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An inverse analysis to estimate linearly temperature dependent thermal conductivity components and heat capacity of an orthotropic medium

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Abstract--An inverse analysis is used to estimate linearly temperature dependent thermal conductivity components $k_x(T)$, $k_y(T)$ and specific heat capacity $C(T)$ per unit volume for an orthotropic solid. Simulated measured transient temperature data are generated by adding random errors to the exact temperatuies computed from the solution of the two-dimensional, direct transient heat conduction problem. An iterative procedure, based on minimizing a sum of squares function with the Levenberg-Marquardt iterative procedure is used to solve the inverse problem.

INTRODUCTION

There are many natural and man-made materials such as crystals, wood, thermo-plastic-matrix composites, etc., in which the thermal conductivity varies with direction as well as temperature. The analysis of heat conduction in a general anisotropic solid is quite complicated; but significant simplifications occur in the analysis for orthol:ropic materials that have a diagonal thermal conductivity matrix [1]. Composite materials enjoy an increasing use in diverse engineering applications because of their well-known advantages, such as enhanced physical properties and ease of processing. A wealth of literature exists on the mechanical properties of composites; but only a limited amount of work is available on the determination of their thermal properties. Recently, interest has been increased in the thermal properties of orthotropic materials because of their extended applications in engineering [2].

In this work we present an inverse method of analysis for estimating the linearly temperature dependent thermal conductivity components $k_x(T)$, $k_y(T)$ and the specific heat capacity $C(T)$ for an orthotropic solid by utilizing simulated transient temperature rec-

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ordings taken at three locations on the surface of the solid. Simulated transient temperature data are generated by adding random errors to the exact temperatures obtained from the solution of the twodimensional direct heat conduction problem. The Levenberg-Marquardt iterative procedure is used to solve the inverse problem.

The basic steps in the analysis include the solution of the direct problem, the inverse problem and the solution algorithm as described below.

DIRECT PROBLEM

We consider a two-dimensional transient heat conduction problem in an orthotropic solid confined to a rectangular region $0 \le x \le a$, $0 \le y \le b$. Let, $k_x(T)$ and $k_y(T)$ be the thermal conductivity components along the x and y directions respectively, and *C(T)* be the specific heat capacity of the solid. Initially the solid is at a uniform temperature T_0 . For times $t > 0$, the boundary surfaces at $x = 0$, $y = 0$ are subjected to a constant heat flux $q \text{W m}^{-2}$, while the boundary surfaces at $x = a$ and $y = b$ are kept insulated. The transient temperature recordings are taken at three surface locations as illustrated in Fig. 1.

The mathematical formulation of the direct transient heat conduction problem is given by

Fig. 1. Geometry, coordinates and thermocouple locations.

$$
\frac{\partial}{\partial x}\left(k_x(T)\frac{\partial T}{\partial x}\right) + \frac{\partial}{\partial y}\left(k_y(T)\frac{\partial T}{\partial y}\right) = C(T)\frac{\partial T}{\partial t}
$$

in $0 < x < a, 0 < y < b$, for $t > 0$. (1a)

Subject to the boundary conditions

$$
-k_x(T)\frac{\partial T}{\partial x} = q \quad \text{at } x = 0, t > 0 \tag{1b}
$$

$$
\frac{\partial T}{\partial x} = 0 \quad \text{at } x = a, t > 0 \tag{1c}
$$

$$
-k_y(T)\frac{\partial T}{\partial y} = q \quad \text{at } y = 0, t > 0 \tag{1d}
$$

$$
\frac{\partial T}{\partial y} = 0 \quad \text{at } y = b, t > 0 \tag{1e}
$$

and the initial condition is taken as

$$
T = T_0 \quad \text{for } t = 0 \tag{1f}
$$

in the region where the thermal conductivity components $k_x(T)$, $k_y(T)$ and the heat capacity $C(T)$ are assumed to depend on temperature linearly in the form

$$
k_x(T) = k_{x0} + k_{x1}T
$$
 (2a)

$$
k_{y}(T) = k_{y0} + k_{y1}T
$$
 (2b)

$$
C(T) = C_0 + C_1 T.
$$
 (2c)

Once the boundary and initial conditions and the thermal properties are specified, the direct problem defined by equations (1) and (2) can be solved numerically and the temperature distribution can be calculated as a function of time and position anywhere in the medium.

INVERSE PROBLEM

The thermal properties as defined by equations (2) involve six unknown coefficients, C_0 , C_1 , k_{x0} , k_{x1} , k_{y0} , $k_{\nu l}$, for their determination. The inverse problem considered here is concerned with the estimation of these six coefficients from the knowledge of transient tem perature measurements taken at three different locations on the surface of the region. It is assumed that the temperature data are obtained by three sen sors placed at the locations $(0, 0)$, $(0.4a, 0)$ and $(0, 0)$ 0.4b). The inverse problem can then be regarded as an optimization problem which aims at finding the unknown thermal property vector $P \equiv [P_1, \ldots, P_n]$ P_0]^T = [C₀, C₁, k_{x0}, k_{x1}, k_{y0}, k_y]^T that minimizes the following sum of squares function

$$
S(\mathbf{P}) = \sum_{i=1}^{n_i^* n_i} [T_i(\mathbf{P}) - Y_i]^2 = \mathbf{F}^T \mathbf{F}
$$
 (3)

where

$$
F_i \equiv T_i - Y_i \tag{4}
$$

and n_s is the number of sensors ($n_s = 3$ for the present problem) and n_i is the number of temperature recordings per thermocouple during the experiment. In addition $T_i(\mathbf{P})$ is the computed temperature at the sensor location at time corresponding to the ith measurement and Y_i is the *i*th temperature measurement. The temperature $T_i(P)$ is obtained from the solution of the direct problem defined previously for specified thermal property coefficients. The function F_i is defined by equation (4), vanishes when T_i is computed using the exact values of the property coefficients and Y_i contains no measurement errors.

The parameters P , which minimize the function S defined by equation (3), satisfy the following set of nonlinear algebraic equations

$$
\sum_{i=1}^{n_i^* n_i} \frac{\partial T_i}{\partial P_j} (T_i - Y_i) = 0, \quad j = 1-6 \tag{5}
$$

which are obtained by differentiating equation (3) with respect to each of the parameters **P** and setting these derivatives equal to zero. To solve the resulting system of algebraic equations (5), the Levenberg-Marquardt iterative method is chosen. This algorithm combines the steepest descent and Newton methods. Starting the iterations with a large value of the Levenberg-Marquardt parameter μ , more emphasis is given initially to the steepest descent method, since a good initial guess is not required with this method; but the convergence is slow. As the value of the parameter μ is gradually reduced at each iteration step, the weight is increasingly shifted to the Newton method which converges faster [3, 4].

By expanding T_i in a Taylor series, retaining only the first-order terms and adding the Levenberg-Marquardt parameter μ , we obtain the following formula to compute the search direction for the parameters P

$$
\mathbf{P}^{n+1} = \mathbf{P}^n - (\mathbf{J}^T \mathbf{J} + \mu^n \mathbf{I})^{-1} \mathbf{J}^T \mathbf{F} \tag{6a}
$$

where

$$
J_{ij} = \frac{\partial T_i}{\partial P_j} \tag{6b}
$$

are the elements of the Jacobian matrix J, I is the identity matrix and the superscript n is the iteration index. Setting the parameter μ^n equal to zero, the Newton method is obtained; and as $\mu^n \to \infty$, the steepest descent method is realized. The solution of the inverse problem starts with a suitable guess \mathbf{P}^0 , and the iterations are continued until

$$
|P_i^{n+1} - P_i^n| < \varepsilon, \quad i = 1 - 6 \tag{7}
$$

where ε is a small number.

The elements of the Jacobian matrix J_{ii} , known as the sensitivity coefficients, can be calculated from the following central finite differencing formula

$$
\frac{\partial T_i(\mathbf{P})}{\partial P_j} \approx \frac{T_i(\mathbf{P} + \varepsilon U_j) - T_i(\mathbf{P} - \varepsilon U_j)}{2\varepsilon} \tag{8}
$$

where $U_j = [\delta_{1j}, \ldots, \delta_{6j}]^T$, δ is the Kronecker delta and e is a small number.

STATISTICAL ANALYSIS

The statistical analysis of uncertainty in the inverse solution results is useful in order to estimate the computation accuracy. Assuming that the temperature measurement errors are additive, independent and have zero means with constant variances σ^2 , then the standard deviation of the estimated thermal property P_i is given by [5]

$$
\sigma_{P_i} = \sigma \sqrt{\left\{ \left[\left(\frac{\partial T^T}{\partial P} \right) \left(\frac{\partial T}{\partial P^T} \right) \right]^{-1} \right\}_i}.
$$
 (9)

If we also assume a normal distribution for the temperature measurement errors and 99% confidence bounds for the computed thermal property P_i , then we have

Probability
$$
[P_{i} - 2.576\sigma_{pi}] < P_{i\text{exact}} \\
&< (P_{i} + 2.576\sigma_{pi})] \simeq 99\%.\tag{10}
$$

SOLUTION ALGORITHM

Having established the basic computational steps needed for the solution of the above inverse problem, we now present the solution algorithm.

Let P^n , $T_i(P^n)$, μ^n and S^n values be available at the nth iteration level. The calculations are carried out in the following manner.

- Step 1. Compute the sensitivity coefficients $\partial T_i/\partial P_j$ using equations (1) , (2) and (8) .
- Step 2. Knowing $T_i(P^n)$, Y_i , P^n , μ^n , and the sensitivity coefficients, compute a new set of thermal properties P from equation (6).
- Step 3. Solve the direct problem given by equations (1) and (2) to find $T_i(\mathbf{P})$.
- Step 4. Find a corresponding new S from equation (3).
- Step 5. If $S > S^n$; double the value of μ^n , update S^n to S and go back to step (2) . If not, set $\mu^{n+1} = \mu^n/2$ and go on to the next step.
- Step 6. Check if condition (7) is met. If not, update P^n , $T_i(P^n)$ and S^n to P, $T_i(P)$ and S respectively and go back to step (1).

RESULTS AND DISCUSSION

To demonstrate the validity and accuracy of the method of inverse analysis considered here for the

Table 1. Initial guess is one tenth of the exact value, $\sigma = 0.0$

\boldsymbol{S}	μ	$C_0 \times 10^{-6}$	$C_1 \times 10^{-3}$	k_{x0}	$k_{\rm rl} \times 10^3$	k_{v0}	$k_{y1} \times 10^3$
38508940	100.000	0.1700	0.2608	0.0608	0.0125	0.4752	0.7320
9475679	50.000	0.3242	0.6783	0.0826	0.0982	0.9521	1.7717
1829981	25.000	0.6143	1.2915	0.1356	0.5420	2.0713	2.9610
223980	12.500	1.0527	1.6523	0.3932	0.8631	3.6969	3.4831
12242	6.250	1.5024	1.7858	0.5711	0.9646	4.7407	3.6636
134	3.125	1.7023	1.8247	0.6120	0.9903	5.0828	3.7185
24	1.562	1.7198	1.8396	0.6121	1.0023	5.1446	3.7452
23	0.781	1.7185	1.8569	0.6093	1.0181	5.1456	3.7817
21	0.391	1.7176	1.8934	0.6029	1.0469	5.1348	3.8541
19	0.195	1.7162	0.9616	0.5904	1.1037	5.1131	3.9934
15	0.098	1.7133	2.0810	0.5705	1.1902	5.0755	4.2402
10	0.049	1.7105	2.2400	0.5405	1.3179	5.0174	4.6302
6	0.024	1.7067	2.4344	0.5103	1.4126	4.9436	5.1717
3	0.012	1.7062	2.5192	0.5099	1.2869	4.8771	5.7740
	0.006	1.7044	2.5769	0.5326	0.9572	4.8192	6.3959
0	0.003	1.7013	2.6219	0.5675	0.5419	4.7804	6.8824
$\bf{0}$	0.002	1.7001	2.6188	0.5950	0.2586	4.7615	7.1754
0	0.001	1.7002	2.6101	0.6045	0.1577	4.7530	7.2930
0	0.000	1.7000	2.6082	0.6076	0.1299	4.7519	7.3153
$\bf{0}$	0.000	1.7000	2.6077	0.6081	0.1249	4.7516	7.3198
0	0.000	1.7000	2.6080	0.6081	0.1250	4.7516	7.3200
The solution		1.7000	2.6080	0.6081	0.1250	4.7516	7.3200
Standard deviations		0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
% error		0.0	0.0	0.0	0.0	0.0	0.0

estimation of thermal property coefficients, we present the following numerical experiments.

The dimensions of the physical domain are taken as

 $a=b=5$ cm

thermal conductivity coefficients as

$$
k_{x0} = 0.6081 \, \text{W m}^{-1} {}^{\circ}\text{C}^{-1},
$$
\n
$$
k_{x1} = 0.125 \times 10^{-3} \, \text{W m}^{-1} {}^{\circ}\text{C}^{-2}
$$
\n
$$
k_{y0} = 4.752 \, \text{W m}^{-1} {}^{\circ}\text{C}^{-1},
$$
\n
$$
k_{y1} = 7.32 \times 10^{-3} \, \text{W m}^{-1} {}^{\circ}\text{C}^{-2}
$$

and the heat capacity coefficients as

$$
C_0 = 1.7 \times 10^6 \,\mathrm{J} \,\mathrm{m}^{-3} {}^{\circ}\mathrm{C}^{-1},
$$

\n
$$
C_1 = 2.608 \times 10^3 \,\mathrm{J} \,\mathrm{m}^{-3} {}^{\circ}\mathrm{C}^{-2}.
$$

Initial temperature of the medium is $T_0 = 20$ °C and the applied heat flux $q = 25$ kW m⁻². Thermal conductivity data chosen here are representative of APC-2 (aromatic polymer composite) [6].

The simulated experimental temperature data are generated by solving the direct heat conduction problem defined by equations (1) and (2) with the explicit finite difference scheme taking time increments of $\Delta t = 0.1$ s and space steps of $\Delta x = \Delta y = 1$ cm. Temperature readings were recorded every 5 s for each of the three thermocouples. The first sensor gave the highest temperature at any time despite the geometric symmetry of the rectangular region, the second sensor had readings higher than the third one because of higher thermal conductivity in the y direction. The simulated measured temperature Y_{measured} is obtained by adding an error term $\omega\sigma$ to the computed exact temperature T_{exact} as

$$
Y_{\text{measured}} = T_{\text{exact}} + \omega \sigma
$$

where σ is the standard deviation of measurement errors. Assuming 99% confidence for the measured data, ω lies in the range $-2.576 \le \omega \le 2.576$ and it is randomly generated by using the IMSL subroutine DRNNOR [7].

Tables 1 to 4 are prepared to demonstrate the effects of the initial guess for the values of the thermal property coefficients $P^0 = \{k_{x0}, k_{x1}, k_{y0}, k_{y1}, C_0, C_1\}^0$ and the Levenberg-Marquardt parameter μ^0 on the convergence of the inverse solution. Tables 1 and 2 are for the cases when the initial guess underestimates the values of these coefficients, while Tables 3 and 4 overestimate them. A large number of cases falling between these two limiting situations have also been examined, but the results are not presented here. It is observed that the solution of the inverse problem considered here would converge with an initial guess underestimating the coefficients by as low as one-tenth of the exact values for the case of no measurement error (i.e. $\sigma = 0$) as shown in Table 1. For this case, the starting value of the Levenberg-Marquardt parameter μ^0 should not be less than that taken in this table for convergence. Table 1 also shows that for experimental data with no measurement error (i.e. $\sigma = 0$, the solution produces exact results for the computed thermal properties. Table 2 presents results similar to those given in Table 1, except the experimental data contain measurement errors of standard deviation $\sigma = 1.0$. In this case, the inverse analysis produces the thermal property coefficients with errors

Table 2. Initial guess is one tenth of the exact value, $\sigma = 1.0$

S	μ	$C_0 \times 10^{-6}$	$C_1 \times 10^{-3}$	k_{x0}	$k_{\rm rel} \times 10^3$	$k_{\nu 0}$	$k_{y1} \times 10^3$
38518260.0	50.0000	0.1700	0.2608	0.0608	0.0125	0.4752	0.7320
9463424.0	25.0000	0.3221	0.6830	0.0987	0.0652	0.9360	1.8136
1878993.4	12.5000	0.6012	1.4117	0.1326	0.4684	1.9525	3.2808
232581.5	6.2500	1.0306	1.8715	0.3760	0.8606	3.5953	3.9647
12632.6	3.1250	1.4767	2.0362	0.5665	0.9776	4.7128	4.1702
217.3	1.5625	1.6902	2.0826	0.6003	1.0042	5.0240	4.2243
112.0	0.7812	1.7153	2.1055	0.5956	1.0169	5.0537	4.2531
111.2	0.3906	1.7141	2.1463	0.5902	1.0388	5.0473	4.2993
109.9	0.1953	1.7114	2.2237	0.5811	1.0711	5.0319	4.3920
107.7	0.0977	1.7074	2.3531	0.5632	1.1515	5.0045	4.5516
105.1	0.0488	1.7011	2.5405	0.5425	1.2175	4.9639	4.8131
102.9	0.0244	1.6956	2.7137	0.5268	1.2263	4.9142	5.1762
101.2	0.0122	1.6894	2.8979	0.5199	1.1353	4.8584	5.6345
100.5	0.0061	1.6840	3.0075	0.5309	0.9408	4.8257	5.9540
100.0	0.0031	1.6819	3.0499	0.5474	0.7238	4.7970	6.2767
99.8	0.0015	1.6784	3.0902	0.5718	0.4568	4.7848	6.4768
99.8	0.0031	1.6793	3.0799	0.5668	0.5090	4.7858	6.4536
99.8	0.0015	1.6792	3.0811	0.5674	0.5021	4.7855	6.4591
99.8	0.0008	1.6825	2.9631	0.6034	0.2082	4.7865	6.6168
The solution		1.6794	3.0357	0.5999	0.1977	4.7764	6.6776
Standard deviations		0.0352	0.6299	0.0934	0.8977	0.0858	0.8850
$%$ error		1.2	16.4	1.3	58.2	0.5	8.8

Table 3. Initial guess is five times the exact value, $\sigma = 0.0$

varying from 0.5% to 58%. The worst error occurs m the estimation of the coefficient k_{x1} , which is the smallest of the six different coefficients considered here.

Tables 3 and 4 illustrate the convergence of the solution when the initial guesses overestimate the coefficients by a factor of five. Table 3 presents results for the case of experimental data containing no measurement errors (i.e. $\sigma = 0$) and the inverse solution converges to the exact values of the thermal property coefficients. Table 4 presents results similar to those given in Table 3, except the experimental data contain measurement errors of standard deviation

Table 4. Initial guess is five times the exact value, $\sigma = 0.5$

S	μ	$C_0 \times 10^{-6}$	$C_1 \times 10^{-3}$	k_{x0}	$k_{\rm H} \times 10^3$	k_{10}	$k_{y1} \times 10^3$
710418.5	500.0000	8.5000	13.0400	3.0405	0.6250	23.7580	36.6000
703992.6	250.0000	8.2795	13.0332	2.9568	0.6220	23.7063	36.5981
690061.8	125.0000	6.8273	13.0186	2.7853	0.6145	23.6028	36.5942
656074.5	62.5000	68584	12.9872	2.4070	0.6005	23.3907	36.5862
548150.8	31.2500	4.6586	12.9145	1.5494	0.5655	22.9673	36.5689
295374240.0	62.5000	-0.4325	12.7252	-0.4292	0.4718	22.2199	36.5348
229995.8	31.2500	1.5649	12.7995	0.3041	0.5075	22.5510	36.5499
79696224.0	62.5000	-0.2929	12.7178	0.8098	0.5100	22.0804	36.5134
136196.4	31.2500	0.0303	12.7322	0.4357	0.5024	22.2969	36.5306
103554.2	15.6250	0.1607	12.6684	1.0639	0.4934	21.9615	36.4846
99603.3	7.8125	0.1696	12.5220	1.5206	0.4545	21.2717	36.4018
95569.9	3.9062	0.1888	12.1970	1.7577	0.3520	19.8646	36.2303
86407.1	1.9531	0.2538	11.5751	1.8000	0.1405	16.8948	35.8834
58414.4	0.9766	0.4274	10.3958	1.5755	-0.3029	10.3477	35.1024
77637.2	1.9531	0.9642	8.3900	0.6597	-1.1351	-0.2036	33.6732
17621.5	0.9766	0.8077	9.2736	0.8641	-0.8315	2.9194	34.1603
4671.3	0.4883	1.3887	9.0697	0.0953	-1.2041	1.7347	33.4952
1326.6	0.2441	1.5582	8.8468	0.2071	-2.1209	1.9881	32.4085
1040.0	0.1221	1.5686	8.5258	0.3524	-3.3632	2.1874	30.6493
727.4	0.0610	1.5503	7.9994	0.5883	-5.0490	2.5450	27.9492
438.1	0.0305	1.5372	7.0320	0.8863	-6.7834	3.0373	24.1392
235.4	0.0153	1.5746	5.3301	1.1333	-7.6694	3.6165	19.5446
108.6	0.0076	1.6190	3.8586	1.1909	-6.6531	4.1410	14.8118
48.4	0.0038	1.6569	3.0927	0.9978	-3.9884	4.5147	10.7510
28.5	0.0019	1.6878	2.6763	0.7421	-1.2055	4.6783	8.3770
25.3	0.0010	1.6890	2.7960	0.6421	-0.2371	4.7385	7.3787
24.9	0.0005	1.6902	2.8271	0.5968	0.2152	4.7599	7.0145
The solution		1.6899	2.8220	0.6013	0.1873	4.7646	6.9824
Standard deviations		0.0176	0.3132	0.0471	0.4613	0.0432	0.4427
$%$ error		0.6	8.2	1.1	49.9	0 ₃	4.6

 $\sigma = 1.0$. The errors involved in the estimation of the thermal property coefficients are small except for the case of the coefficient k_{x1} which has the smallest value. As expected, the errors in the estimated coefficients increase as the standard deviation of the temperature measurement error, σ , increases.

The effect of the sensor location on the accuracy of estimation is also examined by placing the sensors at the inner locations $(0.2a, 0.2b)$, $(0.6a, 0.2b)$ and $(0.2a, 0.2b)$ 0.6b) and conducting computations similar to those discussed previously. The accuracy of the inverse analysis did not seem to be affected by such a change in the sensor location.

The CPU time for the computations with an IBM RS6000 system was of the order of a few minutes.

CONCLUSION

Inverse analysis utilizing an iterative procedure based on minimizing the sum of squares function with the Levenberg-Marquardt method can be used to estimate the thermal conductivity components $k_x(T)$, $k_v(T)$ and the specific heat capacity $C(T)$ varying linearly with temperature in an orthotropic solid.

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