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Parameter estimation in the presence of uncertain parameters and with correlated data errors ☆

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Abstract

Parameter estimation involves fitting experimental data to a model of the system, represented by $F(p, q)$. Here p are the parameters to be estimated and q are other parameters of the model which are assumed to be known. It is usual to assume that q are known precisely. In many cases, q are known only approximately and it is desired to understand (a) how the uncertainty affects the estimates of p, (b) how to eliminate the dependence of p on q. Both effects can be accommodated by the use of Bayesian probability and treating the q parameters as extraneous variables. Because the errors in the model fitting, i.e., the difference between the data and the model, are functions of q, the errors are correlated although they still may be of zero mean. In addition correlation may exist in the data. These correlations have a substantial effect on the precision of the estimated parameters and require more sophisticated analysis than is usually employed in the least square approach to determining p.

This paper presents the fundamentals of considering uncertain parameters and applies them to a hypothetical experiment involving an uncertain, but constant, parameter and to a real experiment in which the data are cross and autocorrelated.

1. Introduction

Model parameters are usually estimated by minimizing the sum of the squares of the differences between measurements and the model predictions. These differences are termed 'errors' and it is common to assume that the errors have zero mean and are independent and identically distributed. Lacking more specific information, the errors are often assumed to be normally distributed. In the case where the measurements are known to have differing standard deviations, a weighted least squares method is used. In either case, the mathematics is straight forward and the minimization of the least squares is not computationally difficult. In some cases, the system of equations is ill-conditioned and some special techniques, referred to as regularization, may be needed for the estimate to converge [1].

The estimation may be made either by minimizing the sum of the errors squared or by solving an equivalent set of non-linear algebraic equations with a weighting matrix which is diagonal. Modern data acquisition systems are capable of sampling at high rates and it is not uncommon for the measurements to be correlated. When this occurs, the weighting matrix is full and the problem is more difficult because

(a) the correlation must be determined, and
(b) the full matrix often leads to a computationally expensive solution.

Typical parameter estimation assumes that all other parameters of the model are known. When they are not, then the problem becomes one of estimating several parameters and the relatively simple minimization problem becomes a more complex multidimensional minimization problem. If the boundary conditions are unknown, then there may be as many unknown parameters as measurements. For example, if the surface heat flux is to be estimated and the model is a finite difference simulation over N time steps, then there are N values of the flux to estimate, all of which may be correlated. This may make the problem practically impossible.

Under some conditions, approximate values of the heat flux may be known. If a measure of the uncertainty of the heat flux is available, it may be possible to take this uncertainty into account and to maintain the problem at a low

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Nomenclature

bc	boundary conditions
B	uncertain parameter
Bi_0	Biot number at $x = 0$
$E[\varepsilon]$	expected value of ε
$f(\varepsilon)$	probability density (pdf) of ε
$f(T\|P)$	conditional probability of T given P
$f_{\mathrm{pr}}(P)$	prior pdf of P
$F(P, B, t)$	model of the system
$[Fb]$	matrix of sensitivities to boundary conditions
Fo	Fourier number
h	convective heat transfer coefficient
ic	initial conditions
k	thermal conductivity
$\mathcal{I}$	information
LS	sum of uncorrelated errors squared
L	sum of correlated errors squared
$l(T)$	likelihood of T
N	number of readings
$N(a, b)$	Gaussian distribution with a mean of a and a variance of b
P	sought after parameter
$\overline{P}$	mean value of P
$\widehat{P}$	estimated value of P
Q	heat flux
t	time
T	temperature
$\{T\}$	column vector of temperatures
$\{T\}^{\mathrm{T}}$	transpose of $\{T\}$
W	covariance matrix of P
ε	noise, error
ρc	product of density and specific heat
σ_B	standard deviation of B
σ_ε	standard deviation of the noise
$\sigma_{\widehat{P}}$	standard deviation of $\widehat{P}$
$\sigma_{\widehat{P}}^{-2}$	precision of $\widehat{P}$
$\sigma_{\mathrm{pr}}[x]$	standard deviation of the prior distribution of x
Σ	covariance matrix of ε

dimensionality. However, doing so introduces an intrinsic correlation into the weighting matrix. This paper describes how to treat uncertain parameters and shows by example how the correlation impacts the information, and thus the precision of the estimated parameter, which can be gleaned from an experiment.

1.1. Parameter estimation

Consider a transient experiment in which temperatures are measured at several locations as a function of time. Let the temperature be expressed in terms of position, time, boundary conditions, initial conditions and properties by $T = F(x, t, bc, ic, k, \rho c)$ where F is the solution of the appropriate field equation. Those parameters which are to be estimated from the measured temperatures will be represented by P and the uncertain parameters by B. B can include spatial location as well as properties, source strengths, etc. For simplicity we will estimate only one parameter, although the method can easily be extended to a vector of parameters.

The temperatures measured at time t_i, denoted by T_i, will differ from those predicted by the deterministic model by additive measurement noise, ε_i, according to

$$T_i = F(P, B, t_i) + \varepsilon_i \tag{1}$$

Estimation is usually done through the Least Squares approach in which we choose $\widehat{P}$ to be such that the weighted sum of the squares of the errors, LS, is minimized where

$$LS = \sum_{i=1}^{N} w_i \varepsilon_i^2 = \sum_{i=1}^{N} w_i \big(T_i - F(P, B, t_i)\big)^2 \tag{2}$$

where the weights are usually taken to be $w_i = 1/\sigma_i^2$ [2].

Although $\widehat{P}$ can be found by minimizing LS using standard routines, it is more common to determine it by linearizing the problem as follows: Let $\overline{P}$ be the true value of P and expand $T(P)$ in a Taylor series about $\overline{P}$ and retain only the 1st order terms

$$T(P) = T\big(\overline{P}\big) + \left(\frac{\partial F}{\partial P}\bigg|_{\overline{P}}\right)\big(P - \overline{P}\big) \tag{3}$$

Substituting Eq. (3) into Eq. (2) and setting the derivative of LS with respect to P equal to zero yields the equation

$$\widehat{P}_{j+1} = \widehat{P}_j + \frac{\sum_{i=1}^{N} w_i \left(\frac{\partial F}{\partial P}\right)\big|_{t_i, \widehat{P}_j} \left(T_i - F(\widehat{P}_j, B, t_i)\right)}{\sum_{i=1}^{N} w_i \left(\frac{\partial F}{\partial P}\right)^2\big|_{t_i, \widehat{P}_j}} \tag{4}$$

which when iterated to convergence will yield $\overline{P}$ if the errors have zero mean. Although we now have a value of $\widehat{P}$, we have no estimate of $\sigma_{\widehat{P}}$ and Eq. (4) provides no mechanism for including correlated errors. To do this we must look at the problem from a probabilistic point of view.

1.2. Probabilistic point of view—the Bayesian approach

Let the mean and standard deviation of T be represented by

$$E[T] = \int T f(T)\,\mathrm{d}t \tag{5a}$$

$$\sigma_T^2 = \int \big(T - E[T]\big)^2 f(T)\,\mathrm{d}T \tag{5b}$$

where $f(T)$ is the probability density distribution of T. Substituting the one term Taylor series, Eq. (3), into Eq. (5) and

using the relationship between probability density distributions, $f(T)\,\mathrm{d}T = f(P)\,\mathrm{d}P$, yields

$$\sigma_T^2 = \left(\frac{\partial F}{\partial P}\bigg|_{\overline{P}}\right)^2 \sigma_P^2 \tag{6}$$

Looking at Eq. (6) we see that the probability of finding a temperature in the range $\mathrm{d}T$ is simply the probability of ε being in the range $\mathrm{d}\varepsilon$, i.e., $f(T) = f(\varepsilon)$, so that Eq. (6) can be written as

$$\sigma_P^2 = \left(\frac{\partial F}{\partial P}\bigg|_{\overline{P}}\right)^{-2} \sigma_\varepsilon^2 \tag{7}$$

Eq. (7) emphasizes that it is not the relationship of one data point, T_i, to another, T_j, that determines the precision of $\widehat{P}$ but the distribution of the errors, $f(\varepsilon)$, their statistics, σ_ε and the sensitivity of the model to P, $\partial F/\partial P$.

It is reasonable to assume that the best estimate of P is that value for which either $f(P)$ is a maximum or for which some measure of the consequence of an error in $\widehat{P}$ is minimized. Sivia [3] and Lee [4] give very good summaries and practical applications of the Bayesian approach. Let $f(T|P)$ represent the probability of obtaining the specific readings T given a value of the parameter P and $f(P|T)$ be the probability of the occurrence of a specific value of P given a set of data T. Bayes' rule relating these conditional probabilities is

$$f(P|T)f(T) = f(T|P)f_{\mathrm{pr}}(P) \tag{8a}$$

or

$$f(P|T) \propto f(T|P)f(P) \tag{8b}$$

In Eq. (8) $f_{\mathrm{pr}}(P)$ is the prior probability of P which reflects our initial estimate of the distribution of P. $f(T|P)$ is called the likelihood and denoted by $l(T)$.

In the Bayesian approach, $\widehat{P}$ is chosen to be the value of P which maximizes $f(P|T)$. Eq. (8) permits the use of priors which reflect our existing knowledge about P. For example since conductivity must be positive, $f(k) = 0$, $k \leqslant 0$; $f(k) > 0$, $k > 0$. A state of maximal ignorance would be if all that we knew about P were that it was limited by $P_{\min} \leqslant P \leqslant P_{\max}$, leading to the uniform prior $f(P) = 1/(P_{\max} - P_{\min})$. As long as the prior is relative flat near $\widehat{P}$, then $f(P|T)$ will be maximum when $l(T)$ $(= f(T|P))$ is maximum. It proves easier to deal with $\ln(l(T))$ than with $l(T)$, whose maxima occur at the same value of $\widehat{P}$. Thus Bayes' approach reduces to

$$\widehat{P} \quad \text{is defined by} \quad \left(\frac{\partial \ln(l(T))}{\partial P}\right)\bigg|_{\widehat{P}} = 0 \tag{9}$$

which is called the Maximum Likelihood Estimator (MLE). Substituting $f(\varepsilon)$ for $f(T)$ in Eq. (9) and assuming that the errors are multivariate gaussian with zero mean and a covariance matrix of Σ, then

$$\ln\big(l(T)\big) = -\ln\big(\sqrt{2\pi}\,\big) - \ln\big(\det(\Sigma)\big) - \big\{T_i - F(P, B, t_i)\big\}^{\mathrm{T}} \Sigma^{-1} \big\{T_i - F(P, B, t_i)\big\} \tag{10}$$

where $\{T_i - F(P, B, t_i)\}$ is the column vector of ε_i. Maximizing $\ln(l(T))$ is equivalent to minimizing

$$L = \big\{T_i - F(P, B, t_i)\big\}^{\mathrm{T}} \Sigma^{-1} \big\{T_i - F(P, B, t_i)\big\} \tag{11}$$

Comparing Eqs. (11) and (2) shows that the Maximum Likelihood Principle with normally distributed independent errors (i.e., Σ has no off-diagonal terms) is simply the weighted Least Squares method with $w_i = 1/\sigma_{\varepsilon_i}^2$.

Minimizing $L(T)$ may be quite difficult for complex functions F, particularly if the errors are correlated or if the errors are not normally distributed. Using the one term Taylor series approximation for F with multivariate normally distributed errors it can be shown [5,6] that $\widehat{P}$ has the normal distribution $N(\widehat{P}, \sigma_{\widehat{P}}^2)$ where

$$\widehat{P} = \overline{P} + \sigma_{\widehat{P}}^{-2} \left(\frac{\partial F}{\partial P}\right)^{\mathrm{T}} \Sigma^{-1} \big(T_i - F_i(P_0)\big) \tag{12a}$$

where the inverse of the standard deviation

$$\sigma_{\widehat{P}}^{-2} = \left(\frac{\partial F}{\partial P}\right)^{\mathrm{T}} \Sigma^{-1} \left(\frac{\partial F}{\partial P}\right) \tag{12b}$$

is often called the *precision* of $\widehat{P}$. If our prior for P assumes that P is normally distributed with $N(\eta, \phi)$, then maximizing $f(P|T)$, Eq. (8a), yields

$$\widehat{P} = \eta + \overline{P} + \sigma_{\widehat{P}}^{-2} \left(\frac{\partial F}{\partial P}\right)^{\mathrm{T}} \Sigma^{-1} \big(T_i - F_i\big(\overline{P}\big)\big) \tag{13a}$$

where

$$\sigma_{\widehat{P}}^{-2} = \left(\frac{\partial F}{\partial P}\right)^{\mathrm{T}} \Sigma^{-1} \left(\frac{\partial F}{\partial P}\right) + \frac{1}{\phi} \tag{13b}$$

Eqs. (12a) and (13a) are iterated to convergence. Eq. (13) reduces to Eq. (12) if $\phi = \infty$, the condition for no prior knowledge about P.

2. Uncertain parameters

Now consider the case where there is uncertainty about the parameter B. The uncertain parameter B clearly affects the solution, yet it is a parameter which we are not seeking. Such parameters are called 'nuisance' parameters and their effects are accounted for by integrating over all values of B to obtain the marginal probability $f(T|P)$ which is defined as

$$f(T|P) = \int_B f(T, B|P)\,\mathrm{d}B \tag{14}$$

It is usual to assume that the measurement errors are Gaussian and uncorrelated. On the other hand, $f(B)$ may take a number of forms, e.g., gamma, beta, uniform, laplacian, or gaussian. Lacking specific information about B it is common to assume either that (a) B is a constant but unknown for which $f(B) =$ constant (maximal ignorance) or (b) that B is a random variable with $f(B) = N(\overline{B}, \sigma_B^2)$ [14].

The Taylor series in terms of P and B is

$$T = \overline{T} + \left.\frac{\partial T}{\partial P}\right|_{\overline{P}} (P - \overline{P}) + \left.\frac{\partial T}{\partial B}\right|_{\overline{B}} (B - \overline{B}) + \varepsilon \tag{15}$$

If ε and B are gaussian and are not correlated with each other and if the temperature can be represented by Eq. (15) (i.e., linear in both P and B), the joint pdf $f(T, P, B)$ can be factored to yield

$$f(T|P) = N(\overline{T}, W) \int N\left(A\left(\frac{\partial T}{\partial B}\right)^{\mathrm{T}} \sigma_\varepsilon^2 (T - \overline{T}), A\right) \mathrm{d}B \tag{16a}$$

$$W_{ij} = \sigma_\varepsilon^2 \delta_{ij} + \left(\frac{\partial T_i}{\partial B}\right)\left(\frac{\partial T_j}{\partial B}\right)\sigma_B^2 \tag{16b}$$

where $A^{-1} = \sigma_B^{-2} + (\partial T/\partial B)^{\mathrm{T}} \sigma_\varepsilon^{-2} (\partial T/\partial B)$. The result for B assumed to be a constant, but unknown, is found by setting $\sigma_B = \infty$ in the expression for A but not in the expression for W_{ij}.

If the range of B is wide enough about $\overline{B}$, the integral is equal to unity, since the integral of a normal distribution over the entire space is unity, and thus $f(T|P)$ is dependent upon P only through the term $\overline{T}$. However, if the range of integration is limited, then the integral may be a function of P, and the differentiation required in Eq. (9) can be exceedingly difficult. For a normal distribution, the integral is essentially unity if the range of integration extends from $\overline{B} - 3\sigma_B$ to $\overline{B} + 3\sigma_B$. Thus it will be required that σ_B be such that this range is physically realizable. For example, since the convective heat transfer coefficient must be positive, this limits the uncertainty in h to be such that $\bar{h} - 3\sigma_h > 0$. Eq. (9) also requires a knowledge of $f(P)$.

If P is assumed to be constant but unknown, T and B are gaussian variables, and the errors have zero mean, $\sigma_{\hat{k}}$ is given by

$$\mathcal{I} \equiv \sigma_{\widehat{P}}^{-2} \geqslant \left\{\frac{\partial T}{\partial P}\right\}^{\mathrm{T}} W^{-1} \left\{\frac{\partial T}{\partial P}\right\} \tag{17}$$

$\mathcal{I}$, which is a direct measure of the precision of the estimate $\widehat{P}$, was called the Information by Fisher [7]. The Cramér–Rao theorem states that for unbiased errors that Eq. (17) is an upper bound to the precision [8]. In many cases the achievable precision is significantly less [5].

When the errors are correlated, then W is a full matrix of size $N \times N$ which for large sample sizes leads to computational expense and often makes the iteration of Eqs. (12a) and (13a) slowly converging. When a parameter is uncertain, Eq. (12b) shows that there are off diagonal terms which must be recomputed at each step in the iteration. When there is no uncertainty in B and the errors are uncorrelated, W is diagonal and each data point will contribute to the reduction of $\sigma_{\widehat{P}}$. But when B is uncertain, the temperatures are correlated through the off-diagonal terms of W and the precision of our estimate, $\widehat{P}$, will be reduced.

3. An example of an uncertain boundary condition

Consider a one-dimensional problem with constant properties and time independent boundary conditions. The region is a slab of thickness L, an initial temperature of zero, with convection to a zero temperature at $x = 0$ with a convective coefficient of h_0, and at $x = L$ a prescribed heat flux, Q. The transient temperature history will be measured at $x = 0$ and L and the conductivity will be inferred from these measurements. The measured temperatures will be simulated by adding a zero mean, uncorrelated, gaussian noise with $\sigma_\varepsilon / T_{\max}$ of 1% to the theoretical values based upon a flux of $QL/k = 1$ and a Biot number of 1 or 10. There is uncertainty in the convective heat transfer coefficient at $x = 0$.

Fig. 1 depicts the information contributed by each temperature reading as a function of sensor position and sampling time for an applied heat flux at $x = L$ when there is

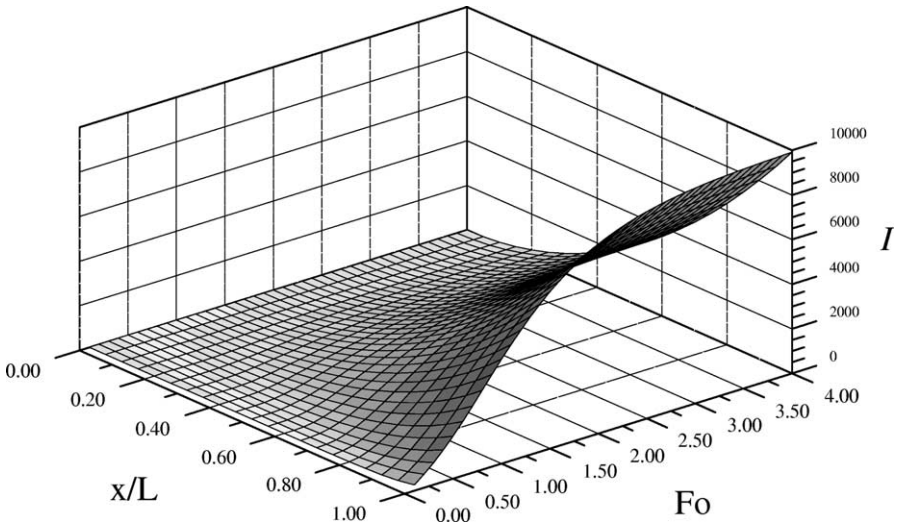


Fig. 1. Information contributed by each temperature reading as a function of sensor position and sampling time for a heat flux applied at $x = L$ for $Bi_0 = 10$ and $\sigma_h = 0$.

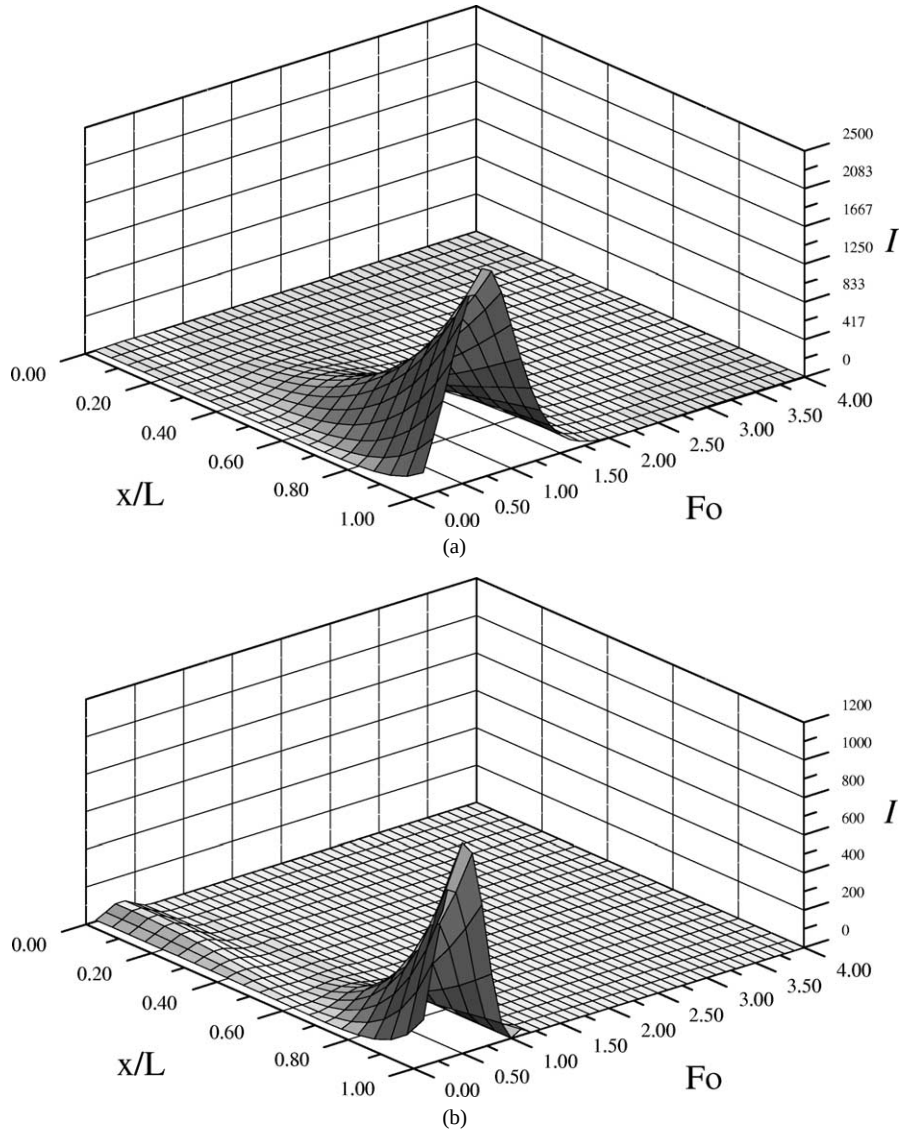


Fig. 2. (a) Information contributed by each temperature reading for a heat flux applied at $x = L$ for $Bi_0 = 10$ and $\sigma_h/\bar{h}_0 = 0.1$. (b) Information contributed by each temperature reading for a heat flux applied at $x = L$ for $Bi_0 = 1$ and $\sigma_h/\bar{h}_0 = 0.1$.

no uncertainty in h for $Bi_0 = 10$. The normalized steady state sensitivities at $x = L$ are $k\partial T/\partial k = -1$ and $h\partial T/\partial h = -1/Bi$ so this experiment is a realistic one for estimating k. Because the temperatures are uncorrelated, the total information is simply the sum of the information provided by each sampled temperature. From the figure it is clear that the ideal sensor position is at $x = L$ and that the readings should be taken at long times. In fact, $\mathcal{I}$ is a maximum at steady state and has the value of $(x/L^2)/\sigma_\varepsilon^2$.

If there is uncertainty about the convection coefficient at $x = 0$, the situation changes dramatically as shown in Fig. 2(a). The information has been reduced by almost an order of magnitude and, more importantly, now shows a definite peak in time. The rapid reduction in information after $Fo = 1$ and the essentially zero information at steady state is due to the correlation caused by σ_B. Clearly the readings should now be concentrated near $Fo = 1$ where the information is maximum and readings should not be taken at longer times where they contribute little to the precision of the estimate of the conductivity.

Because of the low sensitivity to h_0 when $Bi_0 = 10$ the conductivity k can be accurately estimated. However, this low sensitivity does not eliminate the correlation produced by σ_h shown in Fig. 2(a). When the sensitivity to h_0 is high, e.g., for $Bi_0 = 1$, then not only is the information reduced, but it proves to be difficult to estimate k. The information for $Bi_0 = 1$ is illustrated in Fig. 2(b) and a comparison with Fig. 2(a) shows how much the information at $x = L$ has been reduced.

The computation of T_i and $\partial T_i/\partial B$ in Eq. (12) must be done for each sampling time and assumed value of k. For complex systems, the computation can be very expensive. If h is known precisely, then L reduces to LS whose minimization requires only a line search over the possible

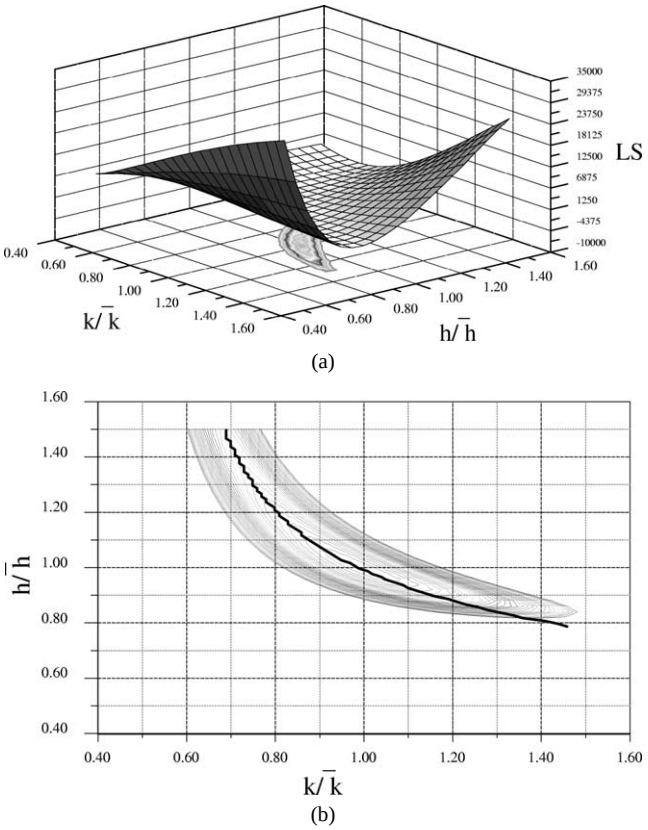


Fig. 3. (a) Values of LS as a function of k and h using 20 temperatures measured at $x = L$ at equal time increments from $Fo = 0$ to 4.0 for $Bi_0 = 1$ and $\sigma_h = 0$. (b) Values of LS as a function of k and h using 20 temperatures measured at $x = L$ at equal time increments from $Fo = 0$ to 4.0 for $Bi_0 = 1$ and $\sigma_h = 0$.

values of k. Furthermore, since h is known, the integration in Eq. (16) is not needed. When h is uncertain, then we must not only perform the integrations, but must search over both k and h to find the minimum point. In addition, minimizing L involves inverting W which, because it is a highly correlated covariance matrix due to the term involving σ_h in Eq. (12b), may be ill-conditioned. Because of the expense of the computations, it is of interest to determine how strongly the value of h affects the results. Fig. 3(a) depicts the variation of LS with k and h when the effect of a variable h is ignored (i.e., $\sigma_h = 0$). The contours, displayed underneath the surface, are shown in Fig. 3(b) with the locus of the minimum values of LS, i.e., the values of k for each h, displayed. It is seen that the estimated value of k varies very strongly with h.

Let us examine what happens when we minimize L where W includes the uncertainty in h. Fig. 4 illustrates this behavior. $\hat{k}$ is now weakly dependent on the value of h, although there are small differences in accuracy as a function of sensor position and time. All of the figures depict equal contour levels. Using temperatures measured at long times, Fig. 4(b), clearly shows the degrading effect of measurements taken when the information content is low.

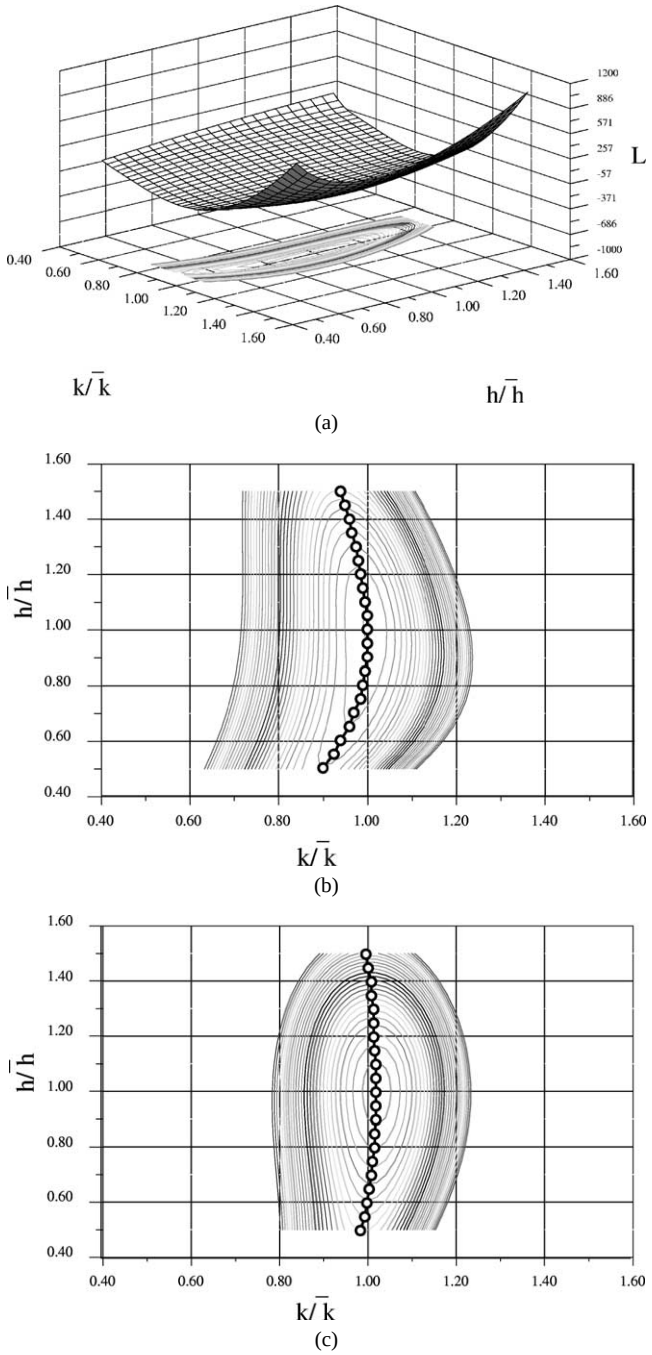


Fig. 4. (a) Values of L as a function of k and h using 20 temperatures measured at $x = L$ at equal time increments from for $Fo = 0$ to 4.0 with $\sigma_h/\bar{h}_0 = 0.1$. (b) Locus of minimum values of L as a function of k and h using 20 temperatures measured at $x = L$ at equal time increments from $Fo = 0$ to 4.0 with $\sigma_h/\bar{h}_0 = 0.1$. (c) Locus of minimum values of L as a function of k and h using 20 temperatures measured at $x = L$ at equal time increments from $Fo = 0$ to 2.0 with $\sigma_h/\bar{h}_0 = 0.1$.

A noticeable improvement occurs when sampling is restricted to times of maximal information, Fig. 4(c). Estimating k using the correct value of h yields accurate values of $\hat{k}$ when using W or Σ (i.e., ignoring σ_h). However, when h is incorrectly specified, the two methods differ substantially as shown in Table 1. It is only when data with the

Table 1
Statistics for estimation of k using $h = 1.1\bar{h}$

x	Fo	$\hat{k}_L$	$\hat{k}_{LS}$	$\sigma_{\hat{k}_L}$	$\sigma_{\hat{k}_{LS}}$
L	0–8	1.025	0.927	1.38	0.23
L	0–4	1.010	0.942	1.12	0.30
L	0–2	1.000	0.967	1.05	0.42
0	0–8	0.932	1.726	3.90	9.21
0	0–4	0.964	1.507	3.37	4.90
0	0–2	0.990	1.240	3.51	2.74

highest information content, $0 < Fo < 2$, are used that ignoring the correlating effect of σ_h leads to acceptable values of $\hat{k}$. On the other hand, the use of W proves satisfactory over a wide range of data. The table also lists estimates obtained using data at $x = 0$. There is so little information available at $x = 0$, so little that it is barely discernable on Fig. 2(b) and 2(c), that the analysis must be restricted to times of highest information and even then, the result is unacceptable. Ignoring the correlating effects of σ_h also substantially overestimates the precision as shown by the values of $\sigma_{\hat{k}}$ for measurements made at $x = L$.

The very good results obtained from the maximum likelihood principle using W from Eq. (12b) and measuring temperatures at times of maximal information, are typical of the different problems that we have examined. These problems involved 1 and 2-D temperature calculations with uncertainties in convective heat transfer coefficients, ambient temperatures, surface emissivity, applied heat fluxes, specific heat capacities, and sensor locations.

3.1. Errors due to linearization and correlated errors

Two common sources of inaccuracies in evaluating the statistics of $\widehat{P}$ are the linearization of the response and the presence of correlated errors. Appropriately accounting for these requires intensive computations.

The effective use of the maximum likelihood principle in determining $\widehat{P}$ and $\sigma_{\widehat{P}}$ requires that the response be linearized, Eq. (3). Ignoring the higher order terms typically gives rise to biased estimators of both $\widehat{P}$ and $\sigma_{\widehat{P}}$ [9]. If a sufficient number of data points are available, then the ML estimator is asymptotically unbiased. Probably the most commonly encountered biased estimator is the estimate of the standard deviation, $\sum_{i=1}^{N}(T_i - E[T])^2/N$. The correct value is $\sum_{i=1}^{N}(T_i - E[T])^2/(N-1)$ and as $N \to \infty$ the bias disappears.

For complex functions $F(P, B)$ which are non-linear with respect to P, the bias is caused by (a) neglecting the higher order terms in the Taylor series expansion and (b) because functions of gaussian distributions, e.g., $f(P)$, are not gaussian. If the 2nd order terms are included in the Taylor series and the distribution of P is gaussian, the 2nd order estimates of the statistics are

$$E[T] = \overline{T} + \underbrace{\frac{1}{2}\overline{\frac{\partial^2 T}{\partial P^2}}\sigma_P^2}_{\text{1st order estimate of bias}} \tag{18a}$$

$$\sigma_T^2 = \left(\overline{\frac{\partial T}{\partial P}}\right)^2 \sigma_P^2 + \underbrace{\left(\frac{1}{2}\left(\overline{\frac{\partial^2 T}{\partial P^2}}\right)^2 + \overline{\frac{\partial T}{\partial P}}\ \overline{\frac{\partial^3 T}{\partial P^3}}\right)\sigma_P^4}_{\text{1st order estimate of bias}} \tag{18b}$$

where the $\overline{T}$ represents evaluation at $\overline{P}$ and the underlined terms are estimates of the bias. The bias is a function of σ_P and can be ignored for small values of σ_P.

However, if $f(P)$ is strongly non-Gaussian, even relatively small values of randomness leads to bias. As an example, consider steady state one-dimensional heat conduction through a slab of thickness L with an electrical heater providing a heat flux $q \propto i^2 R$ at $x = 0$ and a constant temperature at $x = L$. The conductivity can be estimated from

$$k = \frac{qL}{\Delta T} \propto \frac{i^2 RL}{\Delta T} \tag{19}$$

Because of the non-linear form of Eq. (19), especially with respect to ΔT, the distribution of k will not be normal even if ΔT and q are normally distributed. Assuming that the mean values of ΔT, q and i are unity and that $\sigma_{\Delta T} = \sigma_q$ or that $\sigma_{\Delta T} = \sigma_i$, the underprediction of $E[k]$ and σ_k by the *one* term Taylor series approximation are shown in Fig. 5.

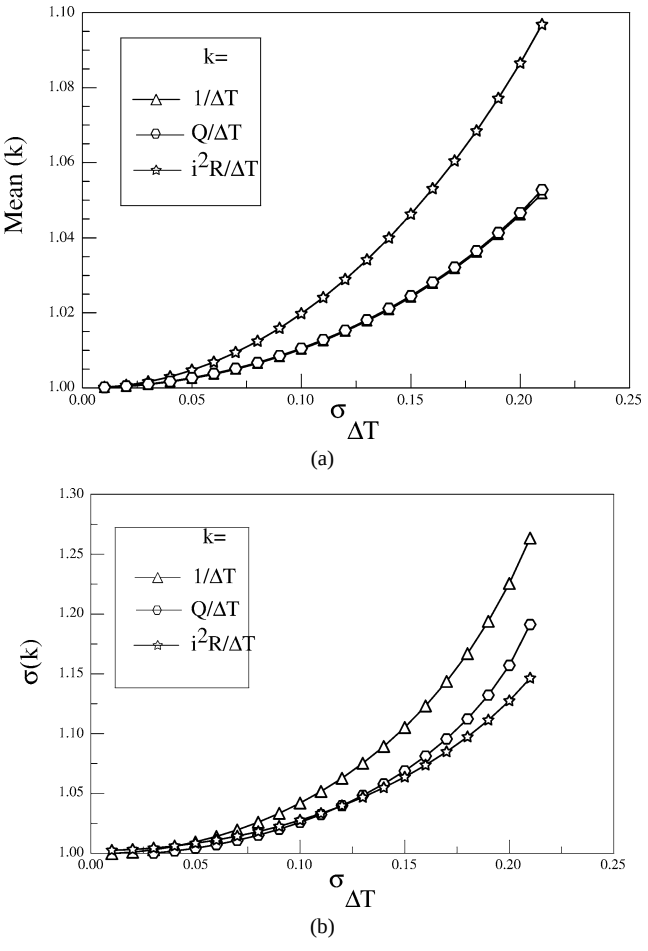


Fig. 5. (a) Ratio of the true mean to that obtained from the one term Taylor series. (b) Ratio of the true standard deviation to that obtained from the one term Taylor series.

The error in estimating $\hat{k}$ is relatively small for reasonable values of σ. However, for accurate estimates of $\sigma_{\hat{k}}$ one should limit the standard deviations in the variables to no more than 10% of the mean values. The stronger effect on the case where $k \propto 1/\Delta T$ is because $f(1/\Delta T)$ is far from gaussian as ΔT becomes large relative to $\overline{\Delta T}$. In the other two cases, the effect of the gaussian distributions of the variables in the numerator tends to ameliorate the effect of the denominator. The only correct way to account for the non-linearities is by evaluating $f(P)$ and determining the value of P which maximizes f after integrating over all nuisance variables. This almost always requires Monte Carlo simulation or numerical integration [9], even for the simplest problems, since very few are problems amenable to analytical solutions. (Even evaluating the statistics of $f(1/\Delta T)$ is difficult.)

Similar computational problems exist when the errors are correlated. Consider the estimation of k for the slab with a prescribed heat flux when the temperatures are read at a high sampling rate and the data acquisition system introduces an error. Let the covariance matrix of the errors be given by

$$\Sigma = \sigma_\varepsilon^2 \begin{pmatrix} 1 & \rho & \rho^2 & \dots & \rho^N \\ \rho & 1 & \rho & \dots & \rho^{N-1} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \rho^N & \rho^{N-1} & \vdots & \dots & 1 \end{pmatrix} \tag{20a}$$

which is representative of many measurement systems with a damped response. This matrix can be easily inverted to give

$$\mathcal{I} = \frac{1}{\sigma_\varepsilon^2}\left[1 + (N-1)\left(\frac{1-\rho}{1+\rho}\right)\right] \tag{20b}$$

Although more readings will increase the information content of the experiment and thus increase the precision of $\hat{k}$ regardless of the value of ρ, the rate of information increase is dramatically slowed when $\rho > 0$. A value of $\rho = 0.5$ means that each additional reading contributes only (1/3)rd as much information as that contributed when the errors are uncorrelated.

Fig. 6 illustrates how the degree of correlation affects the information for our example problem when h is known exactly, compare with Fig. 1. Even small amounts of correlation, 0.5, have a strong negative effect on the precision of $\hat{k}$.

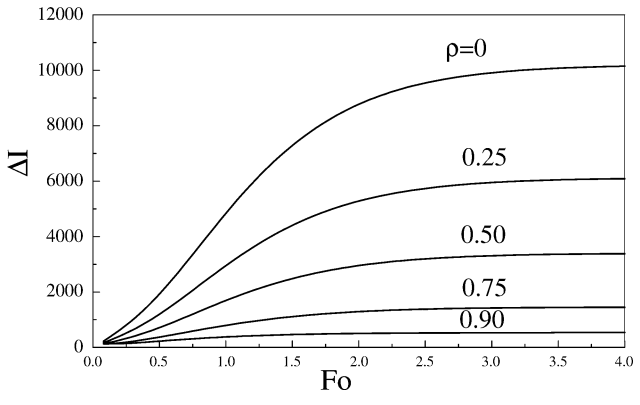
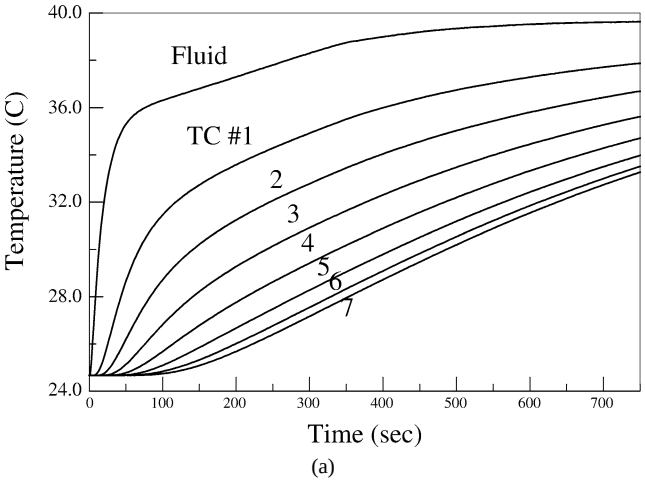


Fig. 6. Effect of correlated errors in the temperatures measured at $x = L$ on the information for a prescribed heat flux at $x = L$, with $k = 1$, $L = 1$ and $Bi = 1$ at $x = 0$.

4. A real experiment

The results presented up to now have used a simulated experiment. Let us look at a real experiment. Blackwell et al. estimated the conductivity of stainless steel by measuring the temperatures in a thin hollow tube of length $2L$. Full details are given in Ref. [10] but a brief description is given here. The tube was installed in an evacuated chamber and space insulation covered the outer surface of the tube and filled the hollow interior to minimize losses from the surfaces and to create a one-dimensional temperature field. The ends of the tube were heated by a fluid which flowed through serpentine channels in copper end blocks. Temperatures were measured at 14 equally spaced axial locations each with 4 thermocouples equally spaced about the circumference. The thermal model of this system by which the thermal conductivity can be estimated would have the circulating fluid temperature as the boundary conditions and would include the thermal characteristics of the copper end blocks, the convection coefficients in the serpentine channels and the contact resistance between the end blocks and the hollow tube. But lacking full details of these characteristics means that the system cannot be modeled. If a heat flux gauge were mounted at the ends of the tube, or if the flux could be estimated, then the problem could be considered as having a known flux history as the boundary conditions. Alternatively one could view the inverse problem as the simultaneous estimation of both the heat flux history and the thermal conductivity. Because the time history of the fluxes is difficult to obtain, as demonstrated in by Beck [11, 12], Blackwell et al. developed a novel approach in which the time varying temperatures measured at the ends, $x = \pm L$ were taken to be the prescribed end boundary conditions and the temperature histories computed using a finite volume code. The measured transient temperatures were then fitted to the numerically computed temperatures as a function of k, x and t and the conductivity estimated using the usual least squares equation, Eq. (2).

Alternatively one can use the measured temperatures in conjunction with reported conductivities to estimate the heat flux history and then estimate k based upon a prescribed boundary heat flux history—this will of necessity involve iterations. Fig. 7 shows the average of the circumferential temperatures measured at each x location and the estimated heat flux. Fig. 8 shows the sensitivities, $\partial T/\partial k$ for the two models. The sensitivities for the temperature boundary condition increase monotonically with time and axial position while those for the prescribed flux model decay at long times and are in general less than those for the temperature *bc*. It would appear to be better to estimate k using the temperature *bc* model, but doing so means that the data at $x = L$



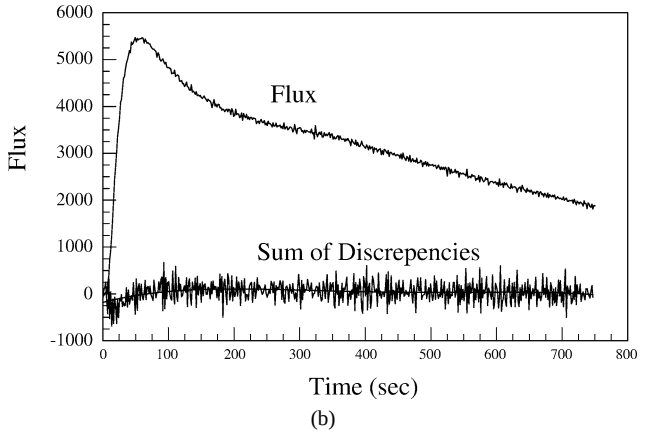


Fig. 7. (a) Measured temperatures. (b) Estimated heat flux.

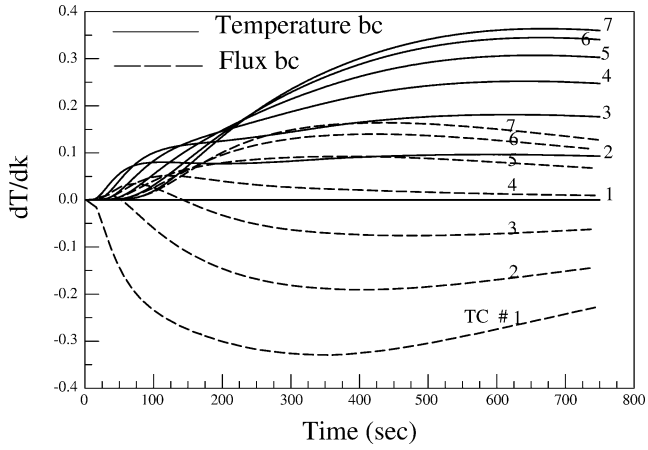


Fig. 8. Sensitivities of the temperature and flux models.

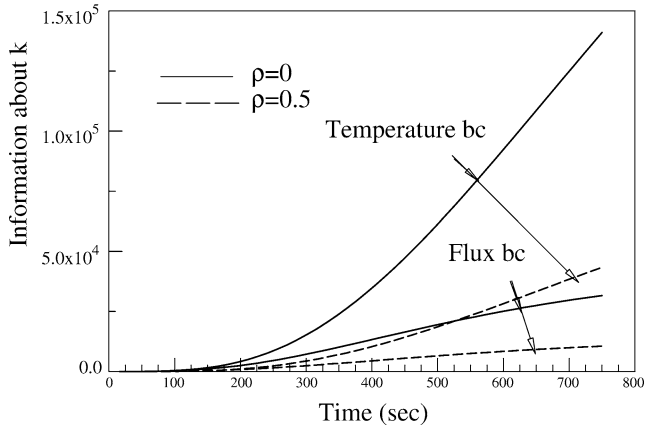


Fig. 9. Information content of the two models for no uncertainty in *bc*.

cannot be used to estimate k. Thus there are fewer sensors, but greater sensitivity for the temperature *bc* model than for the flux *bc* model. On the other hand, the flux model requires that an iterative process be used to estimate simultaneously the flux and the conductivity.

The temperatures read showed high degrees of auto and cross correlation. The 4 circumferential temperatures showed a cross correlation coefficient greater than 0.99 and sensors symmetric in x had values greater than 0.98. The 7 axial stations showed no cross correlation. Thus the 14×4 sensors provided information equivalent to 7 sensors with uncorrelated errors. In addition, each axial station showed considerable auto correlation with $\rho \geqslant 0.5$ which diminished their information content. Care must be taken in extracting the intrinsic statistics of the error, not confusing them with those of the residuals. General methods are suggested in Refs. [13] and [14] and the details for the treatment of this experimental data are given in Ref. [15]. Fig. 9 shows the information content of the two models and it appears that, as suggested by Blackwell, that the temperature *bc* model is to be preferred.

However, Fig. 9 is based upon no uncertainty in the boundary conditions. The errors in the heat flux are easily seen in Fig. 7(b) and have a standard deviation of 42 watts·m^{-2}. Although the temperatures appear to be smooth, the standard deviation of the temperature at $x = L$ is of the order of 0.077 C. Let us evaluate the effect of these errors in the boundary conditions.

Let b_i be the value of the boundary condition (temperature or heat flux) at time t_i. Then following the development of Eq. (12), we obtain

$$W = \Sigma + [Fb]\,\mathrm{cov}(b)[Fb]^{\mathrm{T}}$$
$$Fb_{ij} = \partial F(t_i)/\partial b_j \tag{21}$$

For M sensors, each with N readings, Fb is a $NM \times N$ matrix and W and Σ are $NM \times NM$. For this experiment, $M = 7$ and $N = 500$, and the evaluation of Fb and the inverting of W involve considerable computational expense. Fortunately, the different axial sensors show little cross correlation and the total information is simply the sum of the information from the individual sensors. Thus, treating each sensor individually involves matrices of size $N \times N$ only.

The results of using Eq. (21) are shown in Fig. 10 where we see that the two models yield comparable estimates of $\sigma_{\hat{k}}$. These results are markedly different from those shown on Fig. 9 where the effect of uncertainty in the *bc* was not considered and emphasizes the need to consider all uncertainties in estimating parameters.

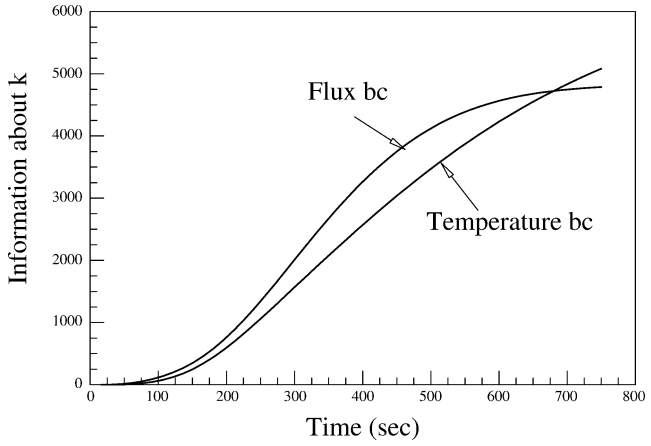


Fig. 10. Information content of the two models when the uncertainty in the boundary condition is considered.

5. Conclusions

It is critical to distinguish between the estimated value, $\widehat{P}$ and the estimate of its standard deviation, $\sigma_{\widehat{P}}$. $\widehat{P}$ is found from Eq. (4) and is primarily a function of the data, T_i, and in general for reasonable accuracies in measurements, is weakly dependent upon the sensitivities, $\partial F/\partial P$. Thus if two different models, $F_1(P, B_1)$ and $F_2(P, B_2)$ yield similar predictions of the temperature and if the errors are small, both models will yield approximately equal values of $\widehat{P}$. This is true because the only effect of the sensitivities is to redistribute the weights. On the other hand, if the errors are large, then the two models will produce substantial differences in $\widehat{P}$. Table 2 lists the different values of the estimated conductivities and those taken from Refs. [10] and [13] considering only the uncertainty in the experiment. In reality, since ρc must be assumed to derive k the full uncertainty in $\hat{k}$ must be increased by the uncertainty in ρ and the specific heat.

The value shown as derived from the measured temperatures was found by an energy balance on the measured temperatures. Because the first two thermocouples are relatively far apart, 13% of the length of the cylinder, the flux estimates are only approximate particularly at the early times when the temperature has not penetrated far. As a consequence the temperatures near $x = L$ at early times have the greatest errors. This when coupled with the sensitivity of the flux *bc* model, which is greatest at $x = L$ (Fig. 8), produces the greatest inaccuracy in $\hat{k}$. The flux determined from the temperature history simulated using the measured temperature *bc*, whose close nodal spacing gives a good representation of the temperature near $x = L$, yields a much closer value to that estimated using the temperature *bc* as expected.

In contrast to $\widehat{P}$, the precision is a function not of the data, but only of the model and the statistical characteristics of the errors. Thus the higher sensitivity of the temperature *bc* model recommends its use. However, when both the autocorrelation and the uncertainties in the boundary conditions are included, both models yield equivalent results — emphasizing the need to consider all uncertainties inherent in the models. It might be thought to be intuitive that since the flux was derived from the measured temperatures that the precisions of the two models would be the same. However unless the flux can be accurately estimated, the resulting values of $\hat{k}$ can be expected to differ. The tabulated values show that the several estimates of $\hat{k}$ are within the expected $\pm 3\sigma$. No estimate of $\sigma_{\hat{k}}$ was made when the flux was derived from the temperature *bc* simulation because of its difficulty and the unlikeliness that this method would be used in reality.

Table 2
Estimated conductivity

Boundary condition	Derived from	$\hat{k}$	$\sigma_{\hat{k}}$
Temperature	experiment	14.62	0.21
Flux	measured temperatures	14.30	0.21
Flux	simulation	14.59	
Incropera (10)		14.97	
Taylor (10)		14.65	1.5

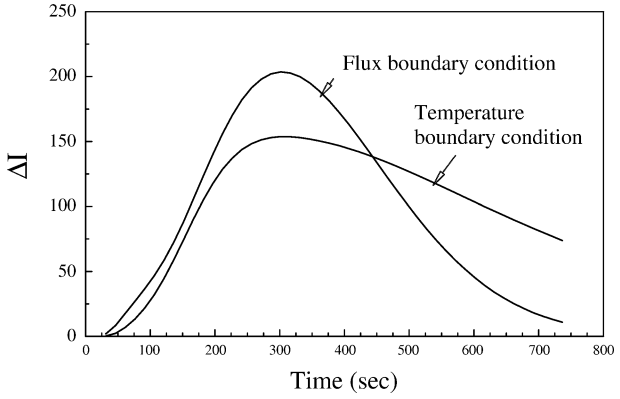


Fig. 11. Increment of information of the two models when the uncertainty in the boundary condition is considered.

If the experimental boundary conditions were a prescribed flux, the higher sensitivity of the temperature *bc* model suggests that the experiment should be analyzed using a measured temperature as a boundary condition. Of course if only a few temperatures are recorded, the loss of the data from one sensor to be used for the boundary condition could result in a significant loss of information.

The increment of information corresponding to Fig. 10 is illustrated in Fig. 11 and illustrates the time value of the data. In this experiment it is clear that as time proceeds the information due to each additional reading diminishes substantially—similar to Fig. 1—and should be considered when planning the experiment.

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