of material properties, boundary conditions, source terms, etc., from field measurements, optimal design of experiments, uncertainty analysis, optimization, and design/analysis studies. Within the context of this work, sensitivity coefficients are defined as partial derivatives of field variables (temperature, displacement, velocity, etc.) with respect to model parameters (conductivity, Young's modulus, viscosity, etc.). In the thermal parameter estimation

arena (including the inverse heat conduction problem), a representative sample of references using sensitivity coefficients can be found in Beck and Arnold (1977); Beck et al. (1985); Blackwell and Eldred (1997); Dowding, et al. (1995); Dowding, et al. (1996); Dowding and Blackwell (1998); Fadale, et al. (1995); Marschall and Milos (1997); Osman, et al. (1997); and Tseng and Zhao (1996). In the optimum design of thermal experiments, a representative sample of references using sensitivity coefficients can be found in Beck and Arnold (1977); Emery and Fadale (1996a); Emery and Fadale (1997); and Emery, et al. (1997). In the thermal uncertainty analysis area, a representative sample of references using sensitivity coefficients can be found in Emery and Fadale (1996b), Fadale (1993), and Fadale and Emery (1994). In the thermal optimization area, a representative sample of references using sensitivity coefficients can be found in Haftka (1981) and Tortorelli and Michaleris (1994). In the structural mechanics arena, see Kleiber and Hien (1992) and Kleiber, et al. (1997). In the reliability and safety arena, see Saltelli and Scott (1997).

This work is directed toward using sensitivity coefficients to guide design and analysis studies and to estimate uncertainty in field variables given uncertainty in model input parameters. To demonstrate the usefulness of sensitivity coefficients, they will be applied to the design and analysis of a thermally activated battery. These so-called thermal batteries have shelf lives of up to 30 years because the electrolyte exists in a solid form, and this inhibits ionic transfer. Battery operation begins when the electrolyte melts following the ignition of pyrotechnic heat pellets that are placed within each electrochemical cell of the battery. The battery continues to operate until the electrolyte cools sufficiently to freeze. Thus the electrochemical performance of a thermally activated battery is governed by its thermal characteristics; in particular the time that the cell remains above the melt temperature of the electrolyte is very important. We focus strictly on the thermal

characteristics and ignore the electrochemical details. The work of Dobranich (1995) suggests this is a valid approach in determining the time over which the battery can operate. An analysis of the electrical output of such a thermal battery would require a more sophisticated model and is not attempted in this work.

In the past the battery design process relied on costly experiments in which batteries were built and tested in a trial-and-error procedure. Currently a computer-based model, Dobranich (1995), that simulates the thermal performance of a battery is used to supplement the design process, thereby reducing the associated time and cost. A computer-based design tool can also provide insight into the model parameters that have the most significant impact on the design. Once the significant parameters have been identified, experiments to reduce the uncertainty in those parameters can be performed, and the overall system uncertainty can be reduced. A new computer code is in development that can be used to facilitate these sensitivity coefficient computations, and results from it will be presented here.

A SIMPLIFIED MODEL OF THE THERMAL BATTERY

The thermal battery of interest consists of ten stacked electrochemical cells. Each cell, in turn, consists of an anode collector, anode, electrolyte binder, cathode, cathode collector, and a heat pellet (Fe/KClO_4). Two additional heat pellets are placed at both the top and bottom of the cell stack to help extend its operation life. A model of the battery with details of the cell would be very complex and was not deemed necessary for this study. Instead materials were lumped together, based on the experiences of the analyst (author DD). A schematic of the simplified axisymmetric

model is shown in Figure 1. The geometry is a cylinder with a 3.72 cm radius and 10.52 cm

Figure 1: Simplified model of the thermal battery.

height. Five materials are identified: 1) outer case, 304 stainless steel; 2) radial sleeve, Min-K®; 3) header/base stack; 4) cell composite; and 5) Fiberfrax®/glass wrap. Because of the lumping of the layered structure in Region 3 (header/base stack) and Region 4 (cell), the effective thermal conductivity of these materials is modeled as orthotropic. The computational mesh is also shown in Figure 1. The effective thermal properties used in the analysis are given in Table 1. The prob-

mat ID	ρc_p , J/m ³ -K	k or k_{rr} , W/m-K	k_{zz} , W/m-K	S_i , W/m ³
1	3.979×10^6	1.591×10^1	-	-
2	3.216×10^5	2.931×10^{-2}	-	-
3	1.281×10^6	2.094×10^0	5.443×10^{-2}	9.480×10^8
4	2.480×10^6	6.657×10^0	8.248×10^{-1}	1.228×10^9
5	1.085×10^5	9.337×10^{-2}	-	-

Table 1. Effective material properties used in the thermal model.

lem is being driven by source terms in both Regions 3 and 4. The source terms were computed from experimental data and the desire to deliver the correct amount of energy to the battery over a time interval of 1 s. This 1 s time interval was chosen somewhat arbitrarily and has little impact on the problem results at the end of a 3600 s simulation time, provided the energy content after the initial burn is correct. The effect of energy change due to melting and solidification of the electrochemical cells and the temperature dependence of thermal properties were ignored for these simulations.

The boundary conditions allow for free convection and thermal radiation from the top and side exterior surfaces. The bottom boundary condition represents the battery sitting on a low conductivity base. The assumed heat transfer coefficients and emissivity are given in Table 2.

location	h , W/m ² -K	ϵ
bottom	2.3	NA
side	5.4	0.25
top	8.0	0.25

Table 2. Boundary condition parameters.

Even though we are assuming that the properties are independent of temperature, the total number of parameters for this rather simple, five-material problem is quite large. There are a total of 19 parameters listed in Table 1 and Table 2. We want to calculate the sensitivity of the temperature field to changes in each of these 19 parameters listed in Table 1 and Table 2. The combination of the temperature field plus the 19 sensitivity coefficients will provide a large amount of information for an analyst or designer to process and interpret.

DETERMINATION OF SENSITIVITY COEFFICIENTS

Sensitivity coefficients are typically determined by one of four methods: 1) analytical differen-

tiation of analytical solutions for the temperature field (termed "analytical"), 2) numerical differentiation of numerical solutions for the temperature field (termed "finite difference"), 3) differentiation of source code to produce new source code to directly calculate sensitivity coefficients (termed "automatic differentiation"), and 4) direct differentiation of governing equations and numerically solving the resulting sensitivity equations (termed "direct differentiation"). Clearly analytical approaches are limited in their scope of applicability due to the lack of analytical solutions for practical problems involving complex geometry. Finite difference methods have been successfully used in many problems; their primary weakness is how to choose an appropriate finite difference step size (in parameter space) to balance truncation and round-off errors. Considerable progress has been made in source code differentiation as evidenced by the availability of the codes ADIFOR, Bischof (1996), and ADIC, Bischof (1997), that take FORTRAN or C code, respectively, as input; however, they could not be readily applied to this problem due to the manner in which the material properties are communicated to the internal data structure of the thermal analysis code. We will focus on the direct differentiation approach for deriving the sensitivity coefficient equations. Additional details on this approach can be found in Blackwell, Cochran, and Dowding (1998); an application of sensitivity coefficients derived in this manner is found in Dowding, Blackwell, and Cochran (1998).

In order to demonstrate the concepts of computing sensitivity coefficients for a multimaterial

problem with multiple sources, we will focus on a simple example given in Figure 2. The devel-

Figure 2: Schematic of two-material problem with sources and convection/radiation boundary conditions.

opment starts from the integral form of the energy equation¹ for a heat-conducting body because the numerical discretization we are using is the control volume finite element method:

$$\frac{\partial}{\partial t} \iiint_{\mathcal{V}} CT d\mathcal{V} + \iint_{\mathcal{A}} \vec{q} \cdot d\vec{\mathcal{A}} = \iiint_{\mathcal{V}} \dot{e}''' d\mathcal{V} \quad (1)$$

where the heat flux vector is given by the anisotropic form of Fourier's Law,

$$\vec{q} = -\tilde{k} \cdot \nabla T \quad (2)$$

and the (orthotropic) thermal conductivity tensor (for 2-D) is given by

1. The volumetric heat capacity is used in the governing equation because it is not possible to distinguish between changes in density and changes in specific heat.

$$\tilde{\mathbf{k}} = \begin{bmatrix} k_{11} & 0 \\ 0 & k_{22} \end{bmatrix}. \quad (3)$$

The initial/boundary conditions for the problem defined in Figure 2 can be written as

$$T(\hat{\mathbf{x}}, 0) = T_o \quad (4)$$

$$-\int \int_{\mathcal{A}_b} (\tilde{\mathbf{k}} \cdot \nabla T)|_{\hat{\mathbf{x}}_b} \cdot d\hat{\mathbf{A}} = \int \int_{\mathcal{A}_b} [h(T - T_\infty) + \varepsilon\sigma(T^4 - T_r^4)] d\mathcal{A}. \quad (5)$$

If Fourier's Law is substituted into Eq (5), we obtain

$$\frac{\partial}{\partial t} \int \int \int_{\mathcal{V}} CT d\mathcal{V} + \int \int_{\mathcal{A}} -\tilde{\mathbf{k}} \cdot \nabla T \cdot d\hat{\mathbf{A}} = \int \int \int_{\mathcal{V}} \dot{e}''' d\mathcal{V}. \quad (6)$$

The source terms are defined as follows:

$$\dot{e}''' = \begin{cases} S_1, \text{ region 1 and } 0 \leq t \leq t_o \\ 0, \text{ region 1 and } t > t_o \\ S_2, \text{ region 2 and } 0 \leq t \leq t_o \\ 0, \text{ region 2 and } t > t_o \end{cases} \quad (7)$$

The first step in the derivation of the sensitivity coefficient equation is to differentiate the energy equation with respect to the parameter of interest. For the sensitivity with respect to the magnitude of the source term S_1 , the result is

$$\frac{\partial}{\partial t} \int \int \int_{\mathcal{V}} C \frac{\partial T}{\partial S_1} d\mathcal{V} + \int \int_{\mathcal{A}} \frac{\partial}{\partial S_1} \tilde{\mathbf{q}} \cdot d\hat{\mathbf{A}} = \int \int \int_{\mathcal{V}} \frac{\partial}{\partial S_1} \dot{e}''' d\mathcal{V} \quad (8)$$

where we have assumed that the limits of integration do not depend on the parameter value. Experience has shown that scaled sensitivity coefficients are useful when comparing the magnitude of different sensitivity coefficients because they have the same units (temperature in this case).

Scaled sensitivity coefficients are defined by

$$T_p = p \frac{\partial T}{\partial p} = \frac{\partial T}{\partial \ln p} \quad (9)$$

where p represents any arbitrary parameter. Multiplying Eq (8) by S_1 and moving this term inside the integral sign (since it is independent of space/time) results in

$$\frac{\partial}{\partial t} \iiint_{\mathcal{V}} CT_{S_1} d\mathcal{V} + \iint_{\mathcal{A}} S_1 \frac{\partial}{\partial S_1} \vec{q} \cdot d\vec{\mathcal{A}} = \iiint_{\mathcal{V}} S_1 \frac{\partial}{\partial S_1} e''' d\mathcal{V}. \quad (10)$$

The right-hand side of Eq (10) will be zero except when integrating over Region 1 and when $0 \leq t \leq t_o$. Consequently, Eq (10) can be written as

$$\frac{\partial}{\partial t} \iiint_{\mathcal{V}} CT_{S_1} d\mathcal{V} + \iint_{\mathcal{A}} S_1 \frac{\partial}{\partial S_1} \vec{q} \cdot d\vec{\mathcal{A}} = \begin{cases} \iiint_{\mathcal{V}_1} S_1 d\mathcal{V}, & 0 \leq t \leq t_o \text{ and region 1} \\ 0, & \text{otherwise} \end{cases} \quad (11)$$

The derivative of the heat flux vector with respect to the source term S_1 is

$$S_1 \frac{\partial}{\partial S_1} \vec{q} = -S_1 \tilde{\mathbf{k}} \cdot \nabla \left(\frac{\partial T}{\partial S_1} \right) = -\tilde{\mathbf{k}} \cdot \nabla T_{S_1}. \quad (12)$$

Eq (12) has the physical appearance of a "Fourier like" law for the diffusion of sensitivity information; thermal conductivity is the appropriate material property for this diffusive effect. The equation describing the transport of the property T_{S_1} can now be written as

$$\frac{\partial}{\partial t} \iiint_{\mathcal{V}} CT_{S_1} d\mathcal{V} + \iint_{\mathcal{A}} -\tilde{\mathbf{k}} \cdot \nabla T_{S_1} \cdot d\vec{\mathcal{A}} = \begin{cases} \iiint_{\mathcal{V}_1} S_1 d\mathcal{V}, & 0 \leq t \leq t_o \text{ and region 1} \\ 0, & \text{otherwise} \end{cases} \quad (13)$$

The initial and boundary conditions for Eq (13) are addressed next. From the initial temperature condition, Eq (4), the initial condition for the sensitivity equation becomes

$$S_1 \frac{\partial}{\partial S_1} T(\bar{x}, 0) = T_{S_1}(\bar{x}, 0) = 0. \quad (14)$$

Similarly the boundary condition for the T_{S_1} equation can be written as

$$\int \int_{\mathcal{A}_b} \left(S_1 \frac{\partial}{\partial S_1} \bar{q} \right) \cdot d\bar{\mathcal{A}} \Big|_{\bar{x}_b} = \int \int_{\mathcal{A}_b} (h + 4\epsilon\sigma T^3) T_{S_1} \hat{n} \cdot d\bar{\mathcal{A}}. \quad (15)$$

We are now in a position to reflect on the equations describing the behavior of T_{S_1} . Eq (13) resembles a conservation equation for the sensitivity T_{S_1} ; the equation contains storage, conduction, and source terms. This will allow us to apply intuition developed for heat conduction problems directly to the transport of sensitivity information, provided we account for differences in the source terms and initial/boundary conditions. Some authors have chosen to differentiate the spatially discretized equations-e.g., Haftka (1981), Fadale (1993)-to derive new equations for sensitivity coefficients rather than differentiating the describing equations. If a consistent discretization method is used, then both approaches should yield identical numerical results. However, we feel that studying the describing equations for the sensitivity coefficient can provide useful insight toward understanding sensitivity related issues.

In comparing the T equations (Eq (4)-Eq (6)) and T_{S_1} equations (Eq (13)-Eq (15)), we draw the following conclusions:

1. The left-hand side of the T and T_{S_1} equations are identical; this has the potential for savings in software development time since the same routines can be used to assemble both global equations.
2. The source terms appear to be similar, but there are subtle differences. If both Regions 1 and 2 have active source terms, then both Regions have a source contribution to the T equations. However, for the T_{S_1} equation, Region 2 has a zero source contribution, even for $S_2 \neq 0$.

3. The initial condition for the T_{S_1} equation is the homogeneous version of the initial condition for the T equation. This suggests some connection between the sensitivity T_{S_1} and the temperature rise $T - T_o$.
4. The boundary conditions for the T_{S_1} equation are homogeneous, while those for the T equation are inhomogeneous. The radiation boundary condition for the T_{S_1} equation has the appearance of a linearization to produce an effective radiation heat transfer coefficient.
5. The only dependence of T_{S_1} on T is through the boundary condition, Eq (15). If convection and radiation were not present, then the T_{S_1} equation would be independent of T .

The previous process is now repeated to determine the sensitivity with respect to the volumetric heat capacity of Material 1. Differentiating Eq (1) with respect to C_1 , multiplying through by C_1 , and simplifying yields

$$\frac{\partial}{\partial t} \iiint_{\mathcal{V}} CT_{C_1} d\mathcal{V} + \iiint_{\mathcal{A}} C_1 \frac{\partial}{\partial C_1} \vec{q} \cdot d\vec{\mathcal{A}} = - \frac{\partial}{\partial t} \iiint_{\mathcal{V}_1} CT d\mathcal{V}. \quad (16)$$

Differentiating Fourier's Law with respect to C_1 and substituting into Eq (16) yields

$$\frac{\partial}{\partial t} \iiint_{\mathcal{V}} CT_{C_1} d\mathcal{V} + \iint_{\mathcal{A}} -\vec{k} \cdot \nabla T_{C_1} \cdot d\vec{\mathcal{A}} = - \frac{\partial}{\partial t} \iiint_{\mathcal{V}_1} CT d\mathcal{V}. \quad (17)$$

The initial/boundary conditions become

$$C_1 \frac{\partial}{\partial C_1} T(\vec{x}, 0) = T_{C_1}(\vec{x}, 0) = 0 \quad (18)$$

and

$$\iint_{\mathcal{A}_b} \left(C_1 \frac{\partial}{\partial C_1} \vec{q} \right) \cdot d\vec{\mathcal{A}} \Big|_{\vec{x}_b} = \iint_{\mathcal{A}_b} (h + 4\epsilon\sigma T^3) T_{C_1} \hat{n} \cdot d\vec{\mathcal{A}}. \quad (19)$$

A comparison of the T equations (Eq (4)-Eq (6)) and T_{C_1} equations (Eq (17)-Eq (19)) reveals the following:

1. The left-hand side of the T and T_{C_1} equations have identical forms, again affording a savings in software development time.
2. While the T equation has an actual source term, the T_{C_1} equation (in the form it is written) has a fictitious source term. In reality this term came from the capacitance term in the energy equation. Note that the integral limits are just over the volume for which Material 1 is active; outside Region 1 this term is zero. This fictitious source term does not depend on T_{C_1} but does depend on the time rate of change of the temperature. If the temperature is increasing with time, this fictitious source term is negative. Problems with a positive $\partial T / \partial t$ tend to have negative T_{C_1} unless there was an earlier cooling phase to the problem.
3. The T_{C_1} boundary conditions are identical in form to the T_{S_1} boundary conditions; see Item 4 above.

In conclusion, the two sensitivity coefficient equations presented are both driven by source-like terms. In one case it is related to the actual source, whereas in the other it is a fictitious source term. In both cases these source-like terms are known once the temperature field is known. This will allow the sensitivity coefficients to be computed on a parallel computing platform, provided the temperature field is determined first.

The other 17 sensitivity coefficient equations can be developed in a similar fashion. The rationale for presenting the development of these two sensitivity coefficients discussed above is that they have the largest magnitude for the thermal battery problem. The equations presented here were solved using a control volume finite element method with a fully implicit time integrator, Hogan, et al. (1996). The solution to temperature and sensitivity verification problems has been previously presented in Blackwell, Cochran, and Dowding (1998).

TEMPERATURE PREDICTIONS

The temperature distribution within the thermal battery is shown in Figure 3 for a series of

Figure 3: Temperature profile in thermal battery at three selected times. Note that the origin of the r - z coordinate system is hidden from view.

times; the back corner (hidden from view) corresponds to the origin of the r - z coordinate system in Figure 1. The lines on the temperature surface are the grid lines that have been displaced from the r - z plane. The two pronounced peaks for the $t = 1.0$ s results correspond to Region 3 (header/base stack), where the volumetric heat capacity is smaller than that for Region 4 (cell composite).

The purpose for this design feature is to insure that the end heat loss is minimized and does not cause premature solidification of the electrolyte. After the very pronounced initial transient, the remainder of the problem is a gradual redistribution of the energy in the system. With the low thermal conductivity insulation (Region 2, radial sleeve) just inside the stainless steel shell (Region 1), the heat loss with time is gradual. The maximum heat loss location in the thermal envelope is the bottom of the thermal battery. Figure 1 indicates that the insulation is thinnest in this Region. Although the bottom of the stainless steel case is hidden in the views shown in Figure 3, it experiences a slight temperature rise.

SENSITIVITY COEFFICIENT AND UNCERTAINTY RESULTS

The sensitivity coefficients were computed for the 19 variables identified in Table 1 and Table 2. The cpu time for the 405 node, 437 time step problem with 20 unknowns per node was 667 s on a SUN ULTRA 2[®] work station. By today's standards this is a very modest amount of computational time. The computer hardware costs attributable to this calculation is minuscule in comparison to the analyst time required to visualize and interpret this volume of information. For this problem, the temperature field and sensitivity coefficients at $t = 3600$ s within Region 4 (cell composite) are of primary interest because of the operational lifetime design requirements. Consequently, we will concentrate on presenting results at $t = 3600$ s.

Of the 19 sensitivity coefficients computed, only four of them have sufficient magnitude at $t = 3600$ s to impact the design: the source terms S_3 in Region 3 (header/base stack) and S_4 in Region 4 (cell composite), volumetric heat capacity in Region 4 (C_4), and thermal conductivity k_2 of Region 2 (radial sleeve). These four sensitivity coefficients are shown in Figure 4 at $t = 3600$ s. All the sensitivity coefficients are scaled so that they all have the units of temperature (K) and are shown with the same scale. This allows their magnitudes to be compared directly. The largest sen-

Figure 4: Four largest sensitivity coefficients at $t = 3600$ s; note that the units of the scaled sensitivity coefficients are K. The origin of the r - z coordinate system is at the bottom back corner of the plot box.

sensitivity coefficient is that for S_4 , and it is positive; an increase in the source term S_4 produces an increase in temperature. Since S_4 is driving the problem, this result is not surprising. For comparison purposes the scaled sensitivity coefficients should be compared to the temperature rise in Region 4 (cell composite); in this region the temperature rise is on the order of 500 K. This indicator confirms that the S_4 sensitivity is a very significant contributor.

The next largest (in magnitude) scaled sensitivity coefficient is that for C_4 (cell composite), and

it is negative; an increase in heat capacity produces a decrease in temperature. Source and heat capacity sensitivities for the same material tend to have opposite signs. For the C_4 sensitivity coefficient, the impact of the smaller insulation thickness on the bottom ($z = 0$) can be seen in the stainless steel shell, Region 1. If the temperature in a Region does not change from its initial value, then the volumetric heat capacity sensitivity will remain zero; see the right-hand side of Eq (17). The volumetric heat capacity of Region 4 (cell composite) is not as influential as the source term in this Region.

The next largest (in magnitude) scaled sensitivity coefficient is that for k_2 (radial sleeve), and it is negative over Region 4; an increase in k_2 causes a decrease in the cell (Region 4) temperature. The sensitivity to k_2 is greater in Region 3 than in Region 4; this makes sense physically since Region 3 is closer than Region 4 to insulation layer Region 2. The stainless steel case (Region 1) shows little sensitivity to changes in k_2 except on the bottom; even there the sensitivity is small.

The last sensitivity coefficient shown is that for the source term in Region 3 (header/base stack), S_3 ; it is positive throughout the computational domain. Even though it is fourth out of 19 of the sensitivity coefficients, it is not a major contributor.

The above four scaled sensitivity coefficients have been evaluated at the lower right-hand cor-

ner of Region 4, Figure 1, and are shown graphically in Figure 5; in this figure the initial condi-

Figure 5: Variation of selected scaled sensitivity coefficients (evaluated at lower right-hand corner of Region 4) with time.

tion for all the sensitivity coefficients was zero. At early time ($t < 60$ s), the sensitivity to volumetric heat capacity C_4 is approximately equal in magnitude but opposite in sign to the S_4 sensitivity. This is because the early time behavior is dominated by capacitance and source effects with diffusion being relatively unimportant. For large times the magnitude of S_4 , C_4 , and S_3 sensitivities are decaying with time, whereas that of k_2 is increasing with time. Relatively speaking the k_2 and S_3 sensitivities are not as important as the other two.

Sensitivity coefficients are important within their own right because they can be used to identify those parameters that are significant. Another use for them is in what is termed "propagation of

uncertainty.” This addresses the question of, given some statistical information about the input parameters to a computational model, what is the uncertainty in the model predictions? Propagation of uncertainty by perturbation methods within computational models has been discussed by Fadale (1993) and Emery and Fadale (1996b). Coleman and Steele (1989) discuss propagation of uncertainty from an experimental perspective; their results are identical in form to the first order results given by Fadale (1993). The equation used here to propagate uncertainty for the above four sensitivity coefficients is as follows:

$$\sigma_T^2 = \left(S_4 \frac{\partial T}{\partial S_4} \frac{\sigma_{S_4}}{S_4} \right)^2 + \left(C_4 \frac{\partial T}{\partial C_4} \frac{\sigma_{C_4}}{C_4} \right)^2 + \left(k_2 \frac{\partial T}{\partial k_2} \frac{\sigma_{k_2}}{k_2} \right)^2 + \left(S_3 \frac{\partial T}{\partial S_3} \frac{\sigma_{S_3}}{S_3} \right)^2 \quad (20)$$

where σ_p is the standard deviation in the input parameter p . The scaled sensitivity coefficients are readily identified in Eq (20). This result requires only first order sensitivity coefficients and hence is restricted to small perturbations or linear functions. Higher order uncertainty propagation equations are given in Fadale (1993). The computational load for first order sensitivity coefficients scales linearly with the number of parameters; for second order the scaling is with the square of the number of parameters. Our limited experience suggests that Eq (20) can be utilized for normalized standard deviations on the order of 0.2-0.3; this depends on the degree of nonlinearity of the problem. Computationally the propagation of uncertainty using Eq (20) is trivial in comparison to the calculation of the sensitivity coefficients. Assuming a normalized standard deviation (σ_p/p) in each input parameter of ± 10 percent, the standard deviation in the temperature was computed for $t = 3600$ s and is shown in Figure 6. Over the primary Region of interest, Region 4 (cell composite), the uncertainty in temperature is roughly 45 K at 3600 s. If the uncertainty is doubled in each of the input parameters, Eq (20) indicates that the overall temperature uncertainty will also double. If the input uncertainties are changed by differing amounts, then Eq (20) must be applied

Figure 6: Temperature uncertainty (K) at $t = 3600$ s; all input quantities had a normalized standard deviation of ± 10 percent.

again. Once the sensitivity coefficients have been computed, then the uncertainty propagation calculation is a postprocessing operation. The consequences of this uncertainty on the thermal battery design are discussed next.

The results of Figure 5 can be put in a dimensionless variance form to better emphasize the contribution of any individual parameter to the overall variance in temperature. Looking at the terms in Eq (20), one can define a relative variance as

$$V_i = \frac{\left(p_i \frac{\partial T}{\partial p_i} \frac{\sigma_{p_i}}{p_i} \right)^2}{\sigma_T^2} \quad (21)$$

where p_i is an arbitrary parameter. Note that the sum of the relative variances must be unity. These results are shown in Figure 7. The dominance of the source and volumetric heat capacity of Region 4 (cell composite) is even more pronounced on this set of coordinates. In fact, for practical purposes all the other sensitivity coefficients can be ignored with regard to the temperature of the cell material at the end of 3600 s of operation.

Figure 7: Relative variance for the four largest sensitivity coefficients. Note that this is evaluated at the lower right-hand corner of Region 4, Figure 1.

Now that the uncertainty in the temperature prediction has been estimated, it is informative to plot a representative cell temperature and its estimated uncertainty as a function of time. These results are shown in Figure 8. The uncertainty bars on the model results are shown at $\pm\sigma_T$. The assumed ± 10 percent uncertainty in the input parameters translates to a potentially large uncertainty in the operational life of the battery. For example, suppose the cell ceases to function at a solidification temperature of 700K. If the lower uncertainty limit on the temperature predictions is used, the time at which the cell temperature reaches 700 K may be as low as 1960 s, instead of the minimum allowable operational time of 3600 s. Due to the slow decay rate of the cell temperature, the relatively small uncertainty of the material properties translates to a very large uncertainty in the operational lifetime of the battery. In order to reduce the uncertainty in the operational lifetime,

Figure 8: Representative cell temperature prediction, its estimated uncertainty, and experimental temperature measurement.

the first step should be directed toward reducing the experimental uncertainty in the source term S_4 and volumetric heat capacity C_4 (Region 4, cell composite). Eventually if these two uncertainties are made sufficiently small, then some of the other input parameters may become more significant (in a relative sense); the methodology used here can be used to address these issues.

For comparison purposes one set of experimental temperature data is shown in Figure 8. The agreement is quite good up to about $t = 1800$ s. At larger times the experimental data exhibits a more rapid temperature decay with time than does the model. Since it is suspected that latent heat effects and temperature-dependent material properties are important, the agreement may be fortu-

itous. However, these results lend some credibility to the validation of the model and the sensitivity coefficient conclusions drawn from these results.

GRID RESOLUTION ISSUES

No grid refinement study was performed as part of this work; however, an earlier study by Dobranich (1995) did address this issue. We feel that the grid presented is adequate for the resolution of the temperature field. However, the grid resolution of the sensitivity coefficients may be another issue. For example, looking at the sensitivity coefficient $k_2 \partial T / \partial k_2$ given in Figure 4, there are very steep gradients in the sensitivity coefficient as you move along the axis of symmetry. If this fine detail is important to the analysis one is performing, then the grid may not be adequate to capture this behavior. We have experienced difficulties with the convergence of optimization methods that use sensitivity coefficients computed from finite differences (as opposed to the direct differentiation approach of this work) when we know that the solution is continuous in the parameter space. Based on the results presented here, it is suspected that the problems we were having were due to the fact that our grid may have adequately captured the temperature field but was inadequate for the sensitivity coefficients. Some of the 19 sensitivity coefficients computed for this study showed gradients that were more pronounced than those in Figure 4. However, since their magnitude was very small relative to the four presented here, their absolute accuracy was not deemed an issue.

SUMMARY

A simplified model of a thermal battery is presented in Figure 1. Sensitivity coefficients were discussed and equations were developed for the two sensitivity coefficients with largest magnitude. For this model which has five materials, constant properties, thermal radiation and natural convection boundary conditions, a total of 19 sensitivity coefficients were computed. Results are

presented for the four largest sensitivity coefficients: these are the source term in Regions 3 and 4 (S_3 and S_4 , header/base and cell stacks respectively); volumetric heat capacity in Region 4 (C_4); and thermal conductivity of Region 2 (k_2 , radial sleeve). Only two of these four sensitivity coefficients had a significant impact on the functional lifetime of the thermal battery. Assuming an input uncertainty of ± 10 percent for all parameter values, the estimated uncertainty in the temperature of cell Region 4 is about 45 K. However, the assumption of ± 10 percent input uncertainty is an engineering guess. From a practical perspective the engineer is unlikely to know the statistical characteristics of all the input and will have to resort to educated guesses. It was pointed out that even though the temperature field may be grid resolved, the sensitivity coefficients may need a more refined grid. However, the usefulness of sensitivity coefficients and uncertainty propagation is not so much to precisely quantify uncertainty as to use them as a means of guiding a design. Having sensitivity coefficients available turns what may have previously been a trial and error, experience-based process into a more formal process with quantifiable results.

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