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ESTIMATION OF A STATE-DEPENDENT MODEL PARAMETER

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Abstract—A numerical algorithm was developed which estimates a state-dependent model parameter on the basis of transient state observation data. The algorithm was presented for the problem of estimating the temperature dependence of thermal diffusivity in a one-dimensional heat equation. The estimation problem was converted into a finite dimensional optimization problem by the least-squares formulation and B-splines representation of the parameter. Numerical experiments were performed using simulated observation data as well as the actual observation data obtained in a heat conduction experiment on rubber compound layers. The performance of the algorithm was discussed in relation to the effect of the parameter representation scheme, the quality and quantity of the data.

Key words: *State-dependent Parameter, Parameter Estimation, B-Splines Representation, Least-squares Method, Temperature-dependent Thermal Diffusivity*

INTRODUCTION

The model equations for a chemical process which are derived from application of the conservation principles are commonly called *state equations*, and the dependent variables of the equations are called *state variables*. The model parameters which represent material properties are usually dependent on the state variables such as temperature or concentration. Temperature-dependent thermal conductivity in a heat equation and concentration-dependent diffusivity in a diffusion equation are examples of the state-dependent model parameters. In modeling chemical processes the state-dependence of the model parameters should not be neglected to get accurate model predictions.

For pure substances the dependence of transport coefficients on temperature or concentration has been the subject of theoretical investigations for many years [Reid et al., 1987]. For compounds, however, theoretical correlations on such dependence are seldom available, or are only of dubious value for practical purposes. In practice the state dependence is usually found by regression. For example, in the tire industry the temperature dependence of thermal conductivity of a rubber compound is found by regression of several conductivity values each of which was measured under isothermal condition using a special apparatus. This procedure can be replaced by a simple heat conduction experiment on rubber layers followed by direct estimation of the dependence on the basis of transient temperature observation data [Toth et al., 1991].

This study aims to develop a numerical algorithm to estimate the state dependence of a model parameter on the basis of transient state observation data. The following one-dimensional heat equation is considered as a specific example

$$\frac{\partial u}{\partial t}=\frac{\partial}{\partial x}\left[\alpha(u)\frac{\partial u}{\partial x}\right]+f(x,\ t,\ u)$$

$$\text{I.C.: } u(x,\ 0)=u_0(x)$$

$$\text{B.C.: } \beta_0 u(0,\ t)+\delta_0\frac{\partial u}{\partial x}(0,\ t)=\delta_0$$

$$\beta_L u(L,\ t)+\gamma_L\frac{\partial u}{\partial x}(L,\ t)=\delta_L \tag{1}$$

where the state u denotes temperature, $\alpha(u)$ the temperature-dependent thermal diffusivity of the medium. The parameter estimation problem associated with the model (1) can be stated as follows:

When the source term f, I.C., and B.C. are known, estimate the parameter function $\alpha(u)$ on the basis of observation data $u^{obs}(x_i, t_j)$, $i=1,\cdots, n_x$; $j=1,\cdots,n_t$.

Below the estimation algorithm is presented and tested through numerical experiments using simulated data as well as the actual data obtained from a heat conduction experiment on rubber compound layers.

PARAMETER ESTIMATION ALGORITHM

1. Least-Squares Formulation

The estimation problem is formulated as a nonlinear optimization problem of minimizing an objective functional of the form

$$\min_{\alpha}\ J(\alpha)=\sum_{i=1}^{n_x}\sum_{j=1}^{n_t}\{u(x_i,\ t_j;\ \alpha)-u_{ij}^{obs}\}^2 \tag{2}$$

In most cases where the output data are the only information available on the system, a least-squares functional is regarded as the most natural criterion. Depending on the availability of valid statistical assumptions on observation errors or *a priori* information on the parameter, one may use a modified objective functional [Cooley, 1977].

2. B-Splines Parameter Representation

For numerical implementation of the least-squares regression stated in (2) the parameter function $\alpha(u)$ should be *discretized* in the following sense: The conceptually infinite-dimensional function space to which $\alpha(u)$ belongs is to be constricted to a finite dimensional space with a suitable basis [Chung and Kravaris, 1988]. This will effectively converts the optimization problem of (2) into an approximate finite-dimensional one. When the form of the function $\alpha(u)$ is known, our parameter estimation problem simply reduces to the estimation of the constant coefficients ap-

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pearing in the expression of $\alpha(u)$. When such an *a priori* information on $\alpha(u)$ is not available, B-splines are proposed here as an effective means of approximate representation of the parameter.

B-splines representation of the parameter function $\alpha(u)$ in the model (1) proceeds as follows. First, an interval $[u_{min}, u_{max}]$ is chosen such that the expected range of variation of the state variable in (1) is included. The interval is divided into l subintervals to define a break point sequence $b=(b_1, b_2, \cdots, b_{l+1})$ satisfying

$$u_{min}=b_1<b_2<\cdots<b_l<b_{l+1}=u_{max} \tag{3}$$

Next are chosen the order k of piecewise polynomials to be defined on each subinterval and the number of continuity conditions ν to be imposed at each of the interior break points, $b_2, \cdots, b_l$. The space $P_{l,k,\nu}$ of piecewise polynomials thus defined is a linear space with the dimension $N=(k-\nu)\,l+\nu$, and its basis is called the *B-splines* [de Boor, 1978]. The specification l, k, ν of the space $P_{l,k,\nu}$ is used to generate a knot sequence $\xi=(\xi_1, \cdots, \xi_{N+k})$ which satisfies the following:

(1) $\xi_1=\cdots=\xi_k=b_1$, $\xi_{N+1}=\cdots=\xi_{N+k}=b_{l-1}$;
(2) $b_2, \cdots, b_l$ are placed $(k-\nu)$ times, respectively.

Then the i-th spline $B_i(u)$ is defined as

$$B_i(u)=(\xi_{i+k}-\xi_i)[\xi_i, \cdots, \xi_{i+k}](\tau-u)_+^{k-1} \tag{4}$$

where $[\xi_i, \cdots, \xi_{i+k}]$ denotes the k-th divided difference with respect to the dummy variable τ and $(\tau-u)_+^{k-1}$ denotes a truncated power function of order k

$$(\tau-u)_+^{k-1}=\begin{cases}(\tau-u)^{k-1} & \text{if } \tau\geq u\\ 0 & \text{if } \tau<u\end{cases} \tag{5}$$

Finally, the parameter function $\alpha(u)$ is approximated as a linear combination of the B-splines

$$\alpha(u)=\sum_{i=1}^{N}\omega_i B_i(u) \tag{6}$$

The above B-spline representation of $\alpha(u)$ converts the optimization problem of (2) into the following form

$$\min_{\omega} J(\omega)=\sum_{i=1}^{n_x}\sum_{j=1}^{n_t}\{u(x_i, t_j; \omega)-u_{ij}^{obs}\}^2, \text{ where } \omega\in R^N \tag{7}$$

Minimization was performed using the MINPACK routine [Garbow, 1978] which implements the Levenberg-Marquardt algorithm designed for least-squares minimization.

3. Model Solver

The partial differential equation (PDE) of (1) may show severe nonlinearity depending on the form of the state-dependent parameter function $\alpha(u)$. The method of lines (MOL) based on finite difference was employed to develop an efficient solution algorithm to handle the nonlinearity. First the PDE was converted into a system of ordinary differential equations (ODE) by finite difference approximation of the spatial derivatives. Then the nonlinear ODE system was solved using the DGEAR routine [Hindmarsh, 1974] for solving initial value problems.

Finite difference approximation of the spatial derivatives was carried out over N_s equidistant point-centered grids discretizing the domain (0, L). At the interior nodes $(i=2, \cdots, N_s-1)$, the approximation takes the form

$$\frac{\partial}{\partial x}\left[\alpha(u)\frac{\partial u}{\partial x}\right]\Big|_i \approx \frac{\alpha(u)\frac{\partial u}{\partial x}\Big|_{i+1/2}-\alpha(u)\frac{\partial u}{\partial x}\Big|_{i-1/2}}{\Delta x}$$

$$\approx\frac{\alpha(u_{i+1/2})(u_{i+1}-u_i)-\alpha(u_{i-1/2})(u_i-u_{i-1})}{(\Delta x)^2} \tag{8}$$

where

$$u_{i+1/2}\approx\frac{u_i+u_{i+1}}{2},$$
$$u_{i-1/2}\approx\frac{u_{i-1}+u_i}{2} \tag{9}$$

At the boundary nodes ($i=1$ and N_s), a different scheme was used to make use of the boundary condition as follows:

$$\begin{aligned}\frac{\partial}{\partial x}\left[\alpha(u)\frac{\partial u}{\partial x}\right]\Big|_1 &\approx \left[\alpha(u)\frac{\partial^2 u}{\partial x^2}+\frac{d\alpha}{du}(u)\left(\frac{\partial u}{\partial x}\right)^2\right]_1\\ &\approx\frac{2\alpha(u_1)}{(\Delta x)^2}\left(u_2-u_1-\frac{\delta_0-\beta_0 u_1}{\gamma_0}\Delta x\right)\\ &\quad+\frac{d\alpha}{du}(u_1)\left(\frac{\delta_0-\beta_0 u_1}{\gamma_0}\right)^2\end{aligned} \tag{10}$$

$$\begin{aligned}\frac{\partial}{\partial x}\left[\alpha(u)\frac{\partial u}{\partial x}\right]\Big|_{N_s} &\approx\frac{2\alpha(u_{N_s})}{(\Delta x)^2}\left(u_{N_s-1}-u_{N_s}+\frac{\delta_L-\beta_L u_{N_s}}{\gamma_{N_s}}\Delta x\right)\\ &\quad+\frac{d\alpha}{du}(u_{N_s})\left(\frac{\delta_{N_s}-\beta_{N_s}u_{N_s}}{\gamma_{N_s}}\right)^2\end{aligned} \tag{11}$$

NUMERICAL EXPERIMENTS

The performance of the estimation algorithm was tested through numerical experiments. Depending on how the observation data were obtained, our estimation runs are divided into two groups using the simulated data and the actual experimental data, respectively.

1. Simulated Data Generation

Hypothetical observation data were generated for the system governed by

$$\frac{\partial u}{\partial t}=\frac{\partial}{\partial x}\left[\alpha(u)\frac{\partial u}{\partial x}\right]$$

$$\text{I.C.: } u(x, 0)=25$$
$$\text{B.C.: } u(0, t)=u(0.02, t)=150 \tag{12}$$

The true parameter function $\alpha(u)$ was assumed to have the following forms for $u\in[25, 150]$.

$$\alpha_{T1}(u)=1.75\times10^{-7}-3.33\times10^{-10}u \tag{13}$$

$$\alpha_{T2}(u)=1.67\times10^{-7}+3.33\times10^{-9}u-1.67\times10^{-11}u^2 \tag{14}$$

The numerical solution to (12) were obtained using 101 grid points. Random numbers with normal distribution $N(0, \sigma)$ were generated and added to the numerical solutions at the assumed sensor locations in order to simulate the observation error. Several combinations of the error level σ and the number of sensors n_x were used in order to address the effect of the quality and quantity of observation data on the estimation performance.

For an easy grasp of the relative magnitude of numerical values involved, the governing equation was converted into a dimensionless form beforehand. The state variable u was transformed into the dimensionless state $\bar{u}$ according to

$$\bar{u}=\frac{u-u_{min}}{u_{max}-u_{min}} \tag{15}$$

where $u_{min}=25$℃ and $u_{max}=150$℃. The interval $[u_{min}, u_{max}]$ indicates the range of variation of u in the system governed by (12),

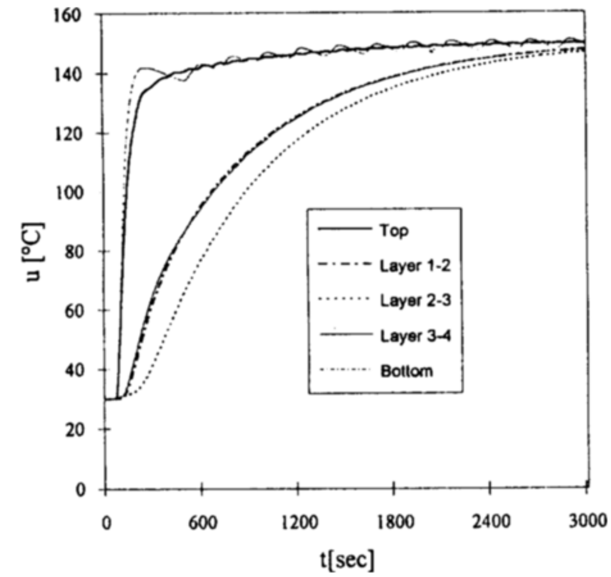

Fig. 1. Measured temperature profiles in a stack of rubber compound layers.

and is also used in the B-spline representation of $\alpha(u)$. The independent variables x, t and the parameter α were scaled by the reference values of 0.02 m, 1500 sec and 1.67×10^{-7} m^2/sec to define the dimensionless quantities $\bar{x}$, $\bar{t}$, and $\bar{\alpha}$, respectively. Under such transformations of variables, the true parameter functions to be estimated can be expressed in dimensionless forms as

$$\bar{\alpha}_{T1}(\bar{u}) = 1 - 0.25\bar{u} \tag{16}$$

$$\bar{\alpha}_{T2}(\bar{u}) = 1.4375 + 1.875\bar{u} - 1.5625\bar{u}^2 \tag{17}$$

2. Actual Data Acquisition

Transient temperature measurements were obtained from a heat conduction experiment on rubber compound layers. Four layers with the thickness 0.0063, 0.0070, 0.0071 and 0.0076 m, respectively, were stacked in folds. The specimen was heated from the top and the bottom surfaces which were to be maintained at constant temperatures in a PI-controlled apparatus. Temperature was measured at every 15 sec for 3000 seconds using five thermocouples which were either attached on the surfaces or inserted between the layers. Fig. 1 shows the measured temperature transients. The aspect ratio of the specimen was large enough for one-dimensional analysis along the thickness direction. In the estimation runs the two temperature curves obtained at the top and bottom surfaces were used as the time-varying boundary conditions for solving the model, while the other curves as the observation data to be compared with the model predictions.

RESULTS AND DISCUSSION

The estimates of the parameter $\alpha(u)$ obtained under varying simulation conditions are presented in Figs. 2-7 in dimensionless forms. Table 1 summarizes the conditions and minimization status of the estimation runs presented in each Figure.

Fig. 2 compares two estimates of α_{T1} obtained under different parameter representation schemes. The 'linear' estimate was obtained by estimating the coefficients a, b in the linear representation a+bu assumed for $\alpha(u)$. Both estimates are close to the true parameter. Furthermore our numerous simulation runs yielded the same estimate in each case regardless of the initial guess $\alpha^{(0)}$, which implies that the global minimum was reached.

Fig. 3 shows α_{T2} and its three estimates with the linear, quadratic, and B-splines representation, respectively. It is clear that the linear estimate cannot adequately describe the variation of the true parameter over the whole range of the state variable. This is also evident from the much larger value of J_{min} in Table 1 compared to the other two estimates. On the other hand, both the quadratic and B-splines estimates are in good agreement with the true parameter. In fact, since the B-splines with the specifica-

Table 1. Summary of conditions and status of estimation runs

Figure No.	True parameter	Observation data specification			Parameter specification	Minimization status			
		σ[°C]	n_x	n_t		$\alpha^{(0)}$	$J^{(0)}$	J_{min}	Iterations
2	α_{T1}	0.5	1	100	Linear	0.9	5.44×10^{-2}	1.52×10^{-3}	6
			@ $\bar{x}$=0.5		B-splines*(1,4,3,4)			1.47×10^{-3}	5
3	α_{T2}	0.5	1	100	Linear	1.5	2.06×10^{-1}	1.93×10^{-3}	8
			@ $\bar{x}$=0.5		Quadratic			1.30×10^{-3}	12
					B-splines(1,4,3,4)			1.25×10^{-3}	5
4	α_{T1}	0.5	1	100	B-splines	0.9	5.44×10^{-2}	1.47×10^{-3}	5
		1.0	@ $\bar{x}$=0.5		(1,4,3,4)		5.94×10^{-2}	5.72×10^{-3}	5
		2.0					7.73×10^{-2}	2.34×10^{-2}	8
5	α_{T1}	0.1	1	100	B-splines(1,4,3,4)	0.9	5.36×10^{-2}	5.60×10^{-5}	6
			@ $\bar{x}$=0.5		B-splines(5,4,3,8)			4.92×10^{-5}	4
					B-splines(10,4,3,13)			4.90×10^{-5}	24
6	α_{T1}	0.1	3	100	B-splines(1,4,3,4)	0.9	1.31×10^{-1}	1.82×10^{-4}	5
			@ $\bar{x}$=0.25		B-splines(5,4,3,8)			1.81×10^{-4}	6
			0.5, 0.75		B-splines(10,4,3,13)			1.78×10^{-4}	10
7	Unknown	Unknown	3	200	Linear	1.0	1.72	5.41×10^{-2}	7
			@ $\bar{x}$=0.23,		Quadratic			5.42×10^{-2}	11
			0.48, 0.73		B-splines(1,4,3,4)			5.40×10^{-2}	13
					B-splines(2,4,3,5)			5.32×10^{-2}	10

*B-splines specification in terms of (l, k, ν, N)

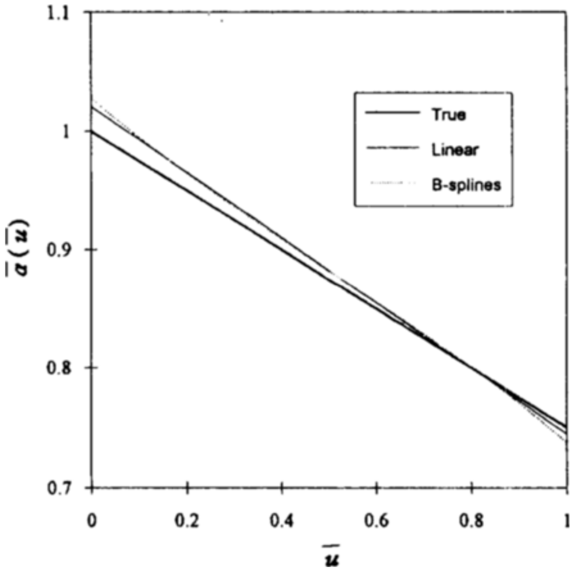

Fig. 2. Linear and B-splines estimates of α_{T1}.

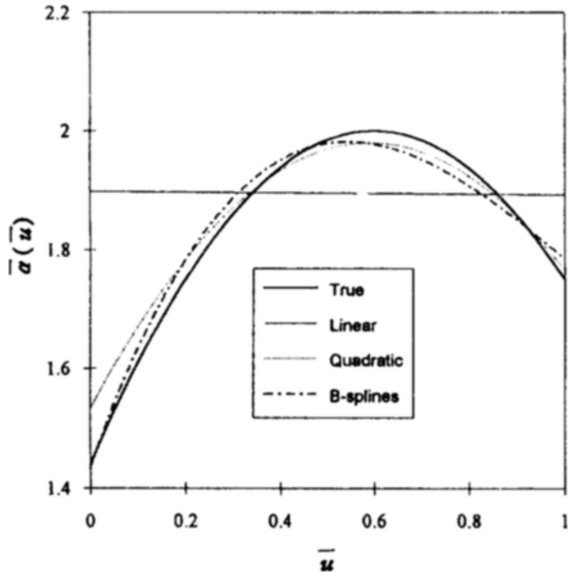

Fig. 3. Linear, quadratic, and B-splines estimates of α_{T2}.

tion (1,4,3,4) is equivalent to a cubic polynomial, it has the capability of describing the state-dependent variation of the true parameters used in our simulation.

Fig. 4 shows the effect of the level of observation error on the estimation performance. As the error level increases, the resulting B-splines estimate becomes more inaccurate.

Fig. 5 shows how the B-splines estimates behave as the level of discretization N is increased for the parameter function. When an excessive number of splines are employed for parameter representation, the estimate shows a symptom of instability in the form of growing oscillations. This is due to the lowered sensitivity of the model output with respect to each spline coefficient. Such ill-conditioned estimates also show up in the estimation of the spatially-varying parameters in distributed parameter systems [Yeh, 1986; Chung and Kravaris, 1988]. Fig. 6 shows that ill conditioning can be alleviated a little when more observation data, obtained using additional sensors, can be utilized in the estima-

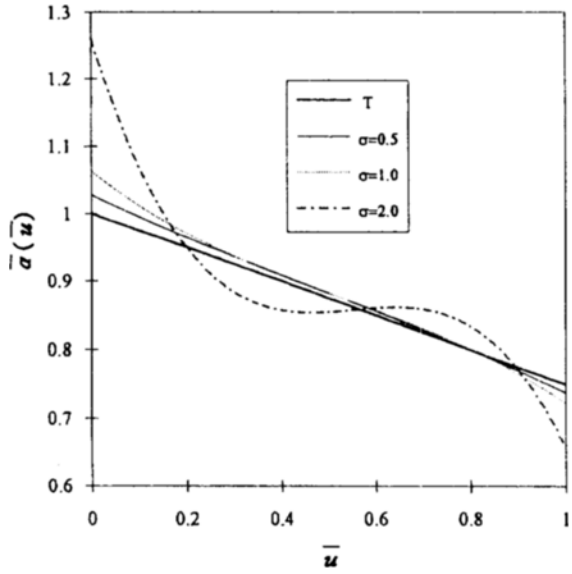

Fig. 4. Effect of the level of observation error on the B-splines estimates of α_{T1}.

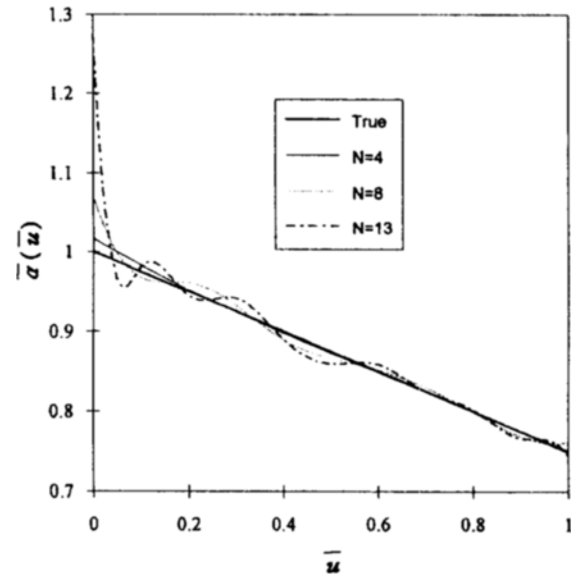

Fig. 5. Effect of the level of discretization on the B-splines estimates of α_{T1} when $n_s = 1$.

tion.

The increasing number of splines facilitate the representation of complex patterns of variation of α(u). It also leads to the smaller values of the objective function in the least-squares estimation as shown in Table 1. However, Figs. 5 and 6 clearly points out that the smaller J_{min} obtained using higher N does not necessarily correspond to the better estimate when error-corrupted data are used in the estimation. It is because the least-squares minimization procedure forces the model output to blindly track even the error components in the data. Such tracking is possible only when the parameter α(u) is allowed to vary freely with u as an element of a high dimensional function space, but the ensuing ill-conditioned estimate is usually contrary to our physical intuition on the expected behavior of the parameter.

The best performance was achieved in Figs. 5 and 6 with the

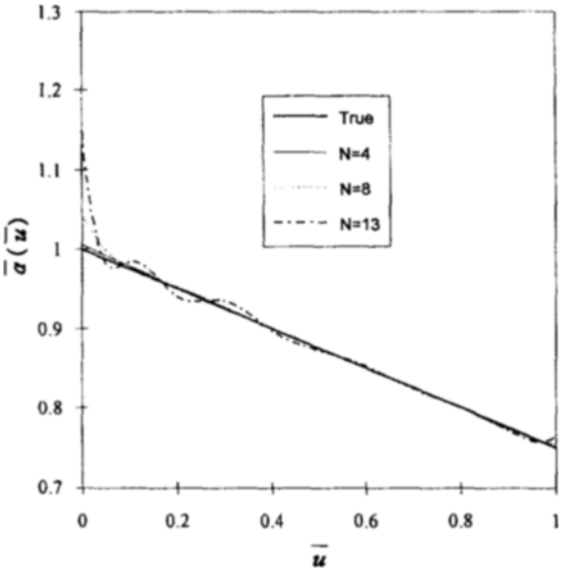

Fig. 6. Effect of the level of discretization on the B-splines estimates of α_{T1} when $n_x=3$.

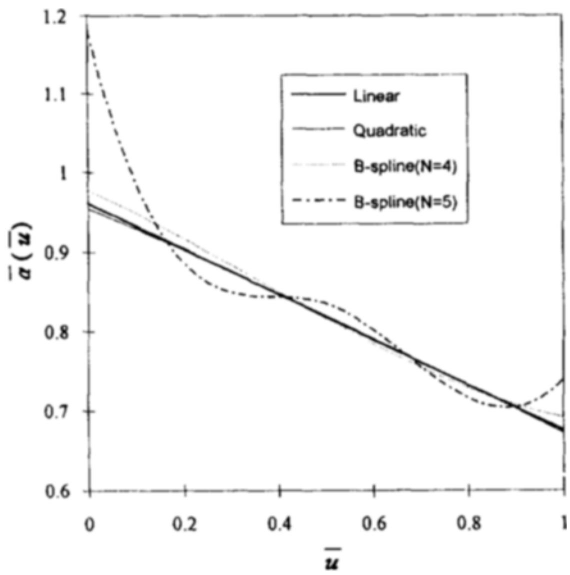

Fig. 7. Estimates of the temperature-dependence of the thermal diffusivity of the rubber compound.

B-spline specification (1,4,3,4) because the simple linear shape of α_{T1} can be sufficiently described by the small number of splines. There is no definitive method of determining the optimal level of discretization when the true parameter is unknown in practice. But it is believed that the state dependence of the parameters encountered in most practical applications can be represented well enough by a small number of splines. The final decision ought to be guided by engineering judgment on the expected behavior of the parameter.

Fig. 7 show the four estimates of the thermal diffusivity of the rubber compound obtained by using the actual data shown in Fig. 1. The dimensionless state variable $\bar{u}$ was based on $u_{min}=30$℃ and $u_{max}=152$℃. The estimation runs were executed in sequence by increasing the number of basis functions one by one. Almost identical estimates were obtained in the first three cases. But the B-splines estimate with N=5 appears to reveal an initial symptom of ill-conditioning: The estimates with higher N were found to be increasingly oscillatory. Considering such behavior of the estimates with increasing N, the B-splines estimate with N=4 was taken as the best one describing the temperature-dependence of the thermal diffusivity of the rubber compound used in the experiment.

CONCLUSIONS

A numerical algorithm was developed which estimates the temperature dependency of the thermal diffusivity in a heat equation. The estimation problem was formulated into a finite dimensional optimization problem by the least-squares method and B-spline approximation of the parameter. A stable solution to the nonlinear model equation was found by the method of lines based on finite difference scheme. The performance of the algorithm was tested through numerical experiments using the simulated data and the actual data. The B-spline approximation using a small number of splines was proposed as a method of representing the state dependence of the parameter when its functional form is not known *a priori*.

ACKNOWLEDGEMENT

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NOMENCLATURE

a, b : coefficients in linear representation of thermal diffusivity $\alpha(u)$ [m^2/sec] and [m^2/sec ℃] respectively
B_i : i-th B-spline function
b : break-point sequence in B-splines representation
f : source term in heat equation [℃/sec]
J : objective function in nonlinear regression
J_{min} : minimized objective function value
k : order of piecewise polynomials
L : length of one-dimensional domain [m]
l : number of subintervals for B-splines representation
N : number of B-splines (dimension of the space)
N_s : # of grid points used in solving state equations
n_x : number of observation points
n_t : number of measurements at each observation point
t : time [sec]
u : temperature [℃]
u^{obs} : temperature observation data [℃]
u_0 : initial temperature distribution [℃]
u_i : temperature at i-th grid point [℃]
x : space variable [m]

Greek Letters

α : thermal diffusivity [m^2/sec]
β_0, γ_0, δ_0 : coefficients in the B.C. at x=0 in (1)
β_L, γ_L, δ_L : coefficients in the B.C. at x=L in (1)
Δx : grid size [m]
σ : standard deviation of observation error [℃]
ν : number of continuity conditions in B-splines representation
τ : dummy variable used in divided-difference
ξ : knot point sequence in B-splines representation

ω : vector of B-spline coefficients

Superscripts

obs : observation data

(0) : initial guess in minimization of objective function

$\bar{}$: dimensionless variable

Subscripts

max : maximum

min : minimum

T : true

REFERENCES

de Boor, C., "A Practical Guide to Splines", Springer-Verlag (1978).

Chung, C.-B. and Kravaris, C., "Identification of Spatially Discontinuous Parameters in Second-order Parabolic Systems by Piecewise Regularization", *Inverse Problems,* **4**, 973 (1988).

Cooley, R. L., "Incorporation of Prior Information on Parameters into Nonlinear Regression Groundwater Flow Models: 1. Theory", *Water Resour. Res.,* **18**, 965 (1982).

Garbow, B. S., MINPACK Project, Argonne Nat. Lab. (1980).

Hindmarsh, A. C., "GEAR: Ordinary Differential Equation System Solver", Lawrence Livermore Lab. Report UCID-30001 (1974).

Reid, R. C., Prausnitz, J. M. and Sherwood, T. K., "The Properties of Gases and Liquids", 4th ed., McGraw-Hill (1987).

Toth., W. J., Chang, J. P. and Zanichelli, C., "Finite Element Evaluation of the State of Cure in a Tire", *Tire Science and Technology,* **19**, 178 (1991).

Yeh, W. W.-G., "Review of Parameter Identification Procedures in Ground Water Hydrology: The Inverse Problem", *Water Resour. Res.,* **22**, 95 (1986).