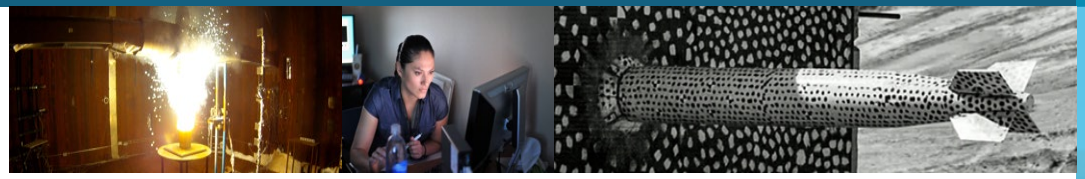
Tutorial: Computational Methods for Inverse Heat Transfer Problems -- Parameter Estimation



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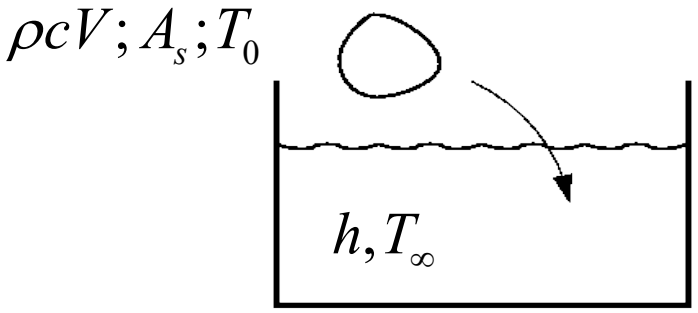
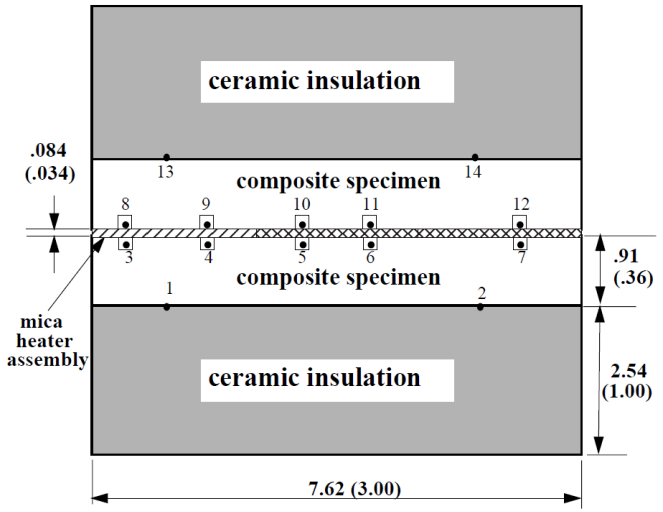
Tutorial Overview: Parameter Estimation

- Basic Concepts
  - Sensitivity Coefficients
  - Parameter Estimation Algorithm(s)
  - Optimal Experimental Design
- Example 1 – Quenching of lumped body
  - Thermal Model & Sensitivity Study
  - Simulated Data & Parameter Estimation
- Example 2 – Estimating Temperature-Dependent and Anisotropic Material Properties
  - Experimental Approach
  - 1D Results
    - Thermal model
    - Estimated parameters and Analysis
    - Uncertainty
  - 2D Results
    - Thermal model
    - Estimated parameters and Analysis
    - Uncertainty





Basic Concepts

What is parameter estimation?

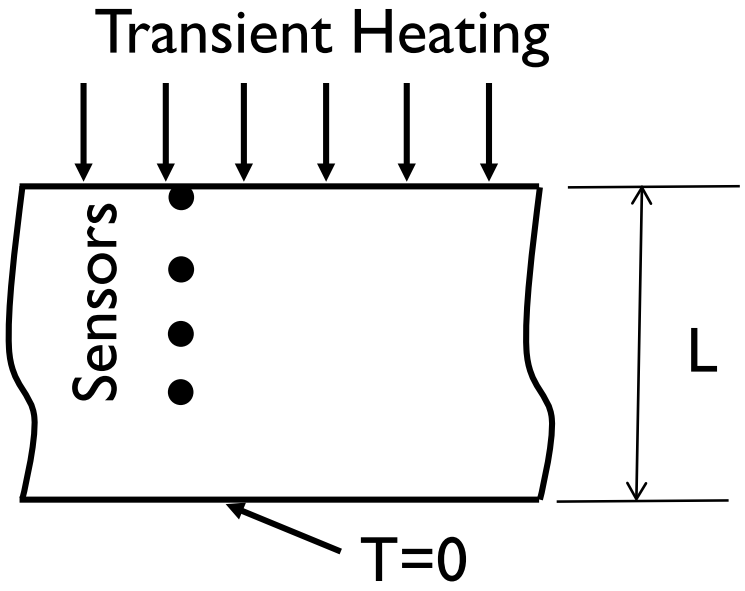
- Efficient use of experimental data for determination of values appearing in a mathematical model of an engineering system.
- Definitions:
  - Data: measurements containing errors (temperature data for heat conduction applications)
  - Model: expression or solution algorithm (for temperature)
  - Parameters may be:
    - Material properties such as density, specific heat, thermal conductivity
    - Coefficients in a formula:

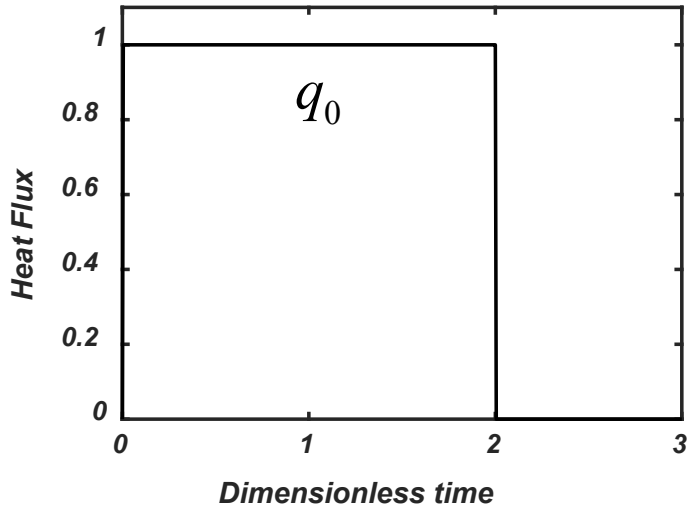
$$Nu = \beta_1 \mathrm{Re}^{\beta_2} \mathrm{Pr}^{\beta_3}$$

    - Constants related to a property

$$k = \beta_0 + \beta_1 T$$

Transient heat conduction experiment:



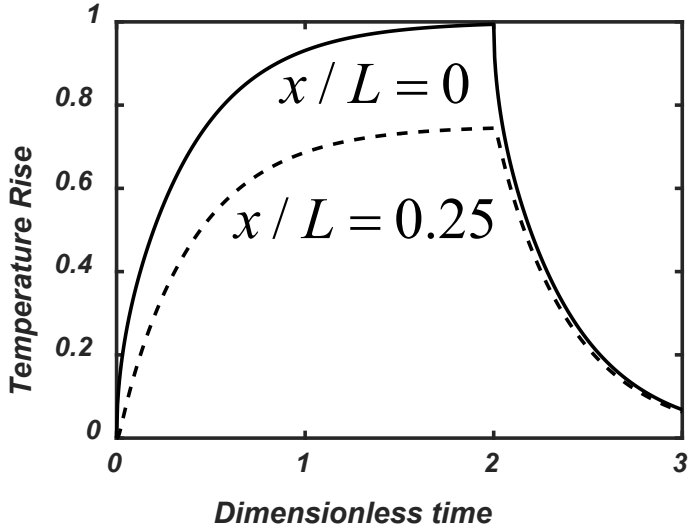


Surface heating:

$$q(t) = \begin{cases} q_0 & 0 < t < t_1 \\ 0 & t > t_1 \end{cases}$$

Temperature data

$$Y(x_1, t_i), Y(x_2, t_i)$$



$$t^+ = \frac{(k/\rho C)t}{L^2}$$

Seek thermal properties *k*, *α* in model

Mathematical Model

$$\frac{\partial^2 T}{\partial x^2} = \frac{1}{\alpha}\frac{\partial T}{\partial t}$$

$$k\left.\frac{\partial T}{\partial x}\right|_{x=0} = -q(t)$$

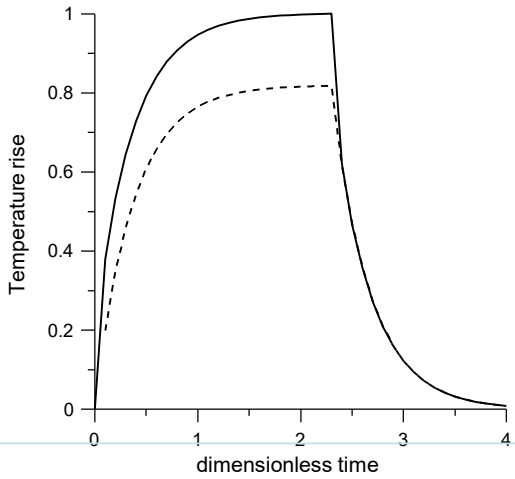
$$T(L,t) = 0$$

$$T(x,0) = T_0(x)$$

Measured Data

$$Y(x_1,t_i),$$

$$Y(x_2,t_i)$$



Parameter Estimation

$$\sum (T_i - Y_i)^2$$

Other names for Parameter estimation:
--Regression analysis
--System identification
--Data analysis

When can several parameters be estimated simultaneously?

- If the measured temperatures are “sensitive” to changes in each of the parameters.
- If you have the “right” data.

Quantify these ideas with sensitivity coefficients:

$$X_{ij} = \frac{\partial T_i}{\partial \beta_j} \text{ where } \beta_j \text{ is the jth parameter}$$

The sensitivity coefficients must be

– large enough

– linearly independent

Scaled sensitivity coefficients are measures for parameter estimation

- Scaled Sensitivity Coefficients

$$T_\beta = \beta \frac{\partial T}{\partial \beta}$$

- Scaled sensitivity coefficients are an important metric for parameter estimation
  - Scale factor is the nominal parameter value
- Scaled sensitivity coefficient will have units of the result (Temperature)
  - Will allow for direct comparison of various parameters
  - Compared to measured response to indicate magnitude

Sensitivity coefficients

Large enough:

$$\beta_j \frac{\partial T_i}{\partial \beta_j} \approx \begin{cases} 1 & \text{then } T \text{ is sensitive to } \beta_j \\ 0.01 & \text{then } T \text{ is insensitive to } \beta_j \end{cases}$$

Linearly Dependent

$$C_1 \frac{\partial T_i}{\partial \beta_1} + C_2 \frac{\partial T_i}{\partial \beta_2} + \ldots + C_p \frac{\partial T_i}{\partial \beta_p} = 0$$

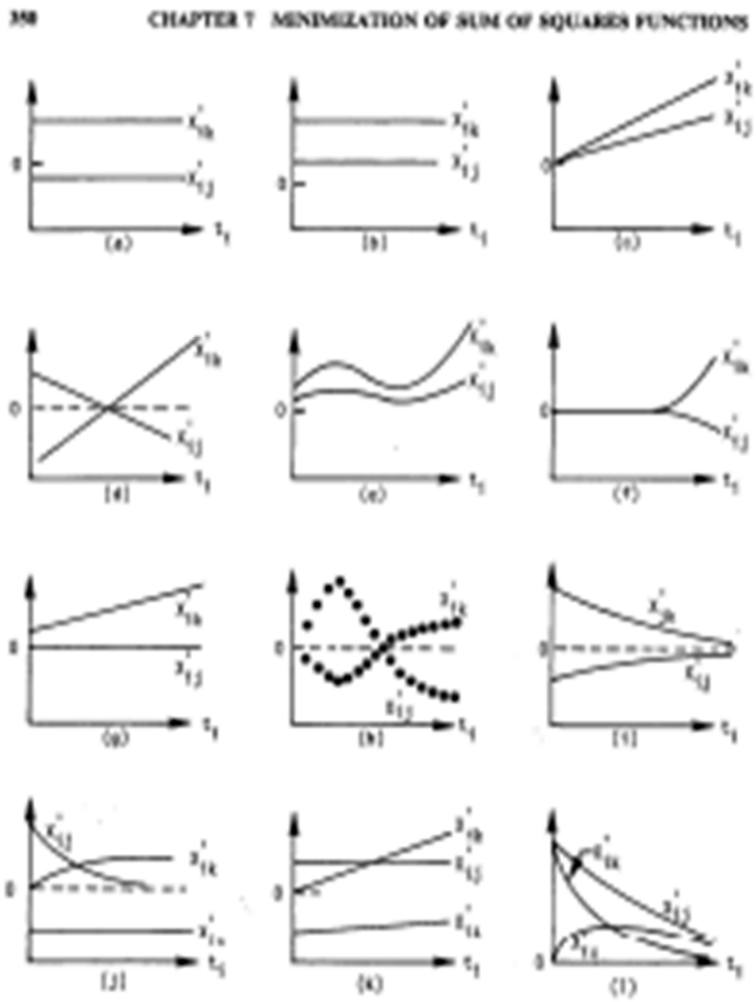
where two or more C_j are not zero

Linearly Independent

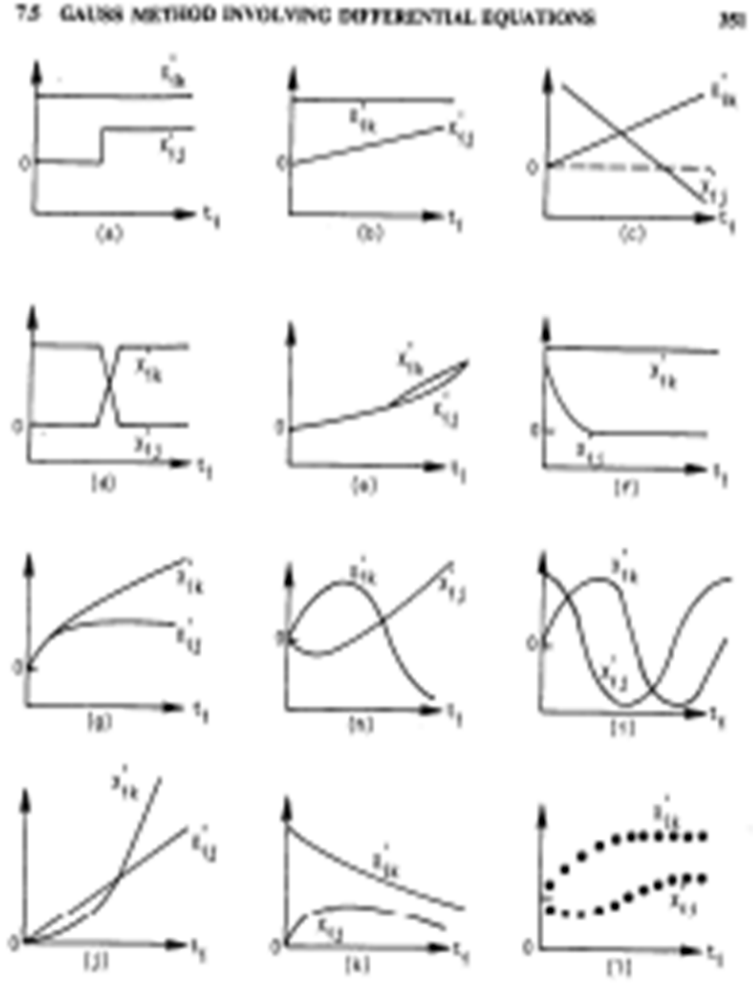
$$C_1 \frac{\partial T_i}{\partial \beta_1} + C_2 \frac{\partial T_i}{\partial \beta_2} + \ldots + C_p \frac{\partial T_i}{\partial \beta_p} = 0$$

only when all $C_j = 0$

Determine linear independence – plots



Linearly dependent



Linearly independent

Determine linear independence – math

Combine all the sensitivity coefficients into a matrix, with *p* columns (for *p* parameters) and *N* rows (for *N* measurements):

$$\mathbf{X} = \begin{bmatrix} \frac{\partial T_1}{\partial \beta_1} & \frac{\partial T_1}{\partial \beta_2} & \cdots & \frac{\partial T_1}{\partial \beta_p} \\ \frac{\partial T_2}{\partial \beta_1} & \frac{\partial T_2}{\partial \beta_2} & \cdots & \frac{\partial T_2}{\partial \beta_p} \\ \vdots & \vdots & \ddots & \\ \frac{\partial T_N}{\partial \beta_1} & \frac{\partial T_N}{\partial \beta_2} & \cdots & \frac{\partial T_N}{\partial \beta_p} \end{bmatrix}$$

The columns of sensitivity coefficient matrix ***X*** are linearly independent if:

$$\det\left|\mathbf{X}^{\mathrm{T}}\mathbf{X}\right| \neq 0$$

Sensitivities and Optimality

- Sensitivities should be as large as possible.
- Sensitivities must be linearly independent to estimate two or more parameters.

Given sensitivity matrix **X**, the optimal experiment is found at the maximum value of the determinant of matrix $\mathbf{X}^T\mathbf{X}$:

$$D = \frac{1}{sn(T_{\max}^{+})^2}\det(\mathbf{X}^{\mathrm{T}}\mathbf{X})$$

s – number of sensors

n – number of time steps

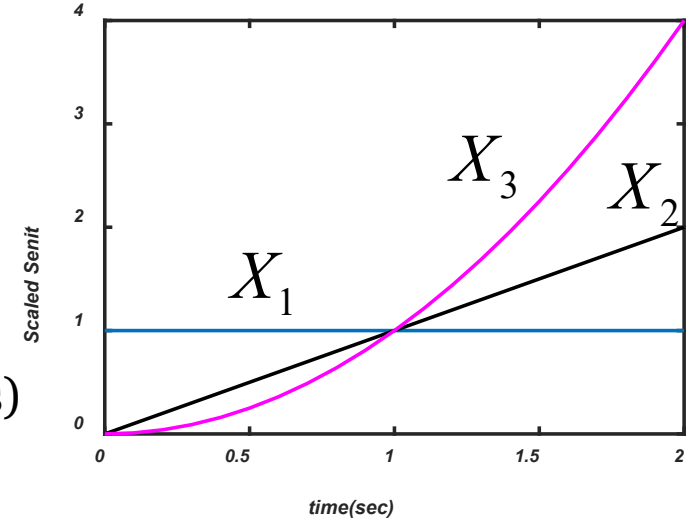
Model linear in parameters

Example. Second-order polynomial in time

$$T(t) = \beta_1 + \beta_2 t + \beta_3 t^2$$

$$X_1 = \frac{\partial T}{\partial \beta_1} = 1; \quad X_2 = \frac{\partial T}{\partial \beta_2} = t; \quad X_3 = \frac{\partial T}{\partial \beta_3} = t^2$$

(Note sens. coeffs. are independent of parameters)



A model linear in parameters can be written:

$$T_i = \sum_j X_{ij}\beta_j \quad \text{with data } Y_i \text{ and } S = \sum \left(Y_i - T_i\right)^2$$

Ordinary least square fitting of the model (minimize *S*) is a matrix solution of the form *Ab* = *B*:

$$\left(X^T X\right) b_{LS} = X^T Y$$

$$b_{LS} = \left(X^T X\right)^{-1} X^T Y$$

where b_{LS} is the least-squares estimate

Most models are non-linear in parameters

For most heat transfer applications

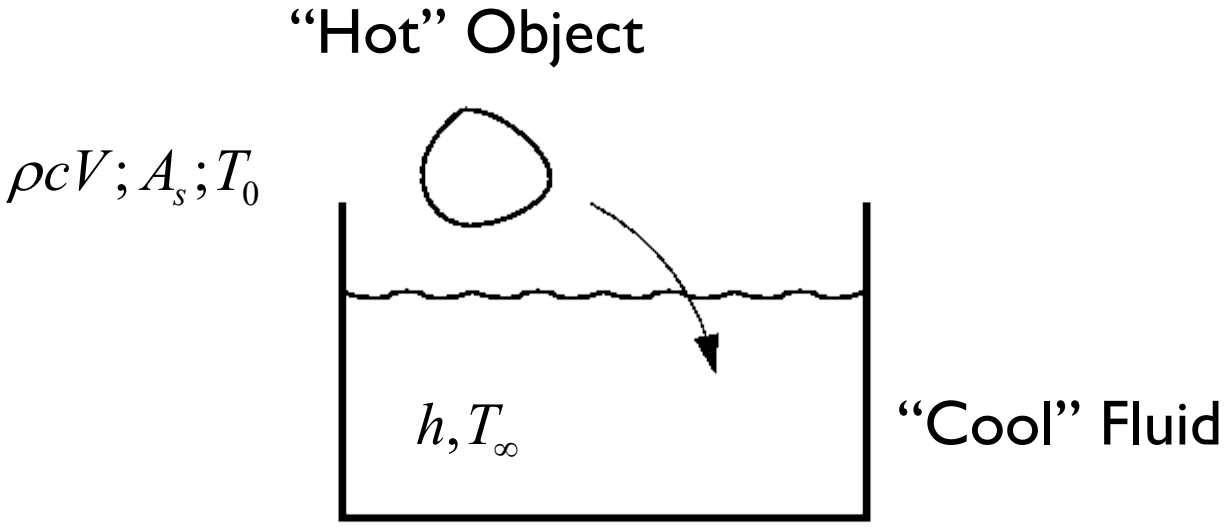
- The model is non-linear in the parameters
- The sensitivity coefficients depend on the parameters
- An iterative solver is needed to fit the parameters
- The iterative Gauss method is well known:

$$b^{k+1} = b^k + \left(X^T X\right)^{-1}\left[X^T\left(Y-\eta\right)\right]$$

for measurements Y and model η

- Most computing environments (Excel, Matlab, Mathematica, etc.) have a non-linear solver

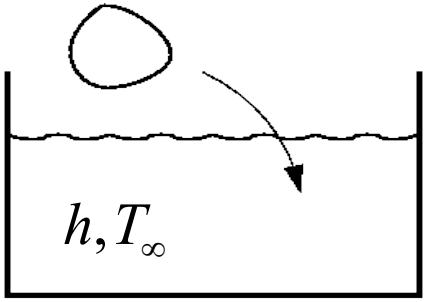
Example 1



Quenching of an object

Example 1. Quenching problem.

$\rho cV; A_s; T_0$



ρ : density
V : Volume
c : Specific Heat
A_s : Surface Area

T_0 : Initial Temperature
h : Convection Coefficient
T_∞ : Fluid Temperature

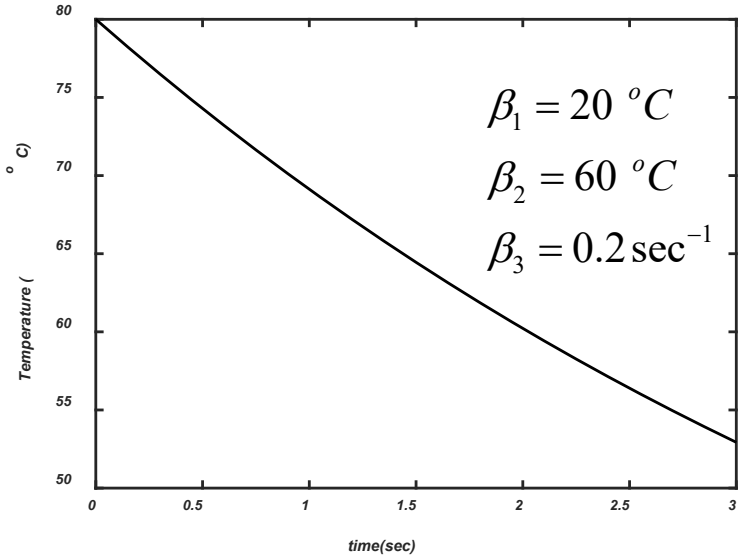
Mathematical Model

$$T(t=0) = T_0$$

$$hA_s\left(T - T_\infty\right) = \rho Vc\frac{dT}{dt}; \qquad t > 0$$

Solution: $T(t) = T_\infty + \left(T_0 - T_\infty\right)\exp\left(-\frac{hA_s}{\rho Vc}t\right)$

or $T(t) = \beta_1 + \beta_2 \exp\left(-\beta_3 t\right)$



Typically, the experiment is conducted and data is collected before studying the model to identify what is possible

Example 1. Quenching problem

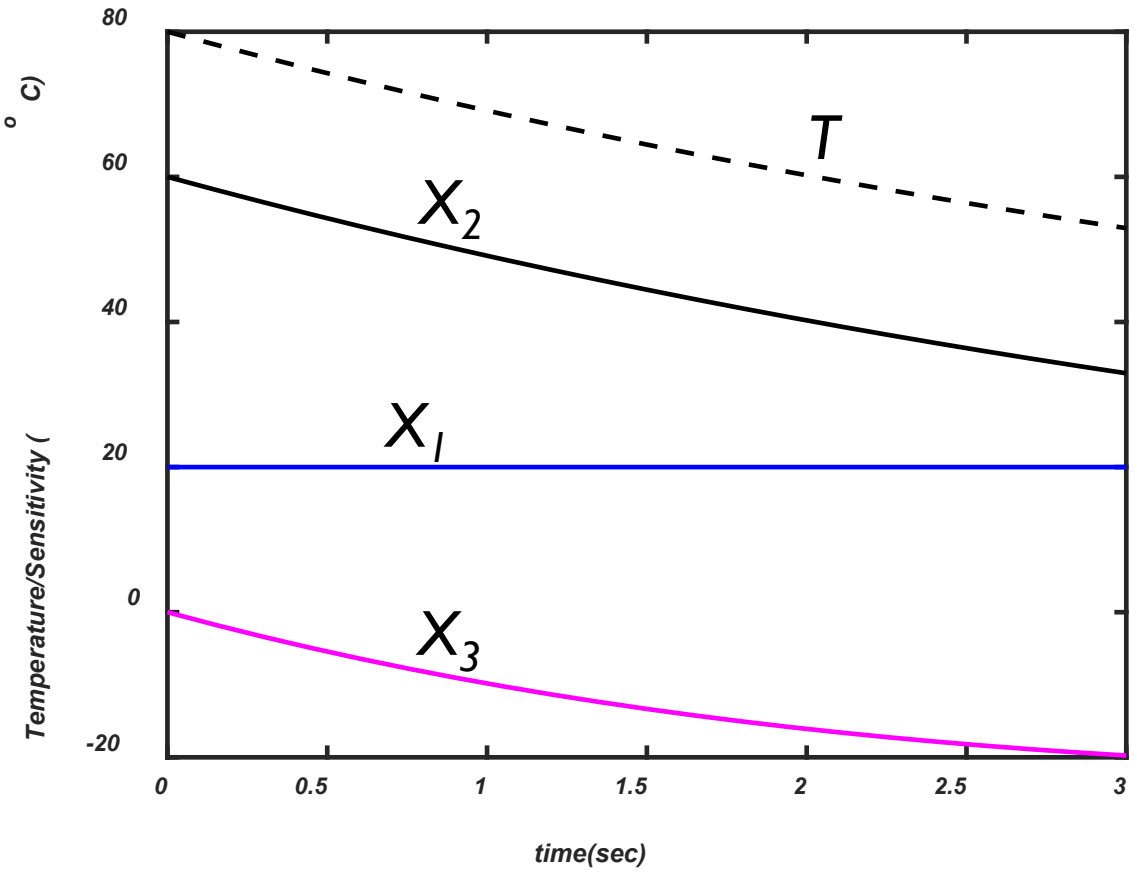
Scaled sensitivity coefficients:

$$T(t) = \beta_1 + \beta_2 \exp\left(-\beta_3 t\right)$$

$$\beta_1 \frac{\partial T}{\beta_1} = \beta_1$$

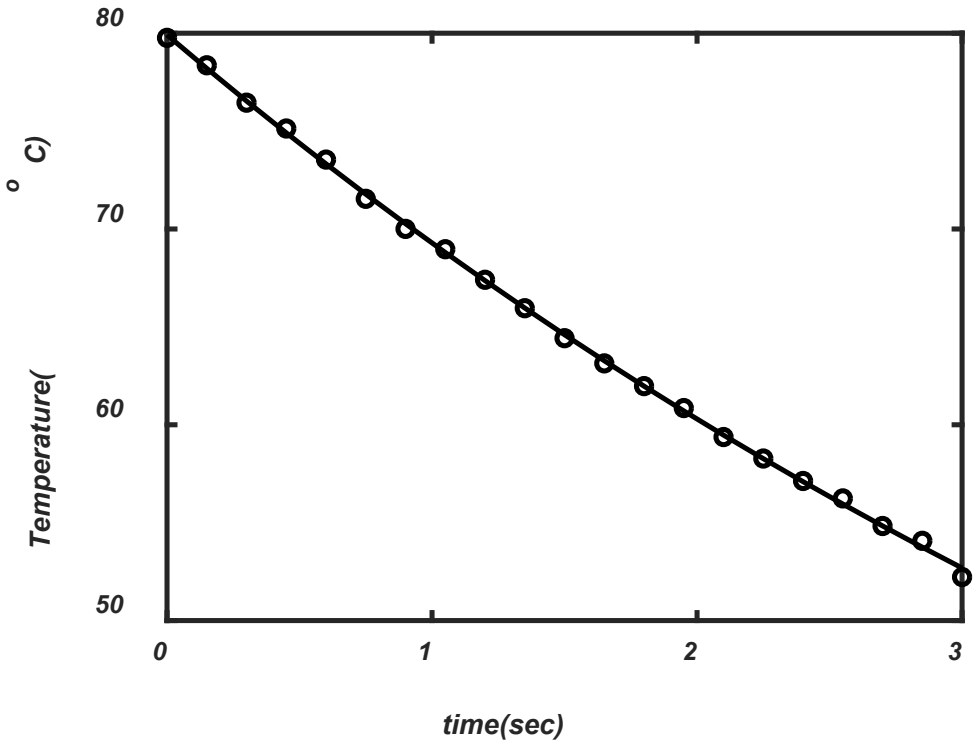
$$\beta_2 \frac{\partial T}{\beta_2} = \beta_2 \exp(-\beta_3 t)$$

$$\beta_3 \frac{\partial T}{\beta_3} = -\beta_2 \beta_3 t \exp(-\beta_3 t)$$



Simulated Experimental Data

Synthetic data 0<t<3 sec
with $\beta_1 = 20$, $\beta_2 = 60$, $\beta_3 = 0.2$
added error $\sigma = 0.25$ C



$$T(t) = \beta_1 + \beta_2 \exp\left(-\beta_3 t\right)$$

$$Y(t) = T(t) + \varepsilon$$

Estimation of parameters from data

Parameter	Estimates Exp 1	Estimates Exp 2
β_1 (20)	10.8841	26.1172
β_2 (60)	69.0291	54.2988
β_3 (0.2)	0.1672	0.2321
$S = \Sigma(Y_i - T_i)^2$	0.7940	0.8353

Matlab results using nlinfit

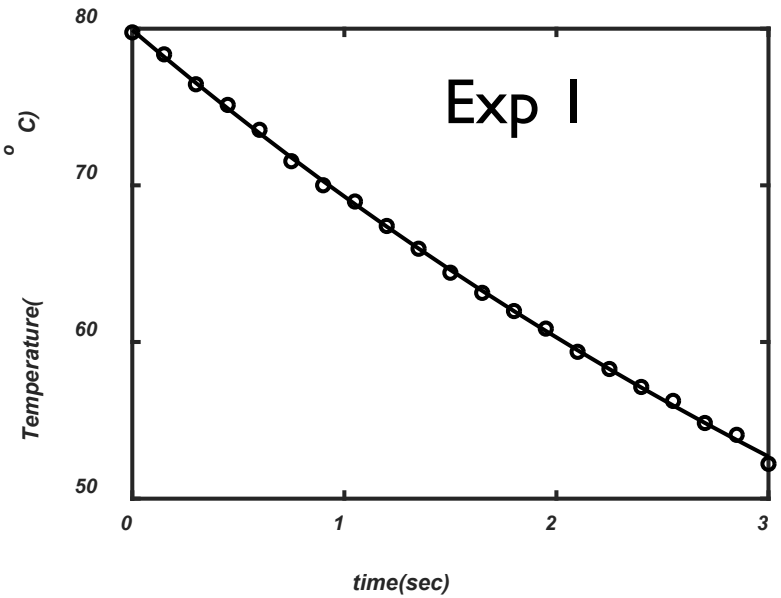
Error in the Estimates:

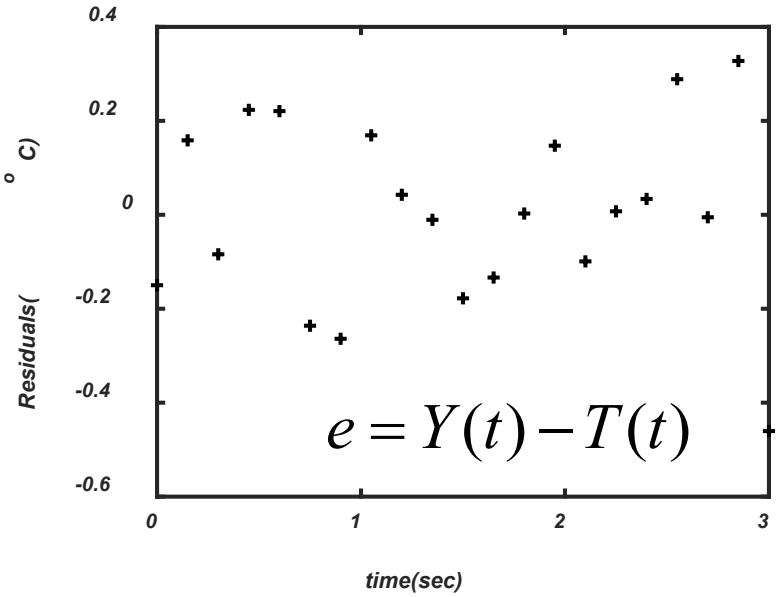
β_1: ~40%

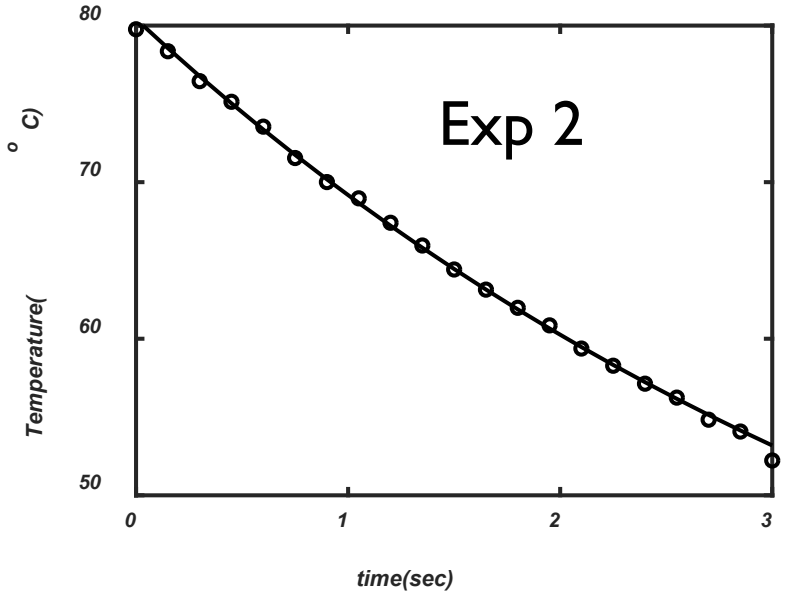
β_2: ~10%

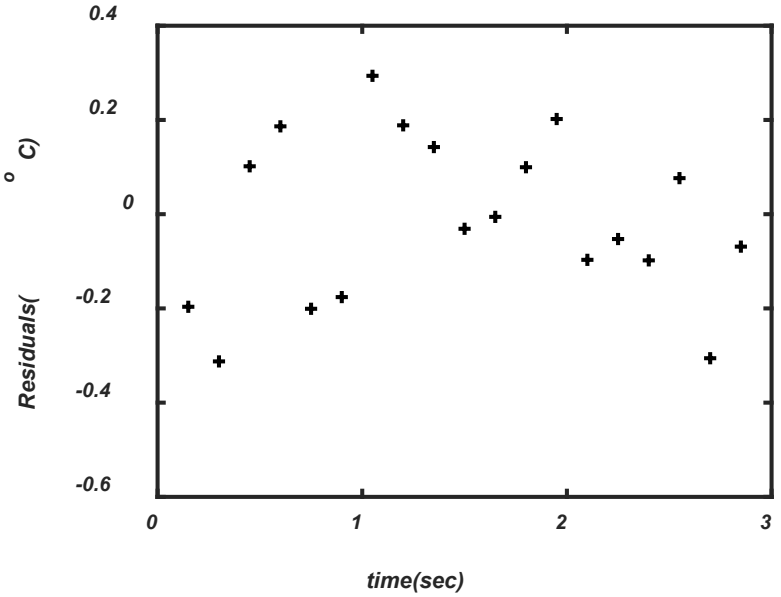
β_3: ~15%

Results for Quenching Example



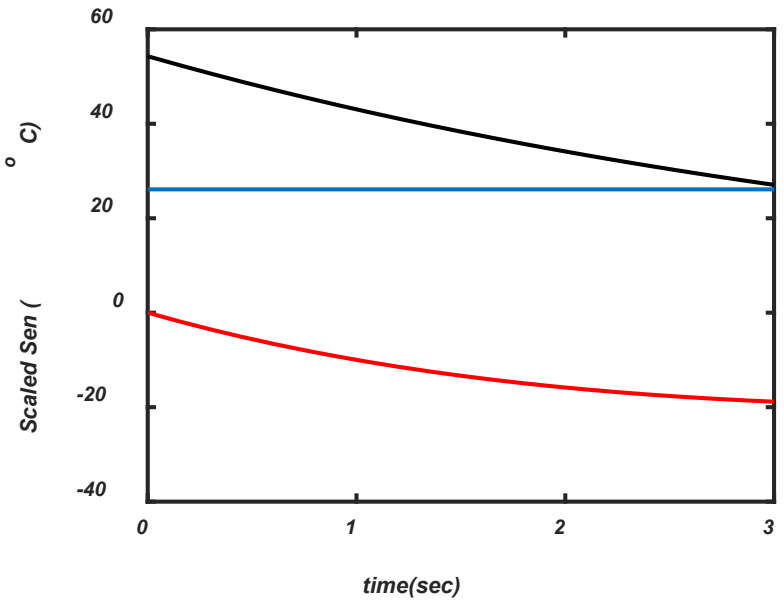


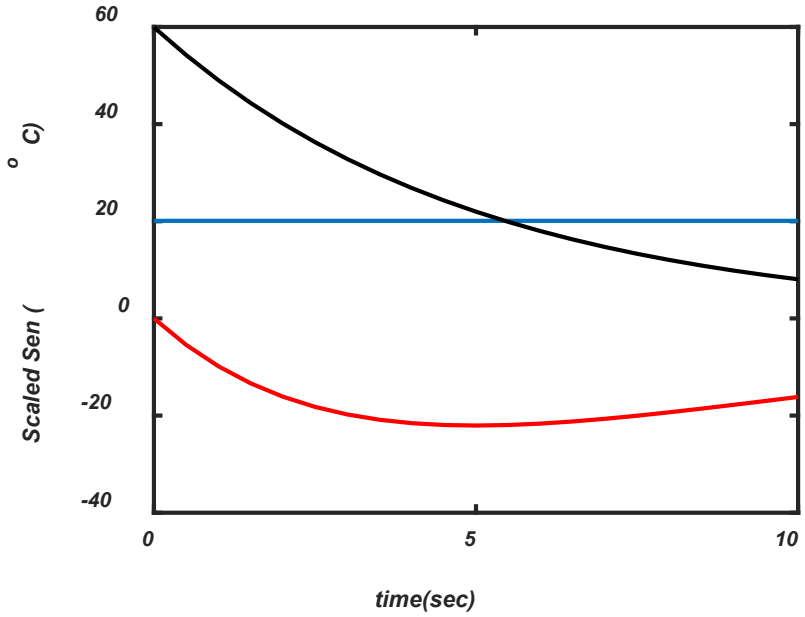




Explain poor fit -- sensitivity coefficients

- Plot sensitivities for the actual parameter values
- Plot sensitivities for the actual time range





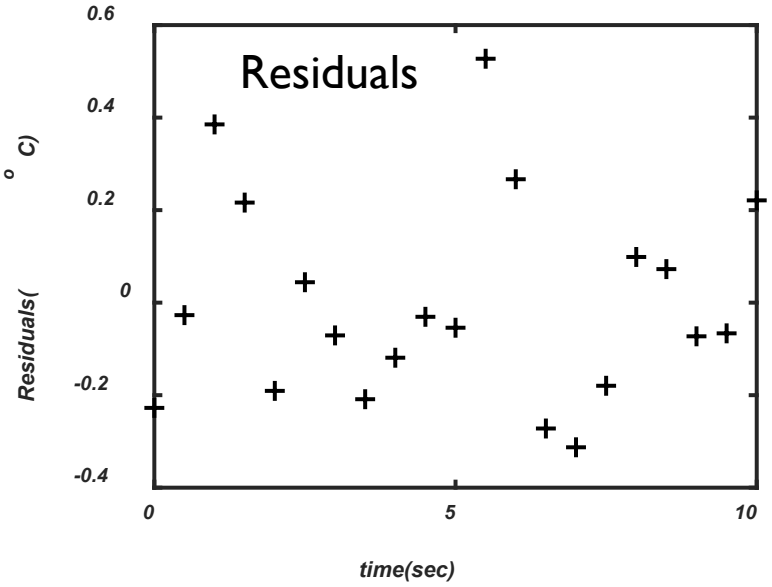
Actual time range 0 < t < 3

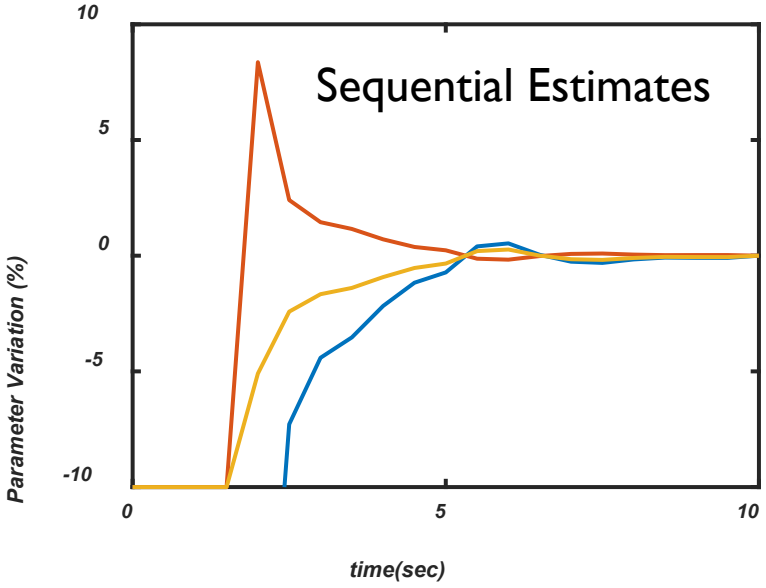
Improved time range 0 < t < 10

Optimal design of experiments is a formal approach to maximize information content

Sequential Estimates

Estimated parameter	0<t<3	0<t<10
β_1	10.8841	20.0913
β_2	69.0291	59.9413
β_3	0.1672	0.2007
$\Sigma(Y_i - T_i)^2$	0.7940	0.9796

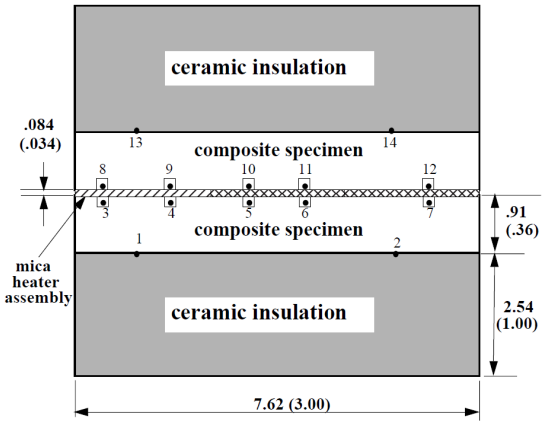


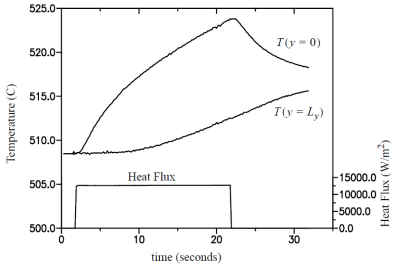


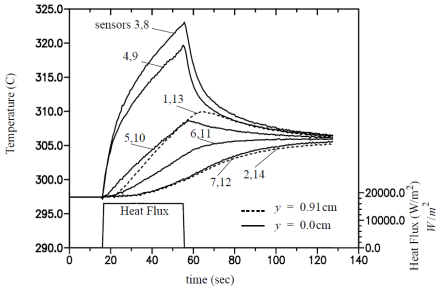
Lessons from quenching example

- Compare shape of the sensitivity coefficients for actual experimental conditions – shape depends strongly on parameters and time range
- Sensitivity coefficients must be large and have different shape to fit several parameters
- Sequential estimates can show if you have the “right” data (i.e. sufficiently long data record)
- Examine residuals to see if errors are randomly distributed (good) or trending/biased (bad)

Example 2: Thermal Properties for Carbon-Carbon Composite







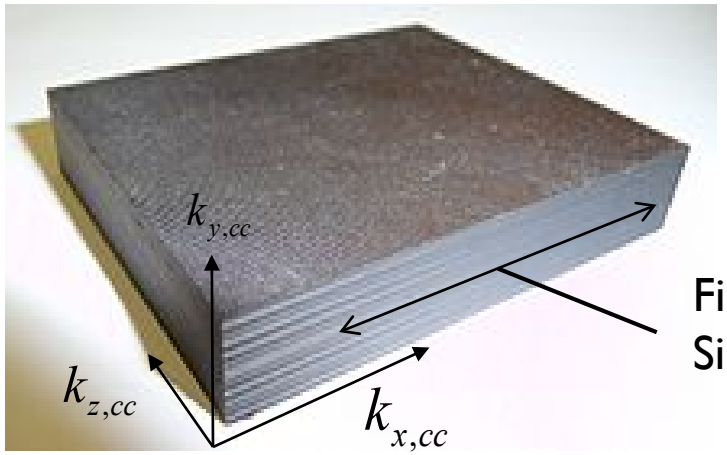
PROP-1D $(k_{y,cc}, \rho C_{cc})$

PROP-2D $(k_{y,cc}, k_{y,cc}, \rho C_{cc})$

Example: Estimating Directionally-Dependent and Temperature-Dependent Properties

Carbon-Carbon has highly anisotropic thermal properties $k_{x,cc} / k_{y,cc} > 10$

High Temperature applications (tested from room temperature to 625 ^{o}C



Fiber-Direction (xz-plane)
Silicon-Carbide Coating

Temperature dependent properties estimated for orthotropic properties

1D Experiments

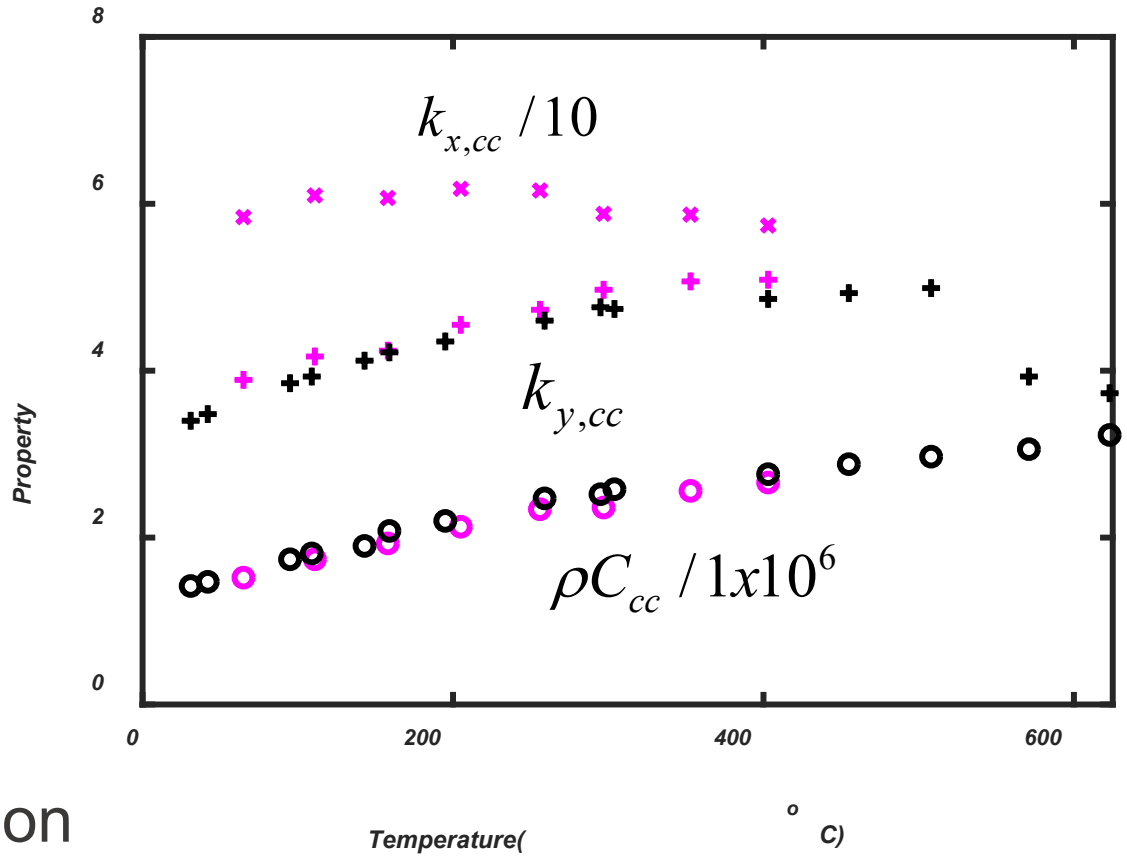
$(k_{y,cc}, \rho C_{cc})$

$25^{o}C$ to $600^{o}C$

2D Experiments

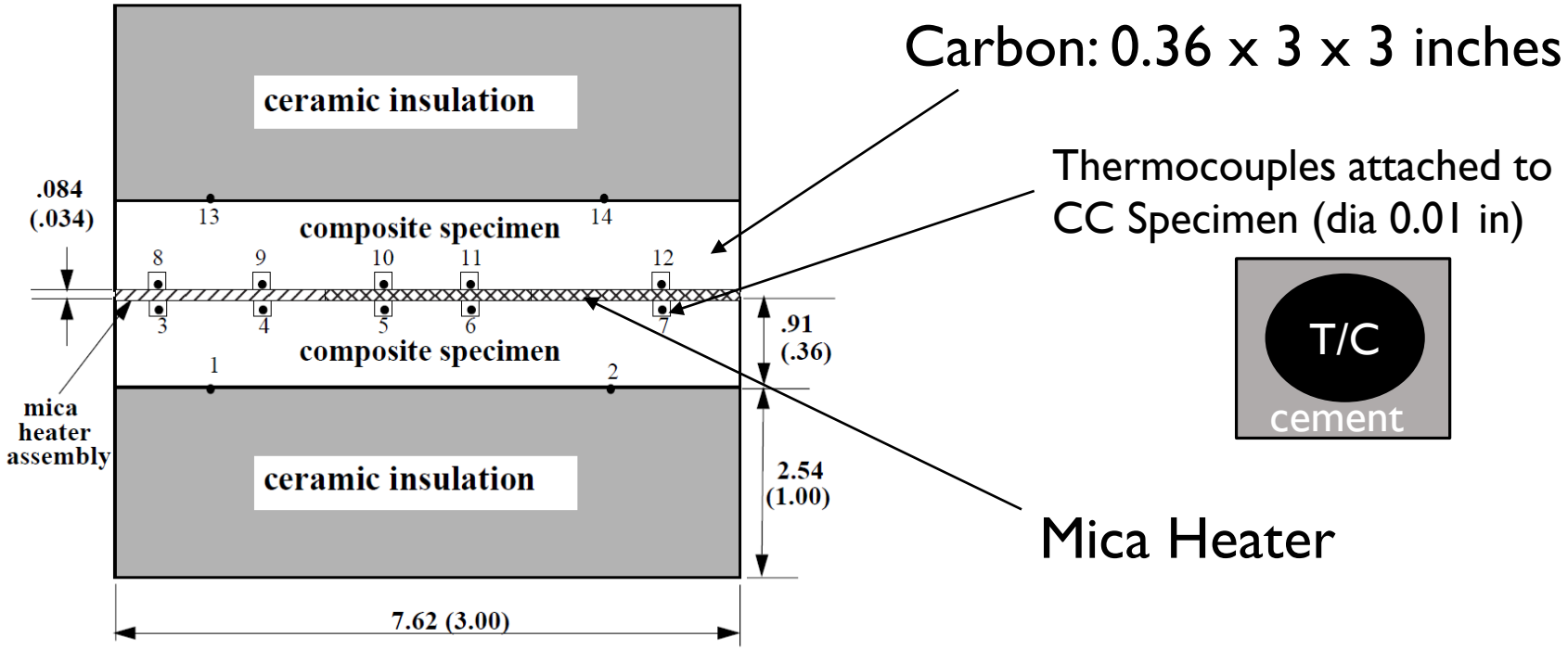
$(k_{y,cc}, k_{y,cc}, \rho C_{cc})$

$25^{o}C$ to $400^{o}C$



- Experimental Discussion
- 1D Approach and Results
- 2D Approach and Results

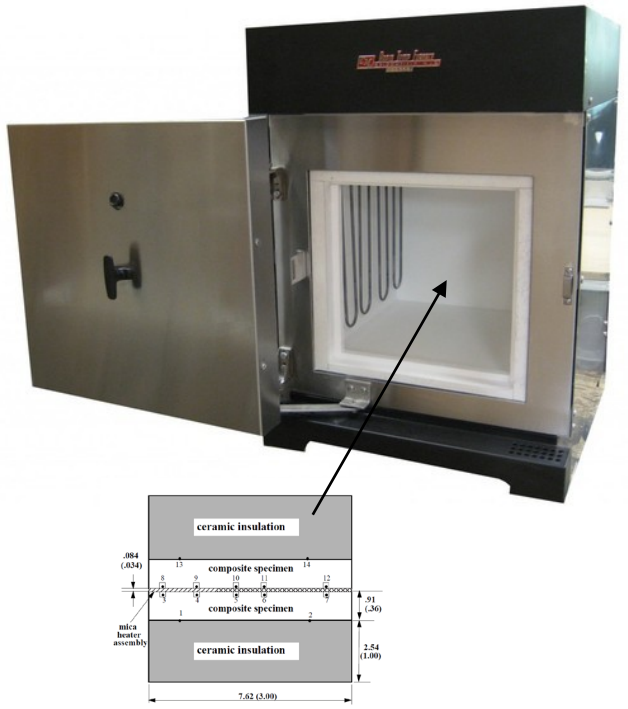
Experimental apparatus designed to estimate properties of anisotropic carbon-carbon



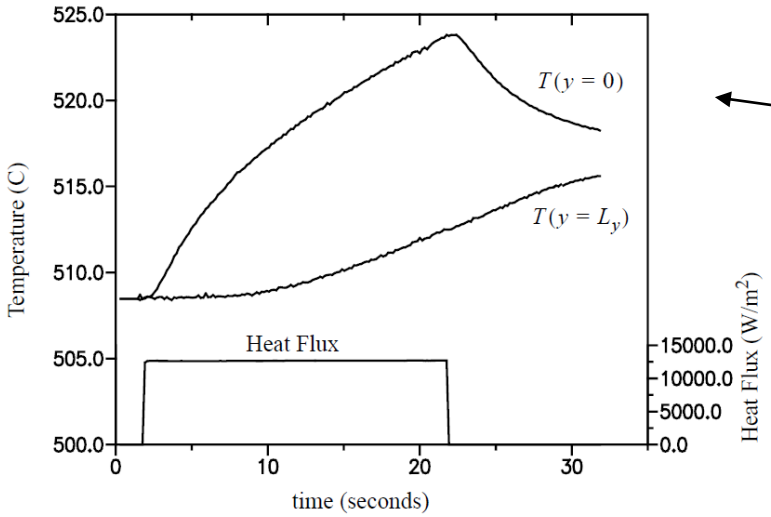
- Design allowed for 1D and 2D heat conduction within the composite sample
  - 3 independently controlled electric heaters (1/3 used for 2D)
- Thermocouples located along heater/composite interface and composite/insulation interface
  - Symmetric implementation
- Designed to estimate properties of a high conductivity material

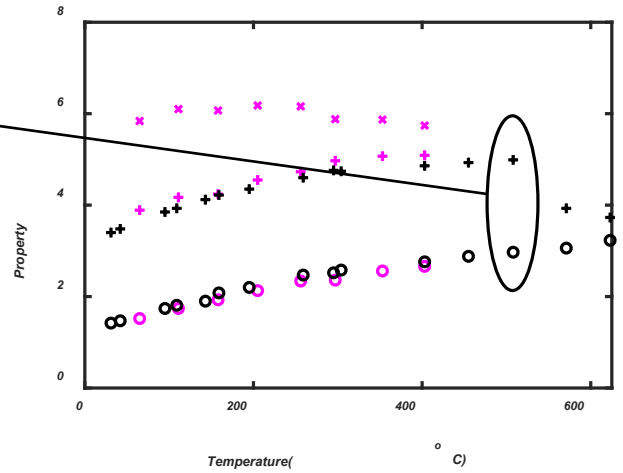
Series of experiments conducted to cover the temperature range

- Apparatus placed in an oven to specify the initial temperature
- Electric heaters activated to impose a transient
- Experimental design
  - Specify heat flux for a “reasonable” ΔT
  - Experimental duration longer than active Heat Flux

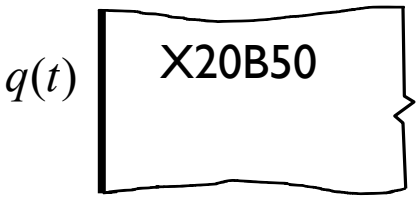


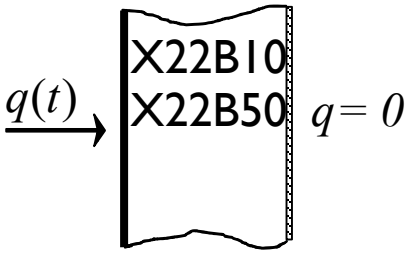
Typical Experiment ΔT = 15-20 °C

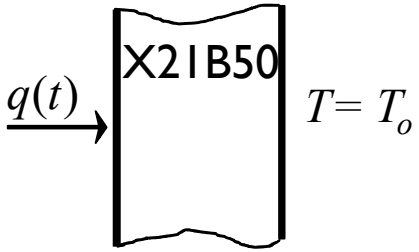




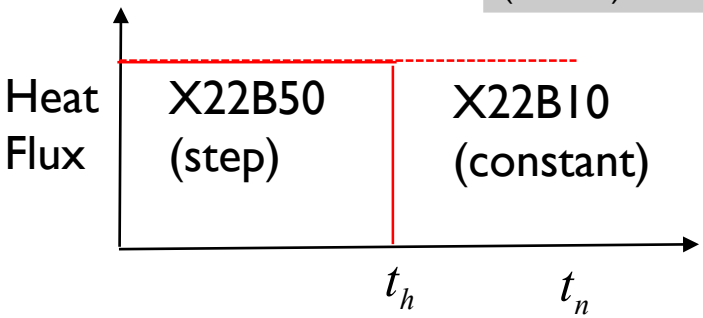
Can maximize the available information with Experimental Design







Geometry	BCs	Sensor	Max D	Opt (t_h)	Opt (t_n)
Semi-Infinite (Beck and Arnold)	X20BIT0	Heated Surface In-depth	0.00263	1.5	1.5
Semi-Infinite (Taktak)	X20B5T0	Heated Surface In-depth	0.0055	1.2	1.2
Finite (Beck and Arnold)	X22BI0T0	Heated Surface	0.00098	1.2	1.2
Finite (Beck and Arnold)	X22BI0T0	x = 0 x = 1	0.0058	0.65	0.65
Finite (Beck and Arnold)	X22B50T0	x = 0 x = 1	0.0088	0.4	0.6
Finite (Taktak)	X21B50T0	Heated Surface	0.020	2.25	2.98
Finite (Taktak)	X21B50T0	Heated Surface	0.012	7	7



Optimality Criteria (Beck and Arnold, 1977)

$$D = \frac{1}{sn(T^{+}_{\max})^2}\det(X^T X)$$

Analysis of the One Dimensional Experiments

Thermal model of apparatus (1D)

- Mica heater assembly (1/2)

- Ceramic Insultation

PROP1D (Beck Engineering Consultants)

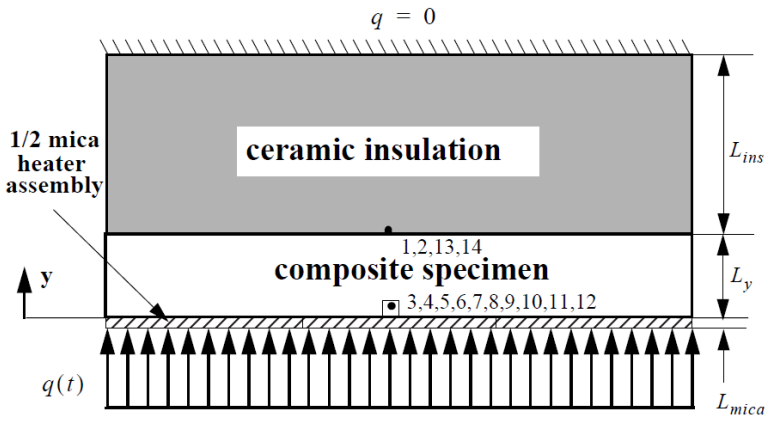
- Finite difference numerical solution

- Integrated with a Gauss method to estimate parameters

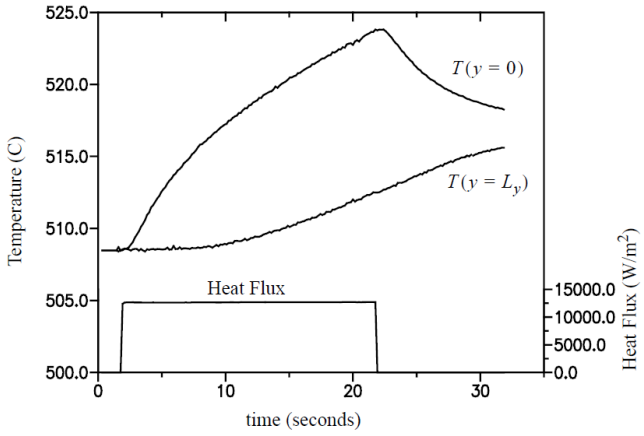
$$b^{k+1} = b^k + P\left[X^T W \left(Y - \hat{T} \right) + U(u - b^{(k)}) \right]$$

$$P^{-1} = \left(X^T W X + U \right)$$

for measurements Y and model $\hat{T}$



Thermal Model - $\hat{T}$



Exp Measurements - Y

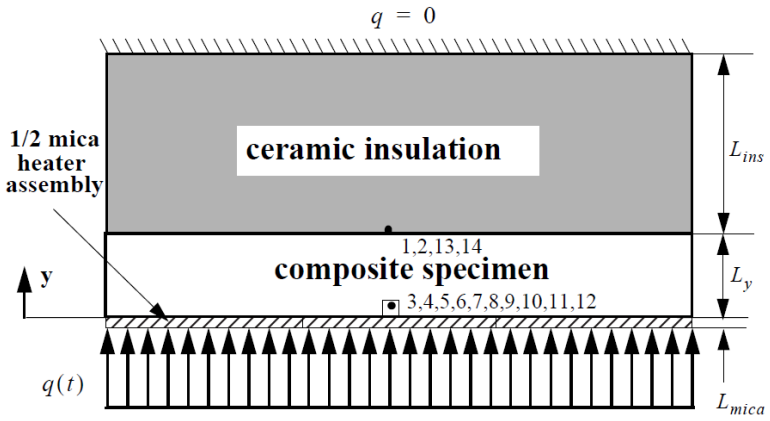
Thermal model includes ancillary materials that will affect the estimated parameters

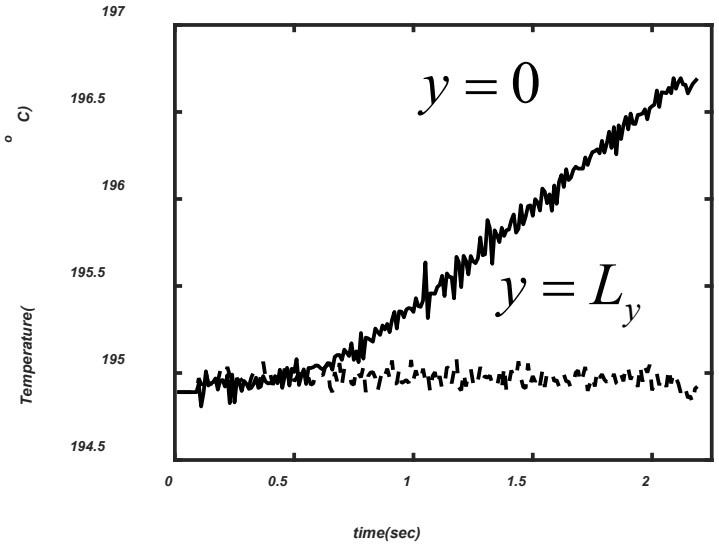
Heater Assembly

- Electric heater imbedded in a mica assembly
- Contact conductance between heater and composite is unknown
- Short duration experiment conducted to estimate effective heater properties
  - Conducted for each experiment

Ceramic Insulation

- Experiments conducted with composite replaced by insulation
  - Estimated for 2 temperatures (40 and 175 ^{o}C)
  - 50% difference from values provided by the manufacture

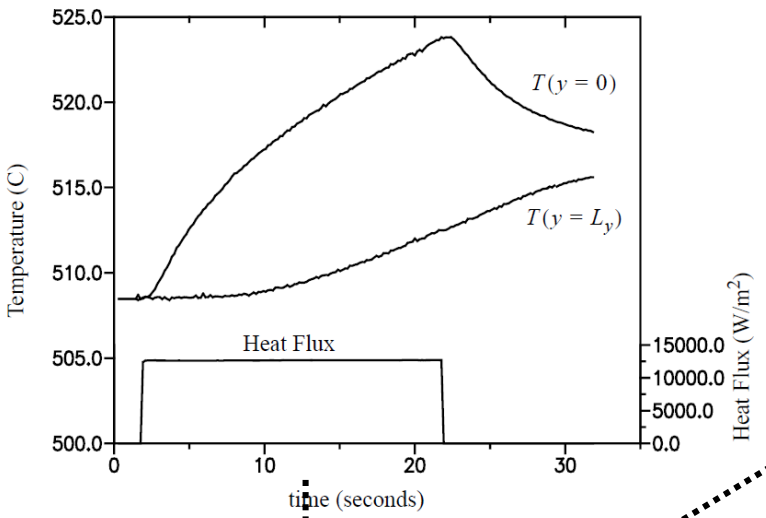




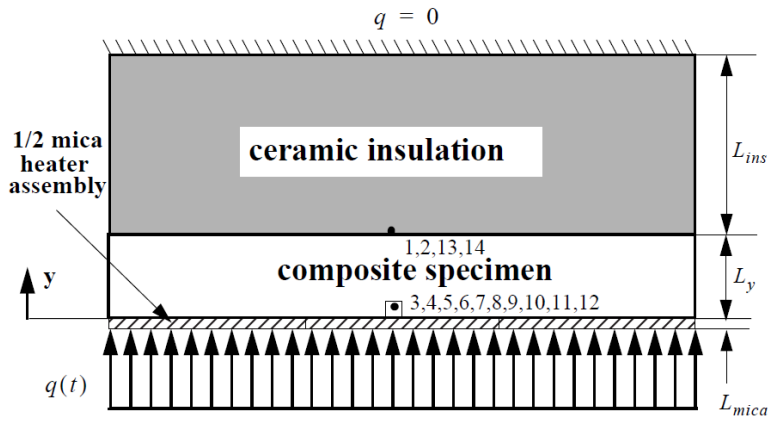
Estimates for One-dimensional Experiment

Typical experiment (T = 508 °C)

Exp Measurements - Y



Thermal Model - $\hat{T}$



PROP-ID

Estimated Parameters

$$k_{y,cc} = 4.99 \pm 0.05 \quad W/m^oC$$

$$\rho C_{cc} = 2.97x10^6 \pm 0.02 \quad J/m^{3o}C$$

Estimates for One-dimensional Experiment

Confidence Intervals

$$\mathrm{cov}(\hat{b}) \approx \left(X^T W X\right)^{-1} s^2$$

$$s^2 \approx \frac{\left(Y-\hat{T}\right)^T \left(Y-\hat{T}\right)}{n-p}$$

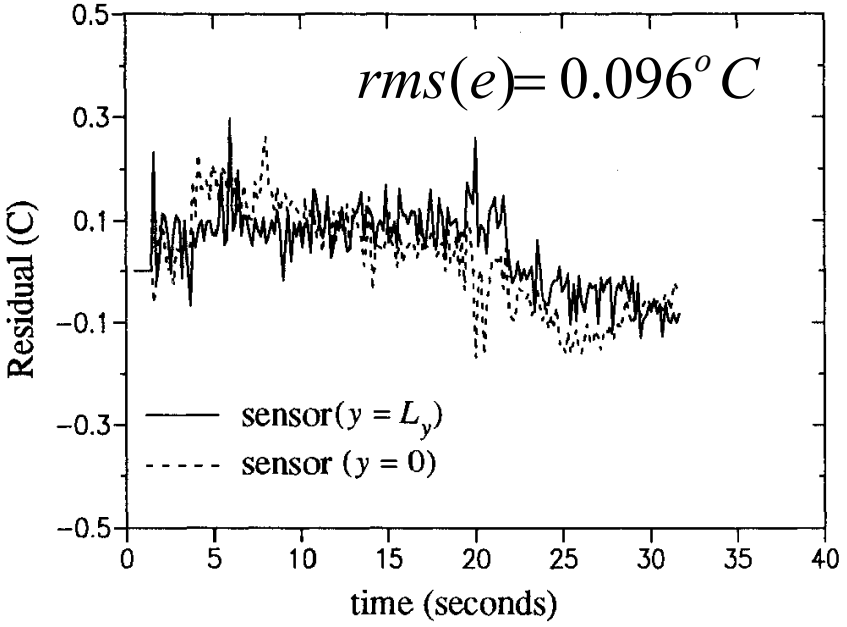
Standard Statistical Assumptions (1111-011)

Estimated Parameters

$$k_{y,cc} = 4.99 \pm 0.05 \quad W/m^oC$$

$$\rho C_{cc} = 2.97x10^6 \pm 0.02 \quad J/m^{3o}C$$

Residuals, $e = Y - \hat{T}$



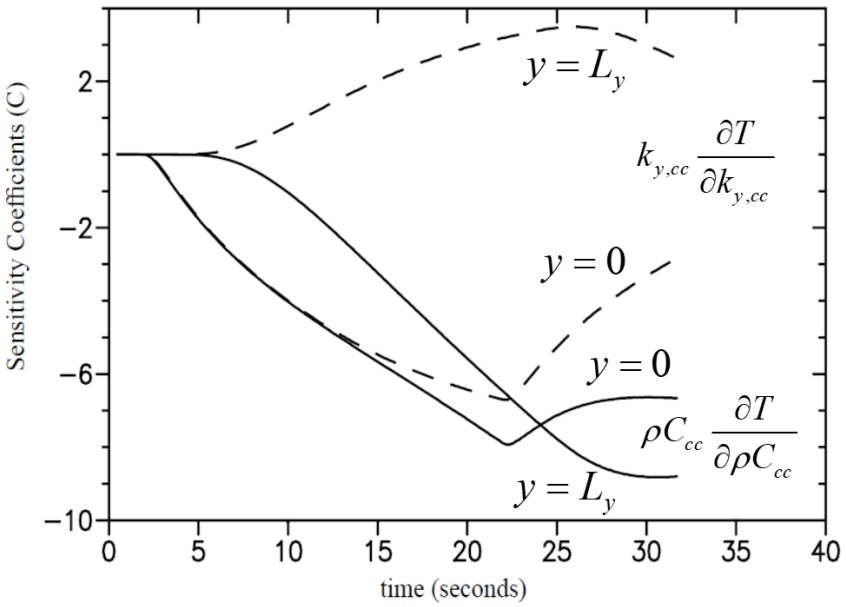
Standard Statistical Assumptions for the Measurement Errors (Beck and Arnold, 1977)

1. Additive measurement errors (1111-011)
2. Zero mean measurement error
3. Constant variance measurement error
4. Uncorrelated measurement error
5. Measurement error is normal
6. Known statistical parameters for measurement error
7. Errorless independent variables
8. Constant parameters

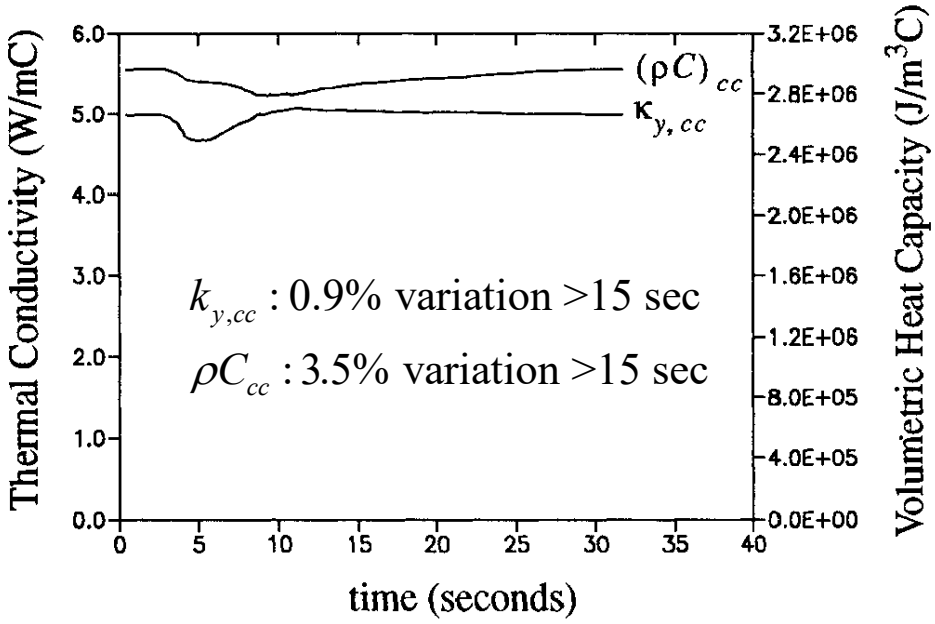
Least-squares estimates are based on the measurement errors

Sensitivity coefficients and sequential parameter estimates assess the quality of the process

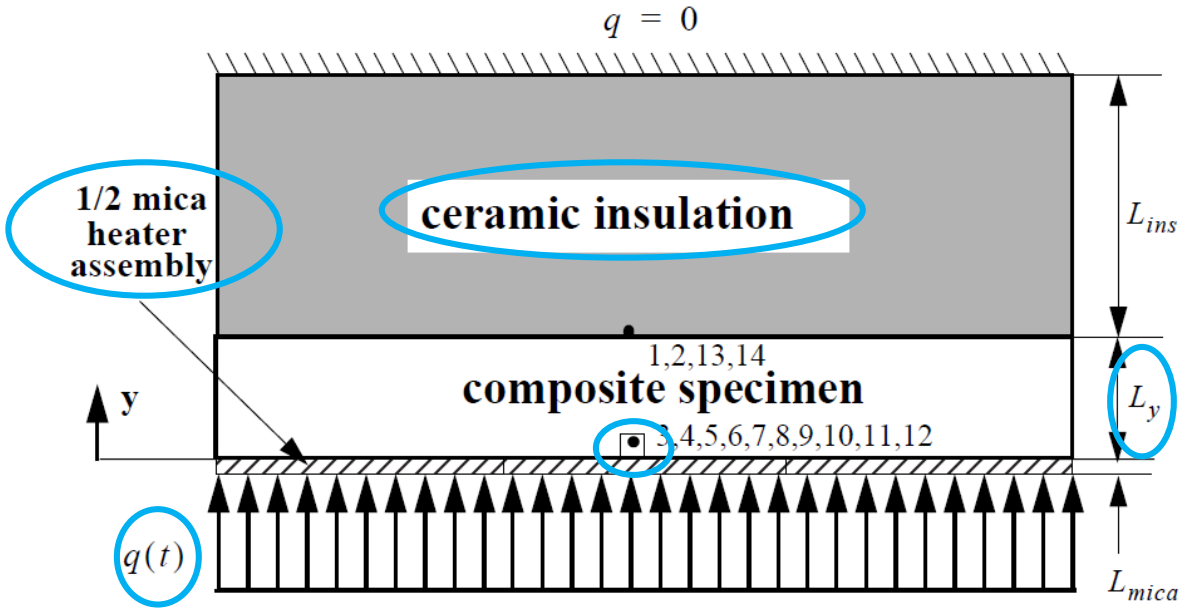
Scaled Sensitvity Coefficients



Sequential Estimates



Uncertainty analysis conducted to assess the effect of experimental uncertainties



$$\Delta_{\hat{b}}^2 = \sum_{i=1}^{N} \left(\frac{\partial \hat{b}}{\partial z_i} \Delta_z \right)^2$$

$$\frac{\partial \hat{b}}{\partial z_i} \approx \frac{\hat{b}(z_i + \Delta z_i) - \hat{b}(z_i)}{\Delta z_i}$$

Uncertainty analysis conducted to assess effect of experimental uncertainty

Exp Parameter	Uncertainty	$\frac{\partial \hat{b}}{\partial z_i}\Delta_z$		$\left(\frac{\partial \hat{b}}{\partial z_i}\Delta_z\right)^2 / \Delta_{\hat{b}}^2$	
z_i	Δ_z	ρC_{cc}	$k_{y,cc}$	ρC_{cc}	$k_{y,cc}$
		J/(m^3 C)	W/(m C)	(%)	(%)
q	125 W/m^2	0.033	0.049	0.162	0.345
L_y	0.05 mm	0.016	0.027	0.038	0.105
y_l	0.025mm	0.014	0.015	0.029	0.032
k_{mica}	20%	0.04	0.0	0.237	0
ρC_{mica}	20%	0.06	0.06	0.534	0.518
k_{ins}	20%	0.0	0.0	0	0
ρC_{ins}	20%	0.0	0.0	0	0
	$\Delta_{\hat{b}} =$	0.082	0.083		

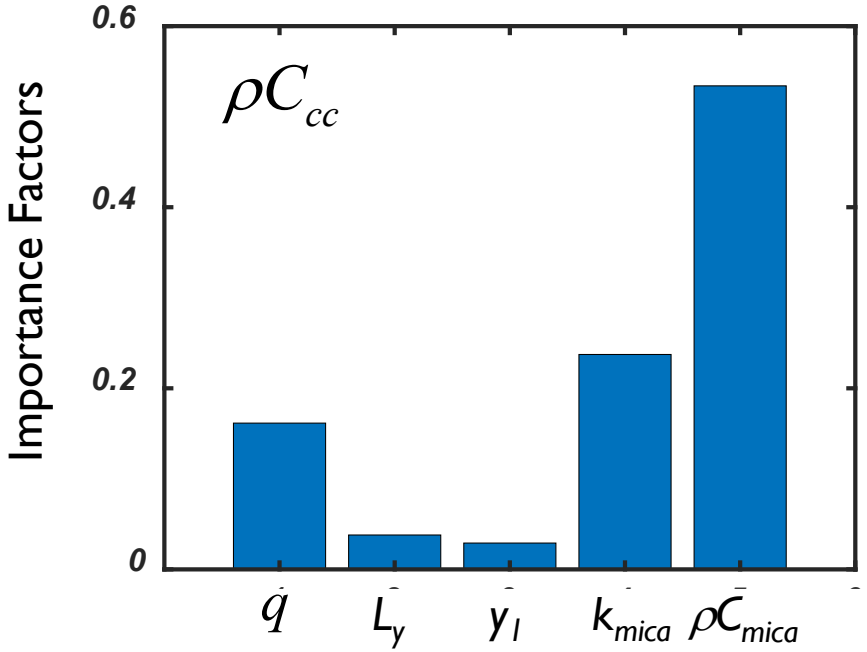
$$\rho C_{cc} = 2.97x10^6 \pm 0.02 \ J/m^{3o}C$$

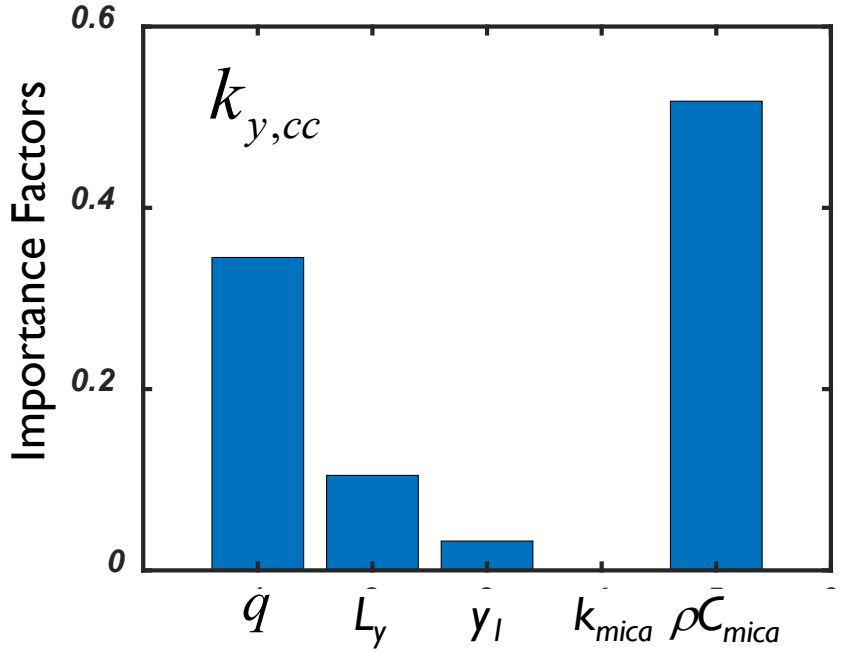
$$k_{y,cc} = 4.99 \pm 0.05 \ W/m^oC$$

Uncertainty due to measurement error

Can identify the main contributors to the overall experimental uncertainty

$$IF_i = \left(\frac{\partial \hat{b}}{\partial z_i} \Delta_z \right)^2 \Big/ \sum_{i=1}^{N} \left(\frac{\partial \hat{b}}{\partial z_i} \Delta_z \right)^2$$

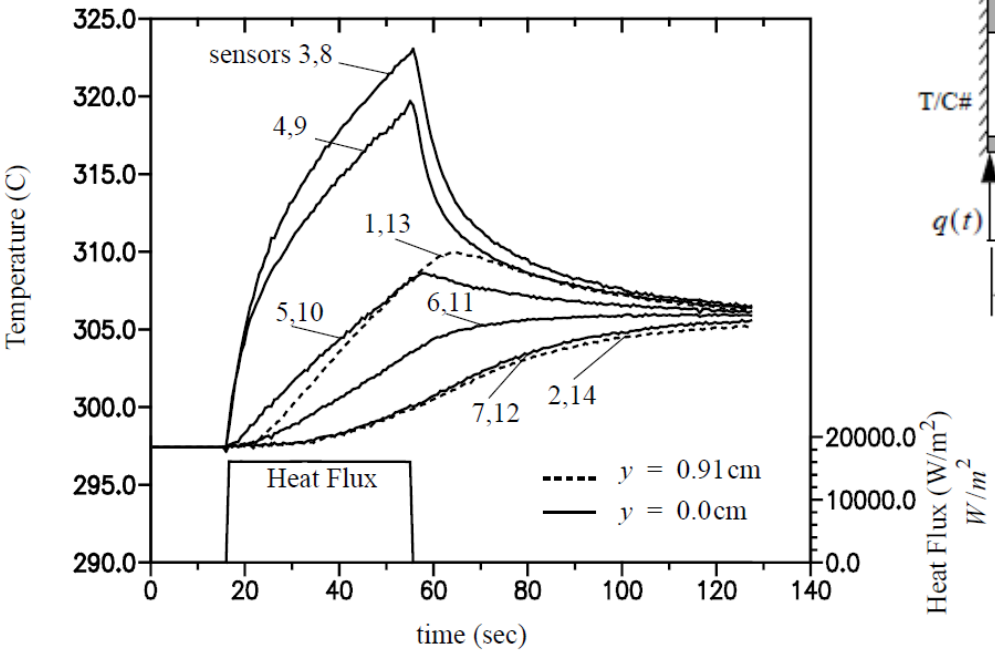


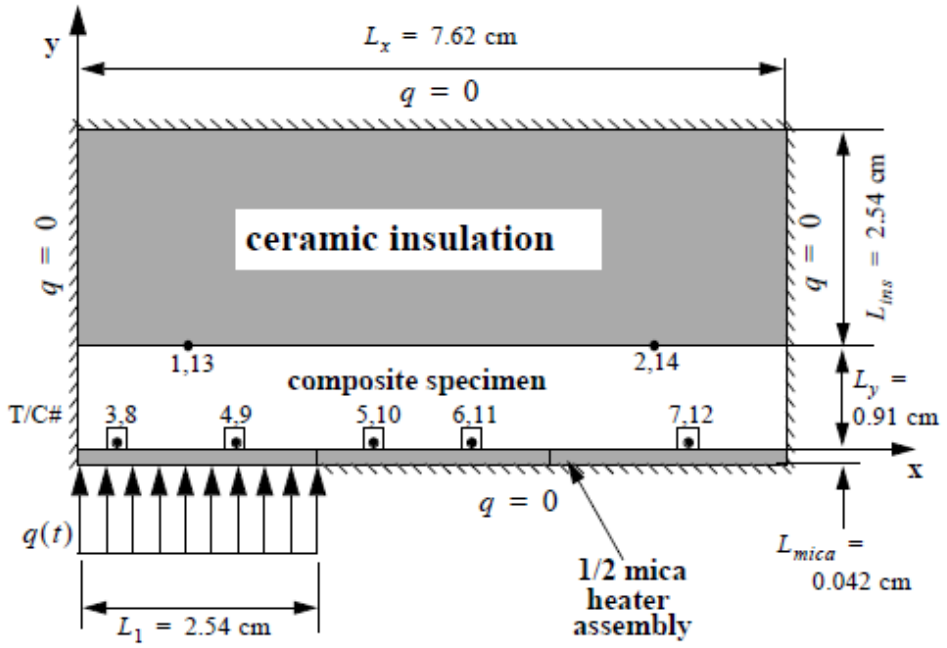


Heat Flux and properties of the (mica) heater are main contributors to uncertainty

Analysis of 2D Experiments

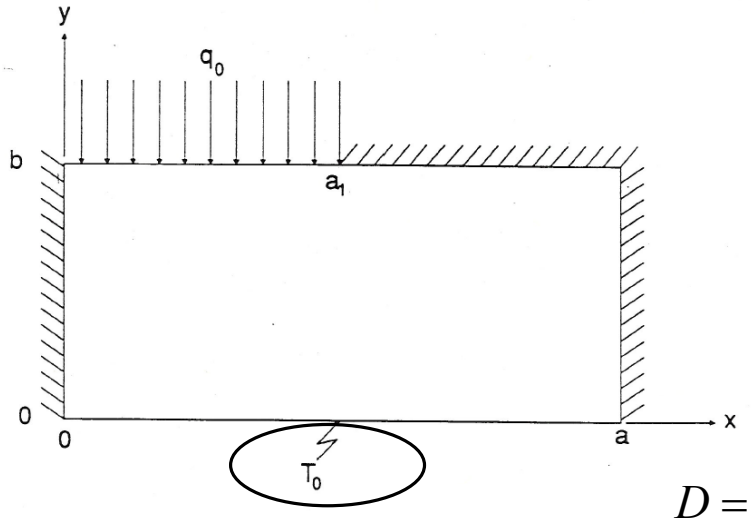
- Need a 2D heat conduction solver
- Estimate three parameters for each experiment





Meas. Sci. Technol. **9** (1998) 877–887.

Design of 2D Experiments (Taktak, 1992)



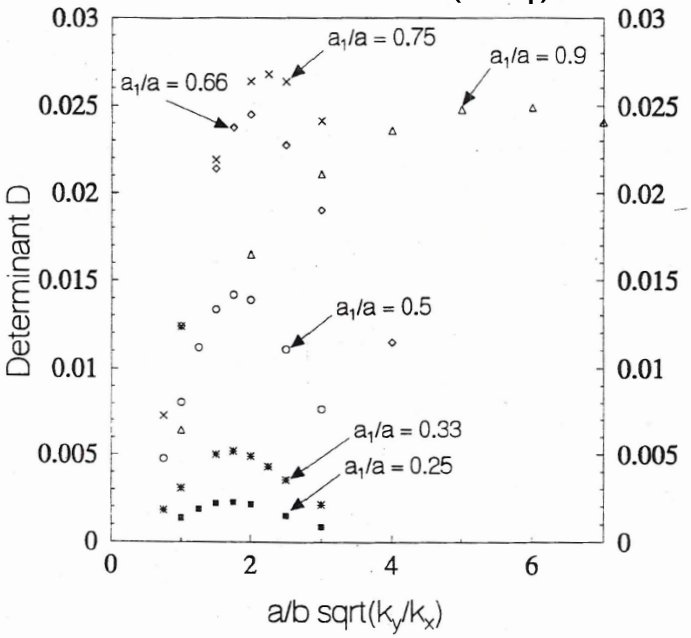
$$T_t^*(x^*,y^*,t^*) = 2a_1^* \sum_{n=1}^{\infty} \frac{(-1)^n}{\lambda_n^2} \sin(\lambda_n y^*) e^{-\lambda_n^2 t^*} + \frac{4}{\pi} *$$

$$\sum_{m=1}^{\infty}\sum_{n=1}^{\infty} \frac{(-1)^n}{m\left(\lambda_m^2 \frac{b^2}{a^2}\frac{k_y}{k_x} + \lambda_n^2\right)} \cos(\lambda_m x^*) \sin(\lambda_m a_1^*) \sin(\lambda_n y^*) e^{-\left(\lambda_m^2 \frac{b^2}{a^2}\frac{k_y}{k_x} + \lambda_n^2\right) t^*}$$

Analytical Solution

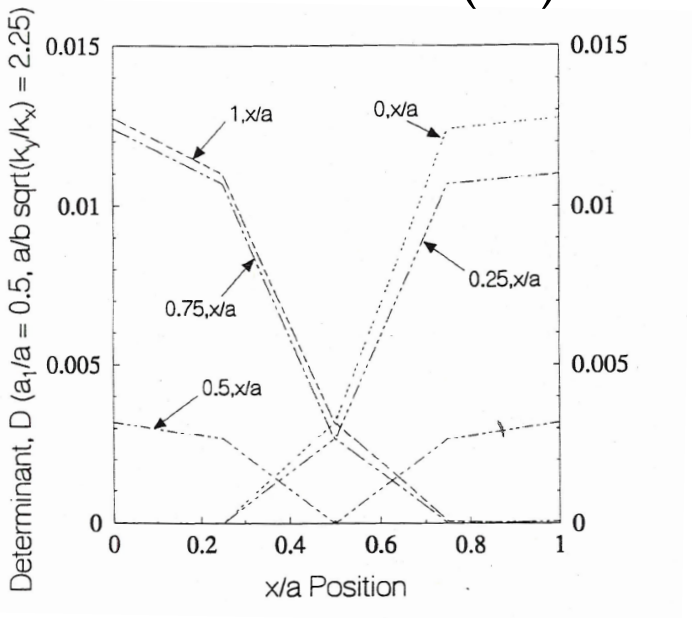
$$D = \frac{1}{sn(T_{\max}^+)^2} \det(X^T X)$$

Heated Area (a/a_1)



$$\frac{a}{b}\sqrt{\frac{k_y}{k_x}}$$

Sensor Locations (x/a)



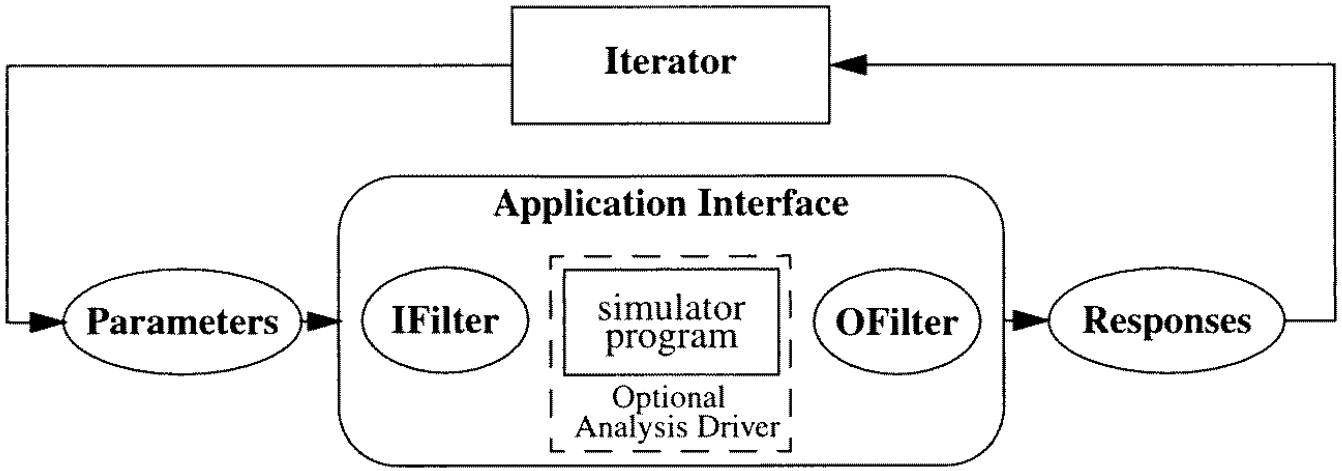
Analysis code for 2D parameter estimation

PROP2D (Developed at Michigan State in 1990s)

- Finite element solution (Topaz2D, LLNL)
- Converted to a subroutine and merged with a least-squares solver

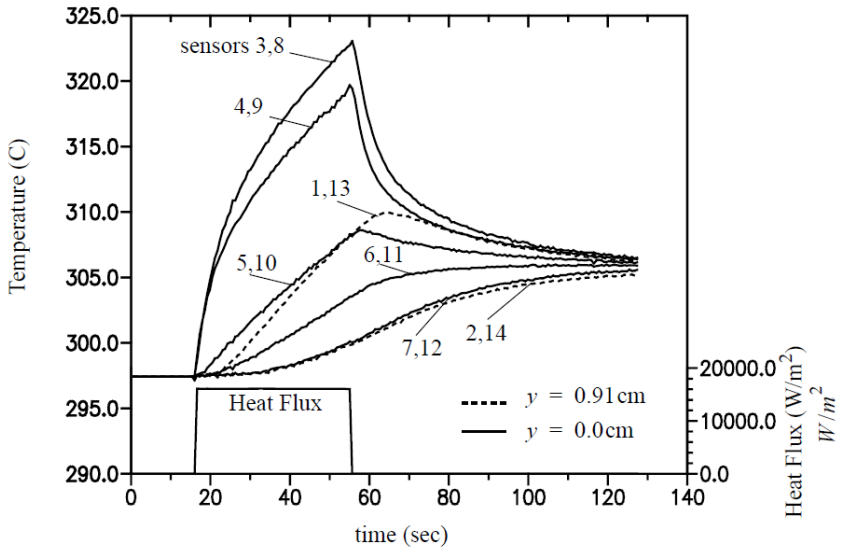
Dakota

- Implements algorithms for optimization, uncertainty, and least-squares
- Leverages existing direct simulation programs

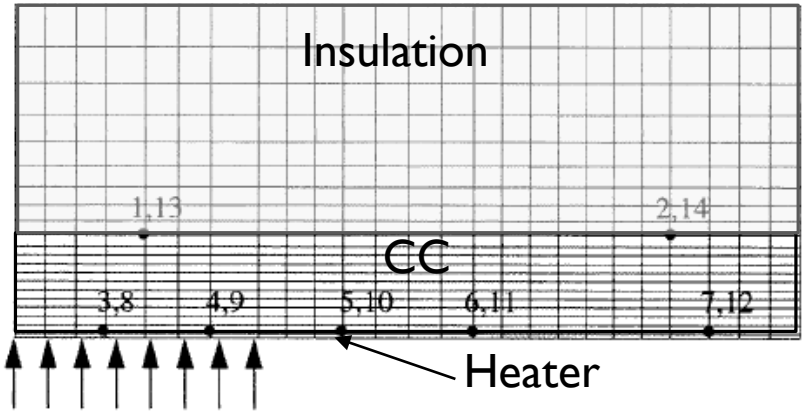


Estimates for Two-dimensional Experiment

Exp Measurements - Y



Thermal Model - $\hat{T}$



PROP-2D

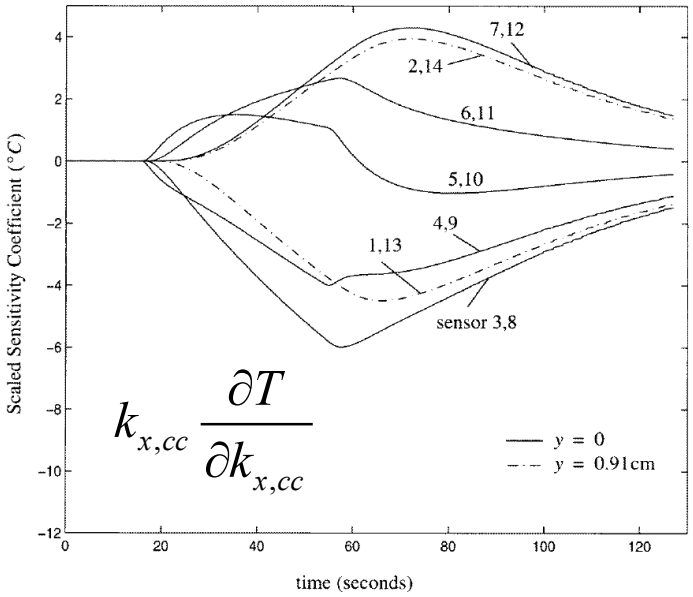
Estimated Parameters

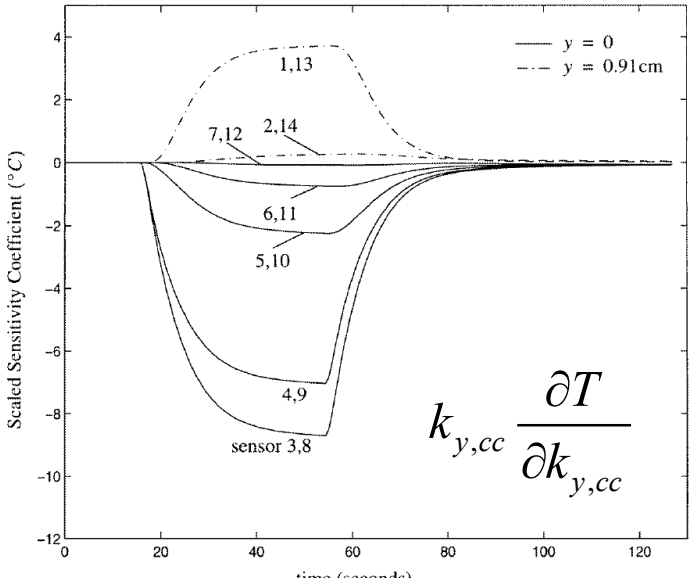
$$k_{x,cc} = 58.8 \pm 0.38 \quad W/m^oC$$

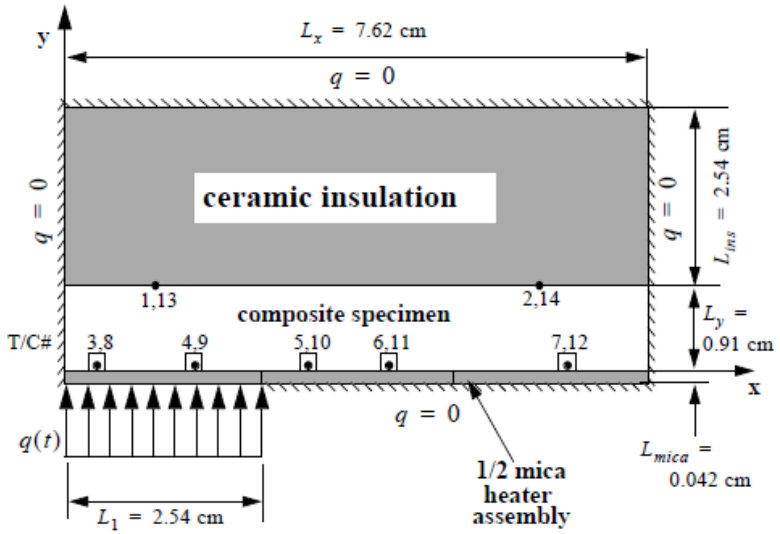
$$k_{y,cc} = 4.97 \pm 0.06 \quad W/m^oC$$

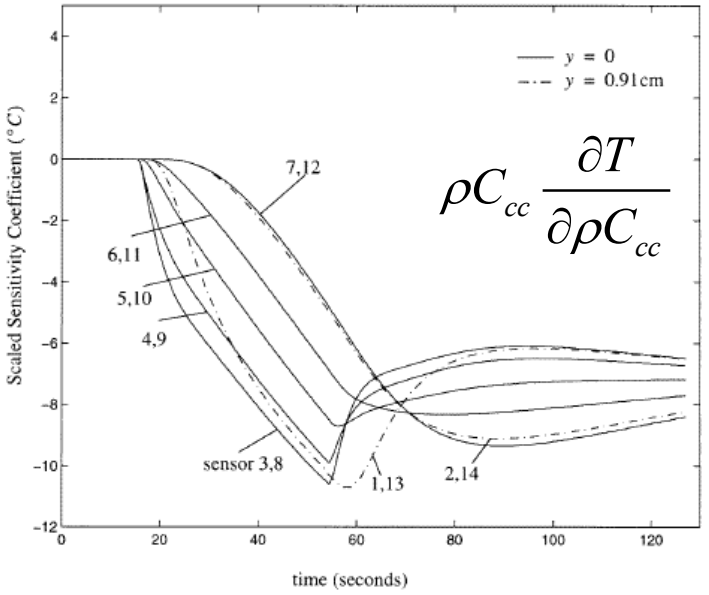
$$\rho C_{cc} = 2.36x10^6 \pm 0.007 \quad J/m^{3o}C$$

Scaled Sensitivity Coefficients

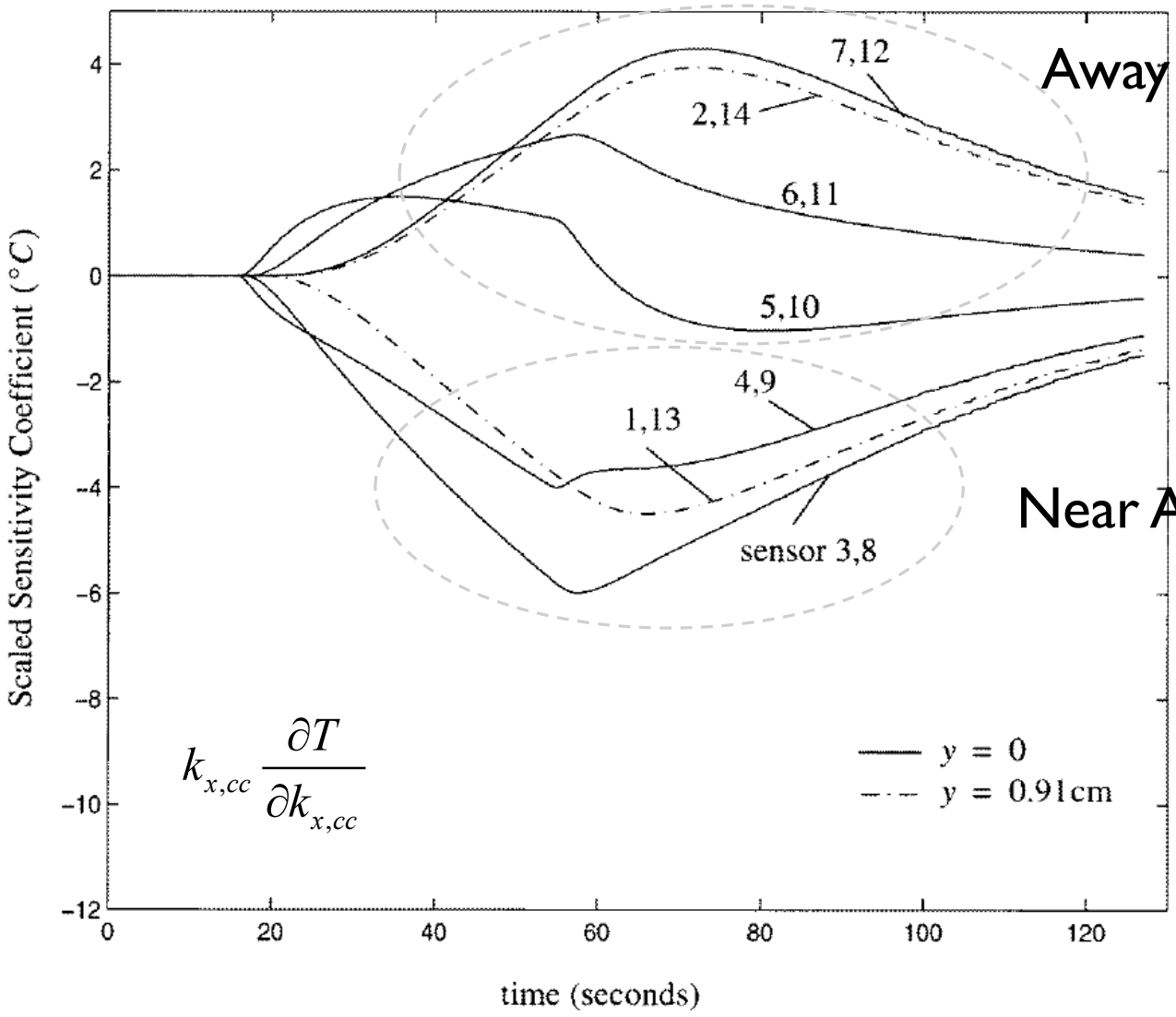








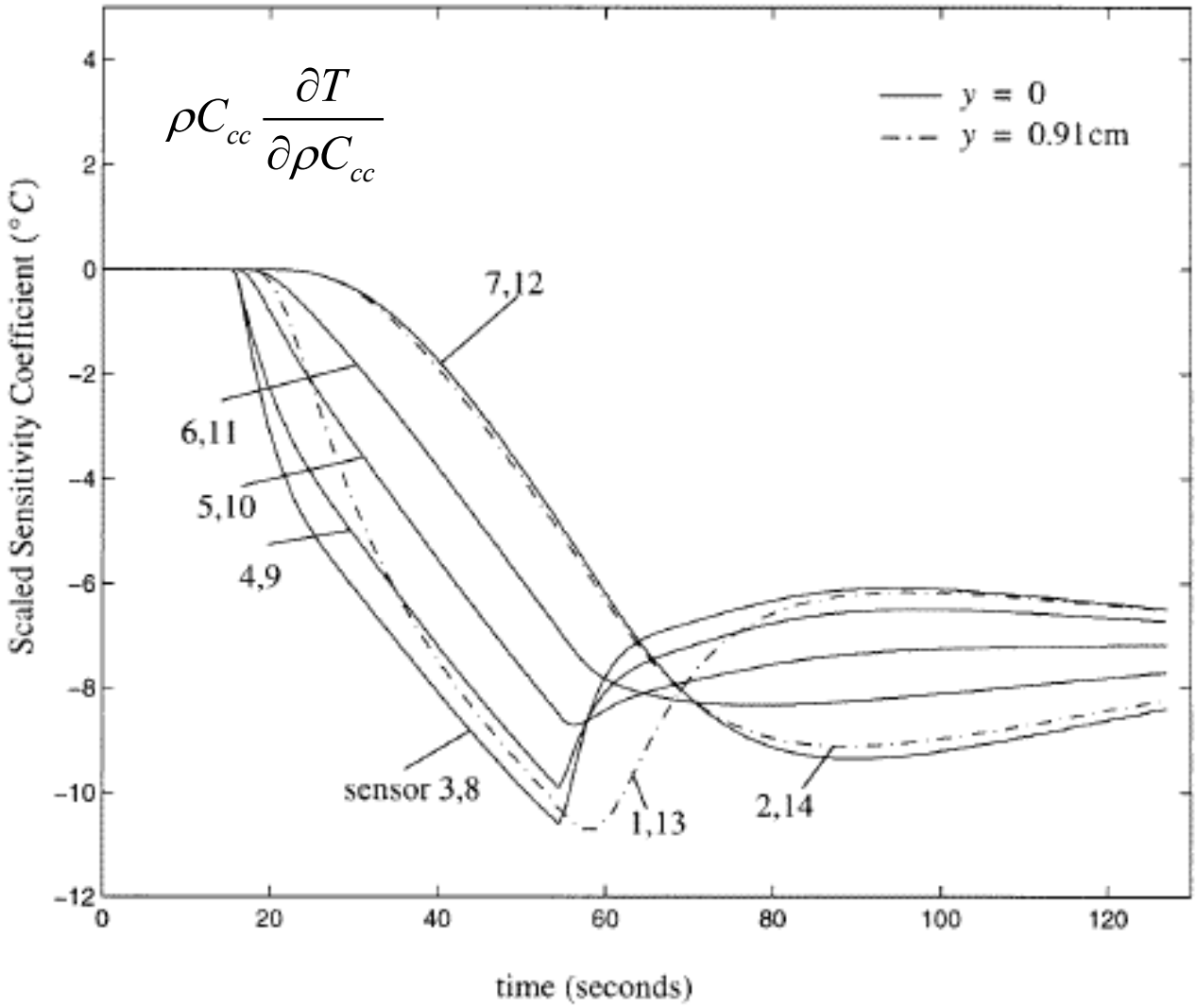
Scaled Sensitivity, $k_{x,cc}\frac{\partial T}{\partial k_{x,cc}}$



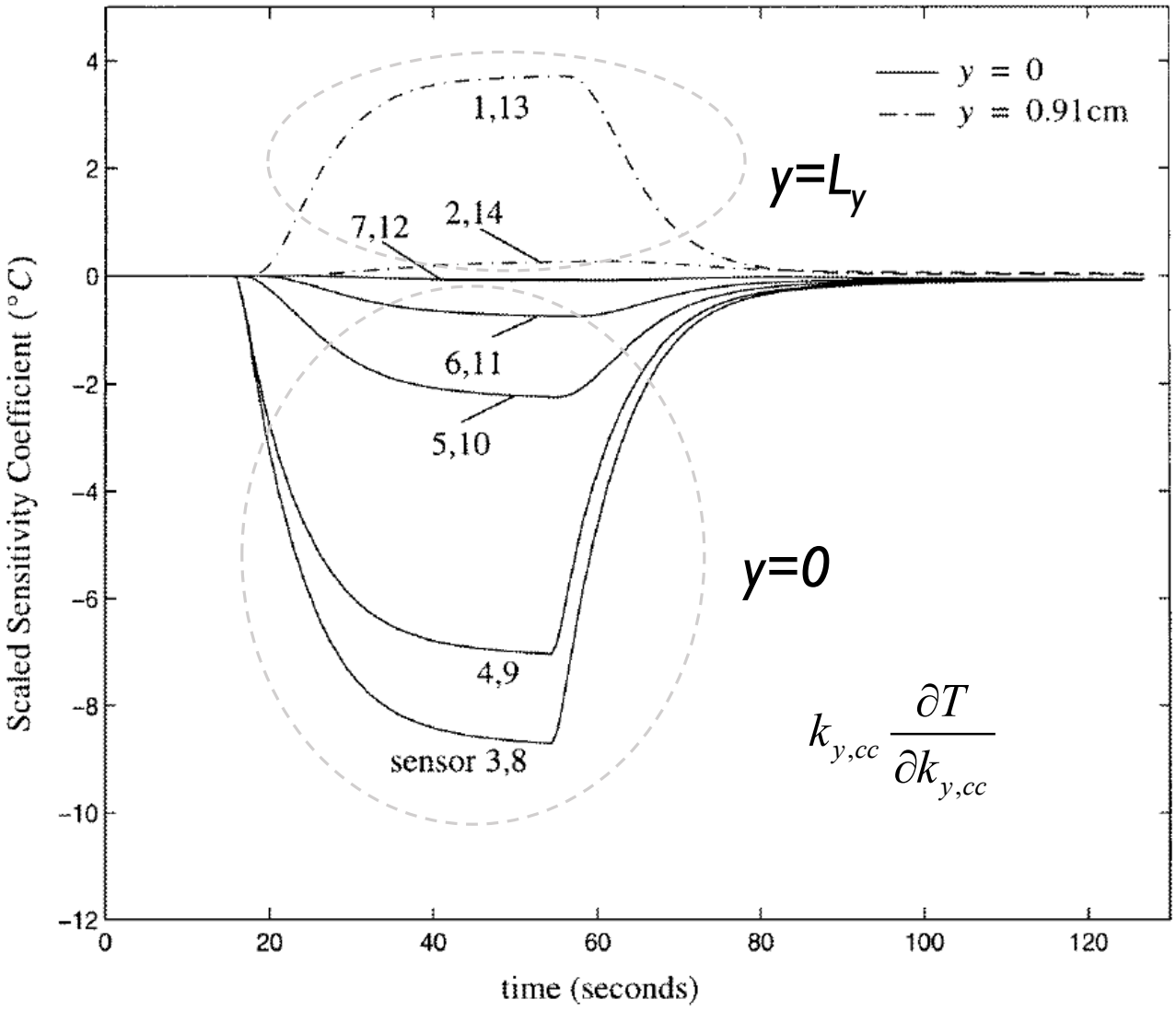
Away from Active Heater

Near Active Heater

Scaled Sensitivity, $\rho C_{cc} \frac{\partial T}{\partial \rho C_{cc}}$

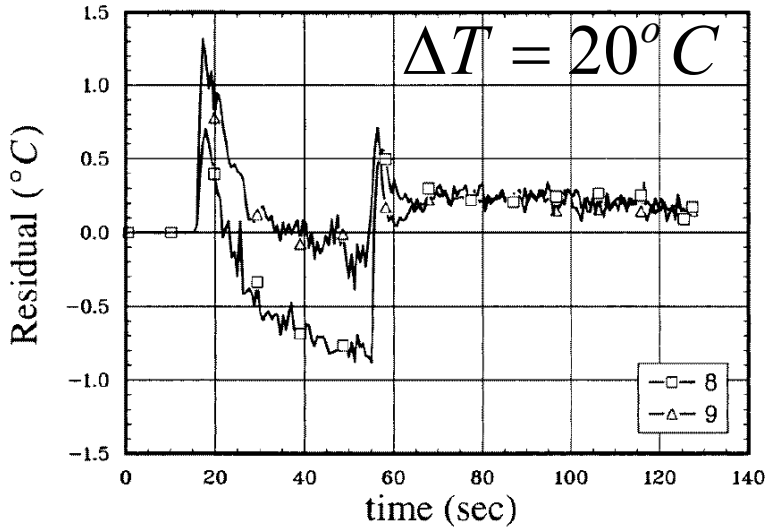


Scaled Sensitivity, $k_{y,cc}\frac{\partial T}{\partial k_{y,cc}}$

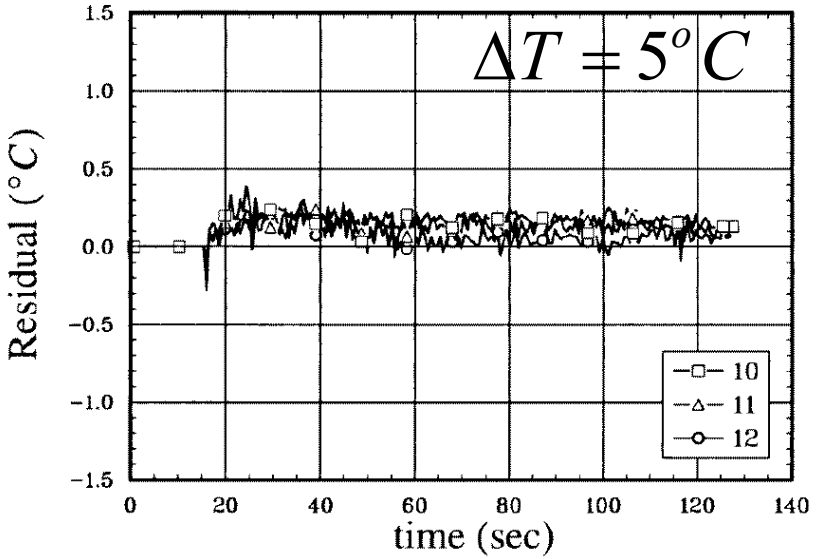


Residuals demonstrate signatures

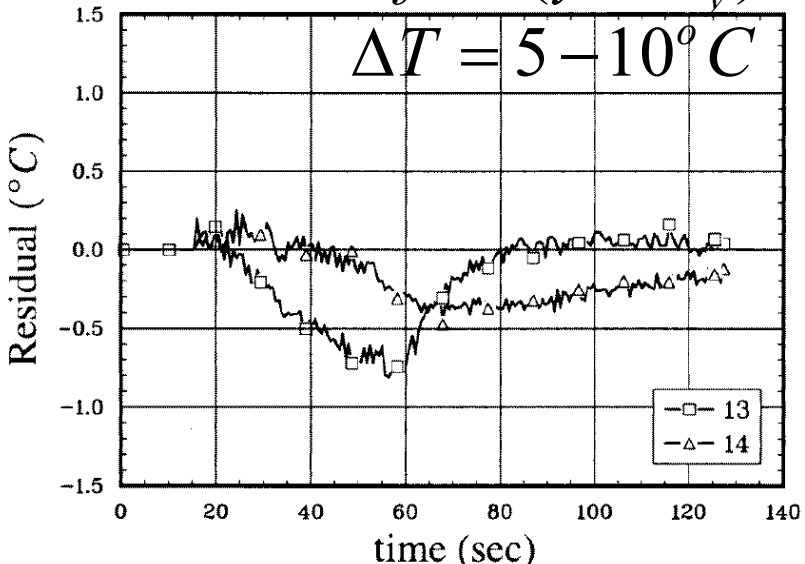
Active Heater $(y = 0)$



Inactive Heater $(y = 0)$



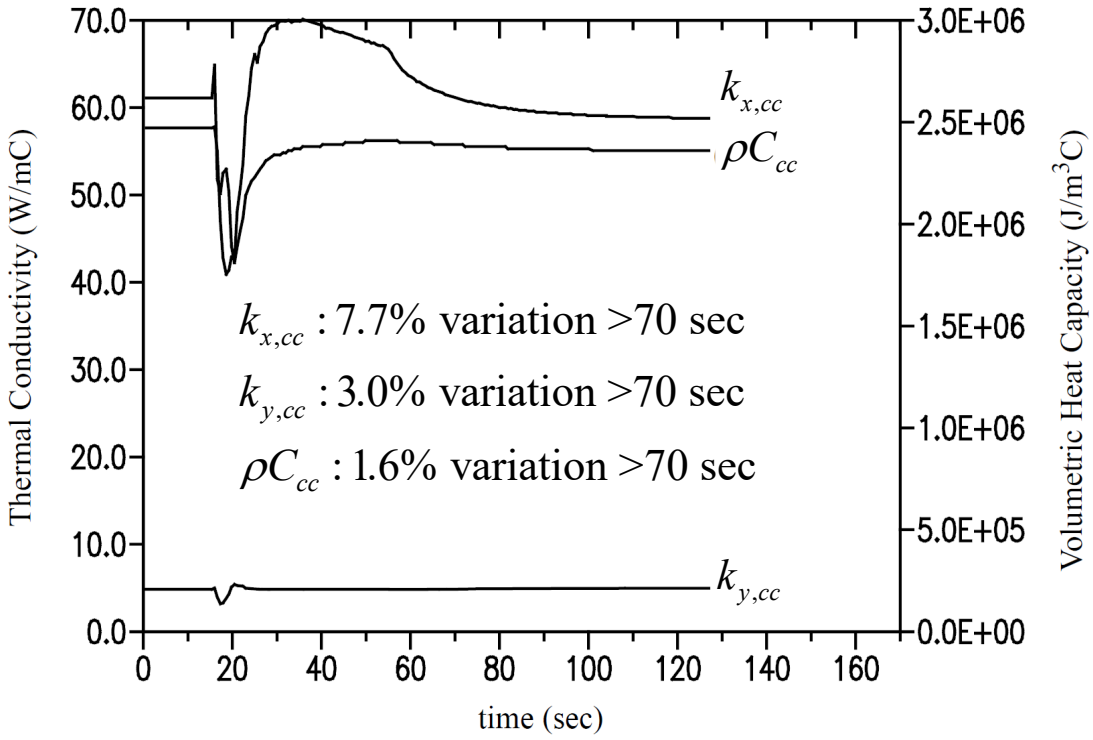
Back surface $(y = L_y)$



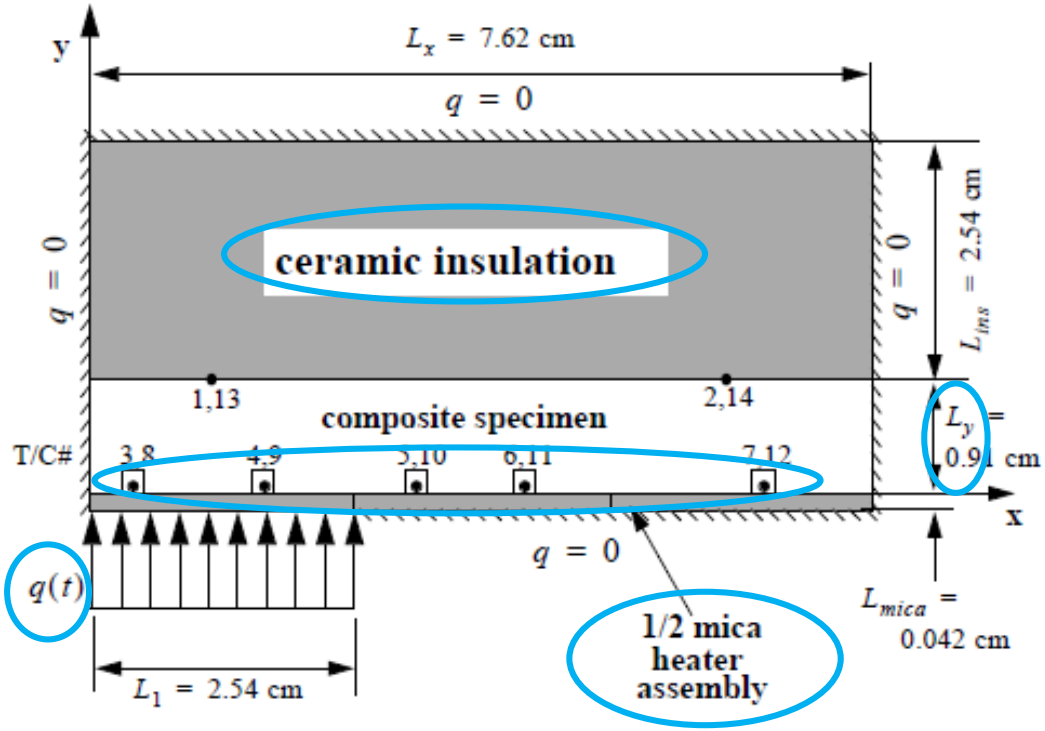
Residuals, $e = Y - \hat{T}$

$rms = 0.30^o C$

Sequential Estimates



Uncertainty analysis conducted to assess the effect of experimental uncertainties



$$\Delta_{\hat{b}}^2 = \sum_{i=1}^{N} \left(\frac{\partial \hat{b}}{\partial z_i} \Delta_z \right)^2$$

$$\frac{\partial \hat{b}}{\partial z_i} \approx \frac{\hat{b}(z_i + \Delta z_i) - \hat{b}(z_i)}{\Delta z_i}$$

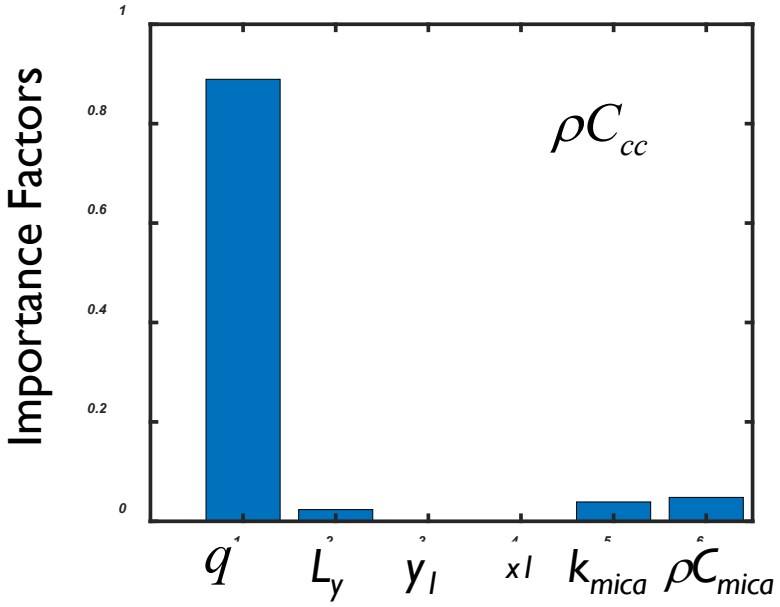
Uncertainty analysis (2D)

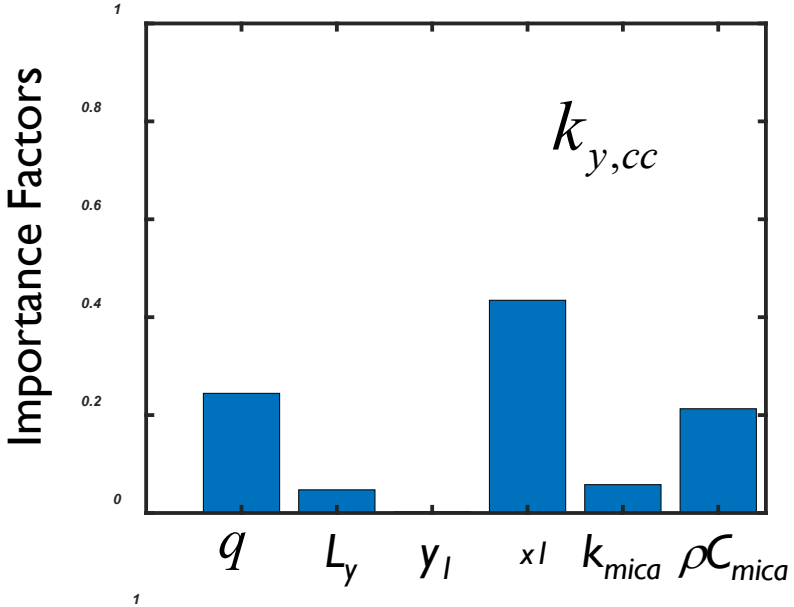
Exp Parameter	Uncertainty	$\frac{\partial \hat{b}}{\partial z_i}\Delta_z$			$\left(\frac{\partial \hat{b}}{\partial z_i}\Delta_z\right)^2 / \Delta_{\hat{b}}^2$		
z_i	Δ_z	ρC_{cc}	$k_{x,cc}$	$k_{y,cc}$	ρC_{cc}	$k_{x,cc}$	$k_{y,cc}$
		J/(m³ C)	W/(m C)	W/(m C)	(%)	(%)	(%)
q	3% (W/m²)	0.086	1.9	0.15	0.89	0.59	0.25
L_y	0.05 mm	0.014	0.43	0.066	0.02	0.03	0.05
y_l	0.025mm	5.5E-4	0.14	0.016	0.0	0.00	0.00
x_j	1.0 mm	8.0E-4	0.72	0.20	0.0	0.09	0.43
k_{mica}	20%	0.018	0.55	0.073	0.04	0.05	0.06
ρC_{mica}	20%	0.020	1.2	0.14	0.05	0.24	0.21
k_{ins}	20%	0.0	0.0	0	0.0	0.0	0.0
ρC_{ins}	20%	0.0	0.0	0	0.0	0.0	0.0
	$\Delta_{\hat{b}} =$	0.091	2.5	0.30			

$$\rho C_{cc} = 2.36x10^6 \pm 0.007 \;\; J/m^{3o}C$$

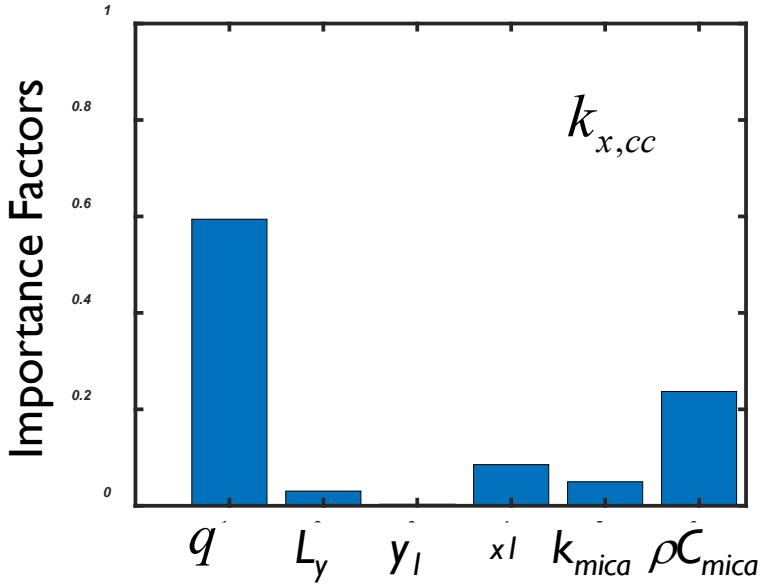
$$k_{x,cc} = 58.8 \pm 0.38 \;\; W/m^oC \qquad k_{y,cc} = 4.97 \pm 0.06 \;\; W/m^oC$$

Experimental Uncertainty Analysis (2D)





$$IF_i = \left(\frac{\partial \hat{b}}{\partial z_i} \sigma_z \right)^2 / \sum_{i=1}^{N} \left(\frac{\partial \hat{b}}{\partial z_i} \sigma_z \right)^2$$



Summary -- Parameter Estimation

- Parameter estimation is using experimental data to find values in a mathematical model – i.e. for finding thermal properties from a heat transfer experiment.
- Examine the sensitivity coefficients, which must be large and independent *for the conditions at hand.*
- Optimality condition D is a formal way to assess the size and level of independence of sensitivity coeffs.
- Examine the residuals ($T_{model} - T_{data}$). Are they normally distributed (good) or biased/trending (bad)?
- Examine sequential estimates to observe the variability in your estimates and to show if you have the “right” data range.
- Study the effect of uncertainties on the estimated parameters

References

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Discussion/Questions

Back-up Slides

Tutorial Overview

Parameter estimation

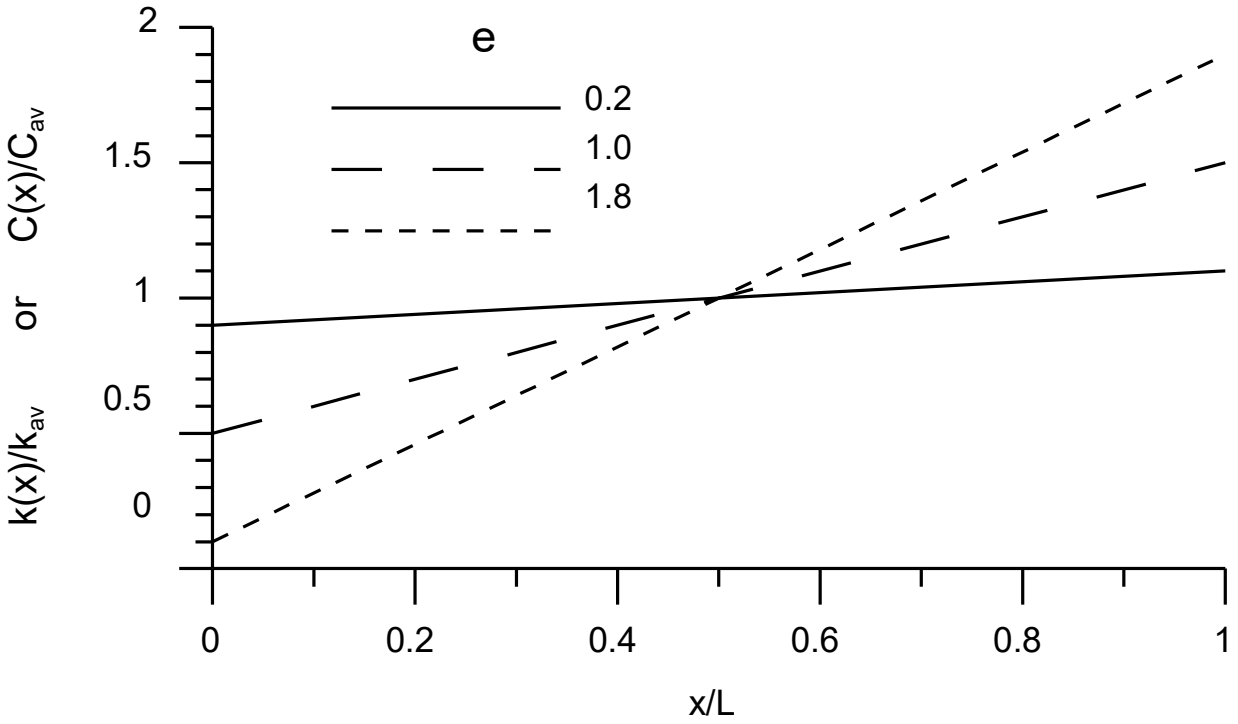
- Basic concepts
  - Sensitivity Coefficients
  - Parameter Estimation Algorithm(s)
  - Optimal Experimental Design
- Example 1 – Quenching of lumped body
  - Thermal Model & Sensitivity Study
  - Simulated Data & Parameter Estimation
- Example 2 – Functionally-graded material
  - Thermal Model
  - Optimal Experimental Design
  - Simulated Data & Parameter Estimation
- Example 3 – Estimating Temperature-Dependent and Anisotropic Material Properties
  - Experimental Approach
  - 1D Results
    - Thermal model
    - Estimated parameters and Analysis
    - Uncertainty
  - 2D Results
    - Thermal model
    - Estimated parameters and Analysis
    - Uncertainty
- Advanced Concepts
  - Sequential over experiments
  - Optimal Design for Temperature varying Properties

Example 2

Example 3
Functionally-graded (FG) material

- Material (or structure) with properties that vary though the thickness
- Graded property values are of interest to improve thermal/mechanical performance
- May include composites, built-up structures, metal foams, or any structure with variations designed into the material
- Application: high-performance thermal insulation for NASA

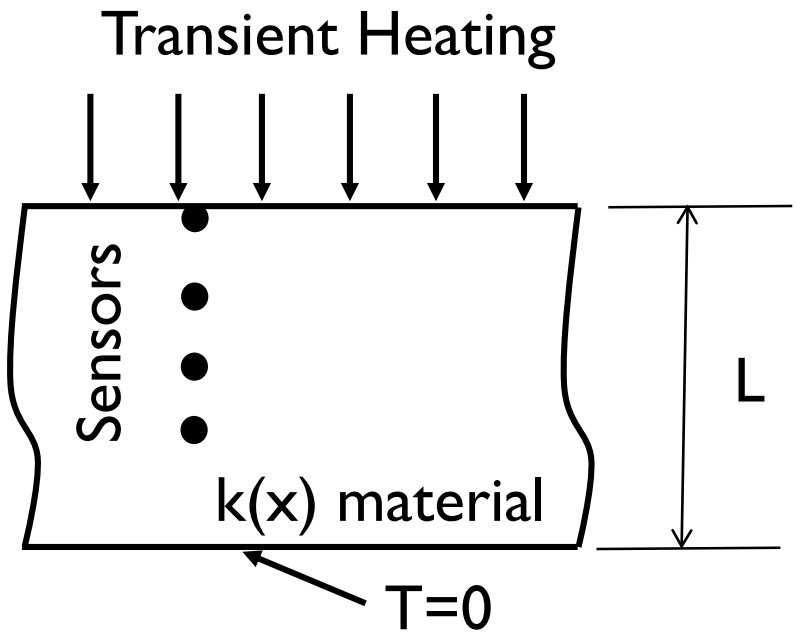
FG Material with conductivity k(x)



- $k(x) = k_{av}\,[1 + e(x/L - 0.5)]$ (W/m/K)
- $C(x) = C_{av}\,[1 + e(x/L - 0.5)]$ (J/m^3/K)
- Parameters sought: k_{av} , C_{av} , e

Experiment for studying FG material

- On-off heating on one side
- Fixed temperature on other side
- Several temperature sensors
- Collect data during heating and continue while unheated
- Analyze data for desired properties with parameter estimation



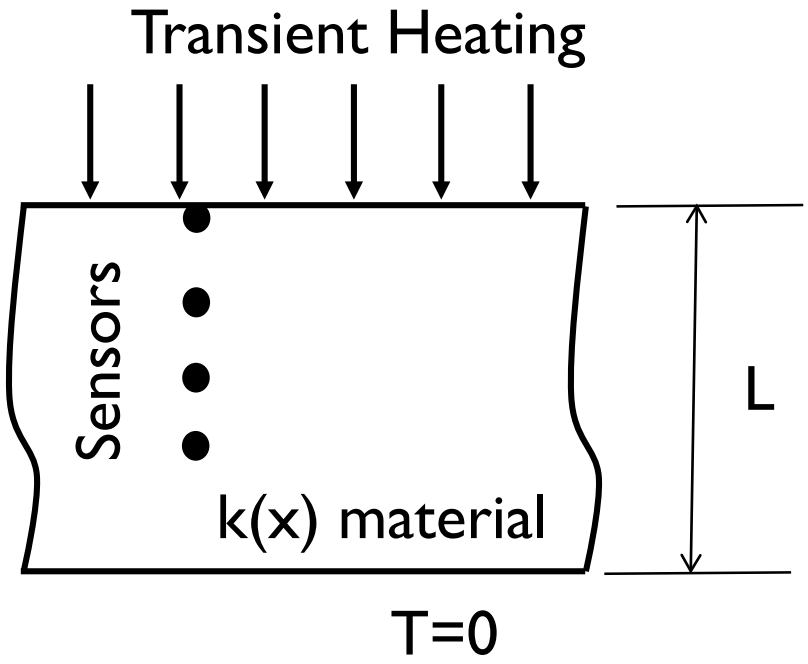
Computational Model (solution method: finite difference)

$$\frac{\partial}{\partial x^+}\left(k^= \frac{\partial T}{\partial x^+}\right) = C^+ \frac{\partial T^+}{\partial \theta} \qquad 0 < x^+ < 1$$

$$k^+ \left.\frac{\partial T^+}{\partial x^+}\right|_{x=0} = \begin{cases} 1 & \theta < \theta_h \\ 0 & \theta > \theta_h \end{cases}$$

$$T(x^+ = 1, \theta) = 0$$

$$T(x^+, \theta = 0) = 0$$



with dimensionless parameters

$$k^+ = \frac{k(x)}{k_{av}}; C^+ = \frac{C(x)}{C_{av}}$$

$$x^+ = \frac{x}{L}; \theta = \frac{k_{av}}{C_{av}} \frac{t}{L^2}; T^+ = \frac{T - T_0}{q_0 L / k_{av}}$$

Sensitivity coefficients

- Minimization of error requires scaled sensitivity coefficients (derivatives wrt parameters b_k)

$$X_{jk}(i) = b_k \frac{\partial T_j^+}{\partial b_k}$$

- Finite difference approximation is used

$$X_{jk}(i) \approx b_k \frac{T_{ij}^+((1+\varepsilon)b_k) - T_{ij}^+(b_k)}{\varepsilon b_k}$$

- Assembled into sensitivity matrix **X**

Sensitivities and Optimality

- Sensitivities should be as large as possible.
- Sensitivities must be linearly independent to estimate two or more parameters.

Given sensitivity matrix **X**, the optimal experiment is found at the maximum value of the determinant of matrix $\mathbf{X^T X}$:

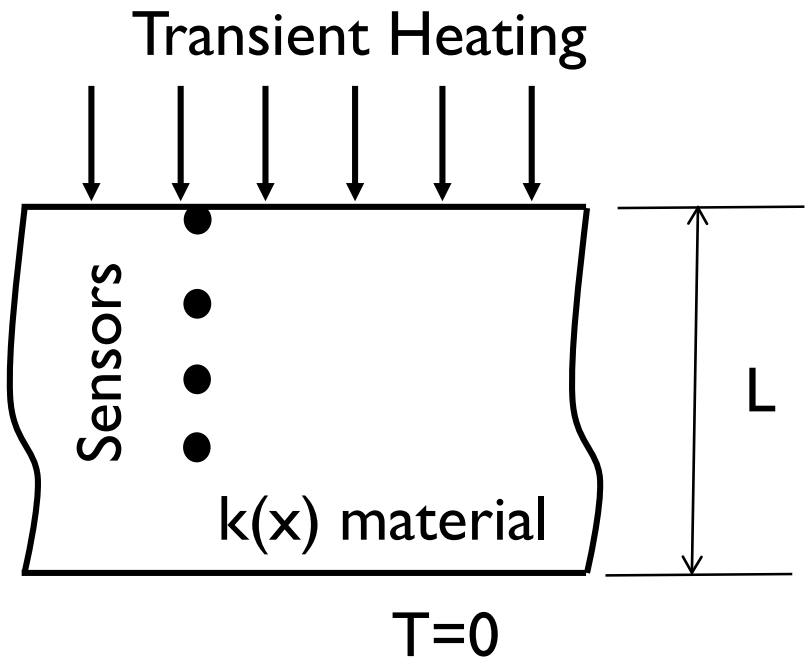
$$D = \frac{1}{sn(T_{\max}^{+})^2} \det(X^T X)$$

s – number of sensors

n – number of time steps

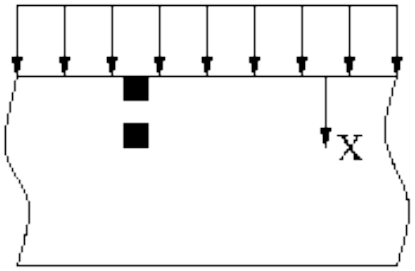
Seek best experiment by varying:

- Number and location of sensors
- Duration of heating period
- Duration of entire data record
- Location of heating (x=0 or x=L)
- Apply to several different spatial variations (slope, e)

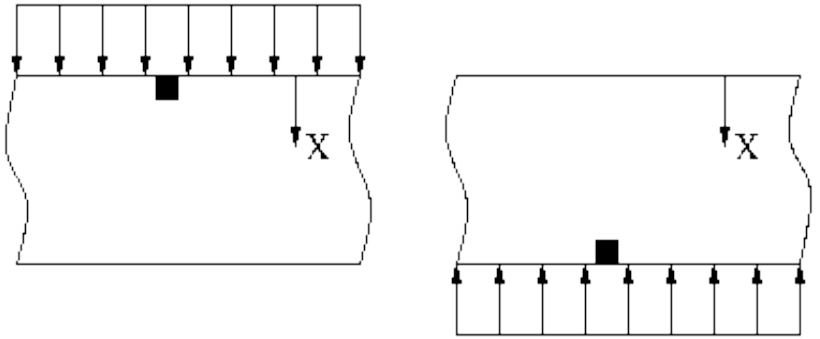


Compare 2 Experimental Designs

Experiment 1:
Heat at x=0
with two sensors:
•Sensor at x=0.
•Sensor at x=L/4.



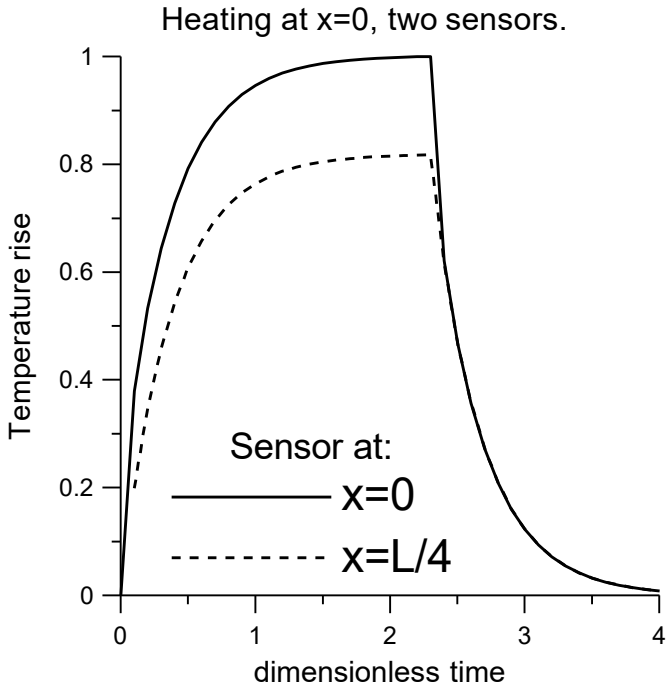
Experiment 2:
Two heating events with one sensor each:
•Heat/sensor at x=0.
•Heat/sensor at x=L.



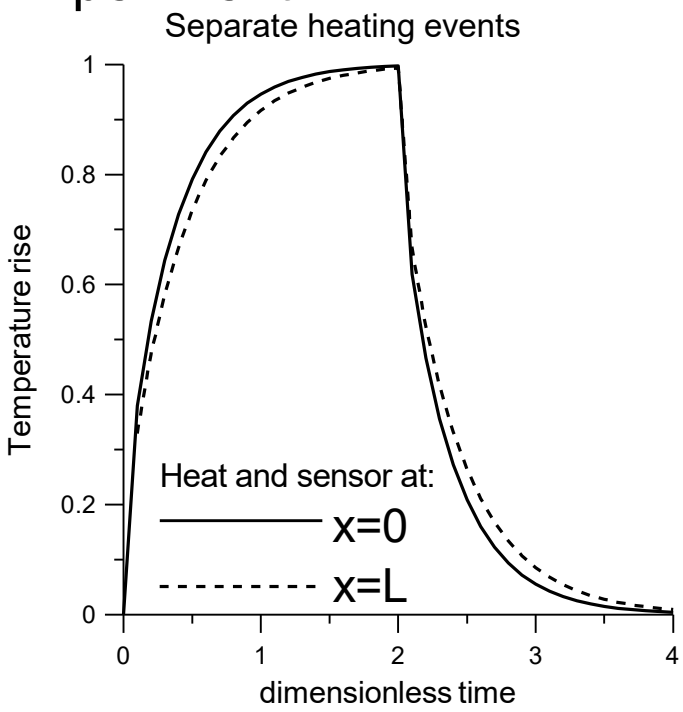
Seek optimum for each experimental design by varying heat duration and data duration, for several values of slope e

Calculated temperatures (e = 0.2)

Experiment 1.

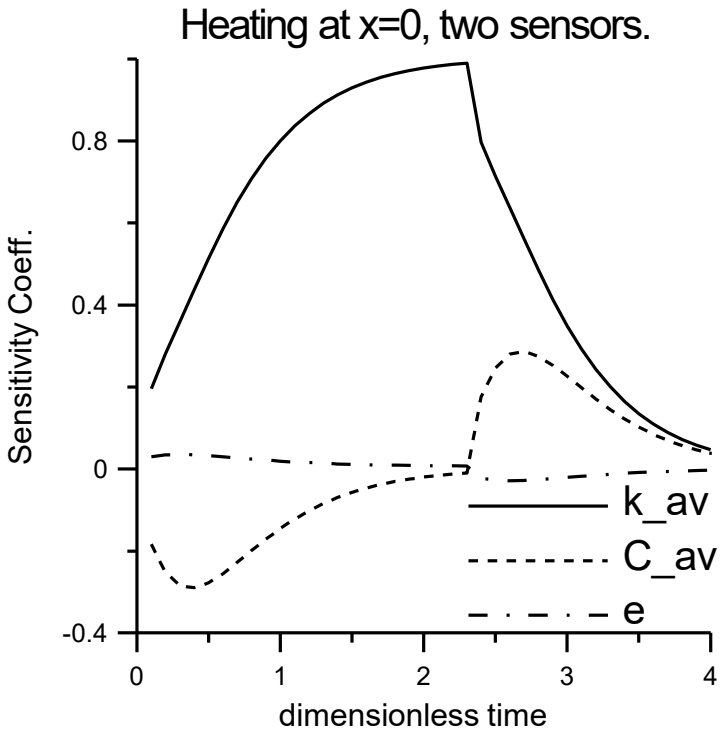


Experiment 2.

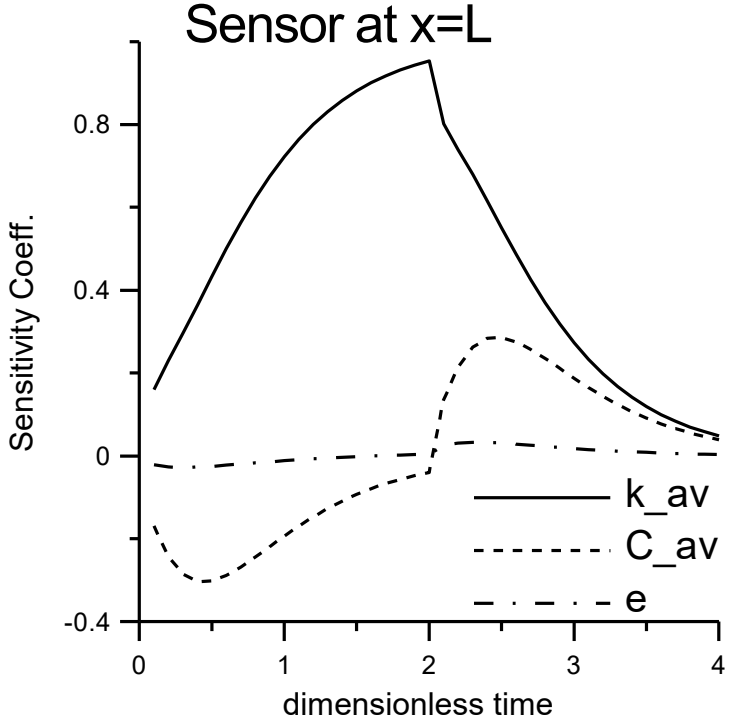


Sensitivity Coefficients (e = 0.2)

Experiment 1.

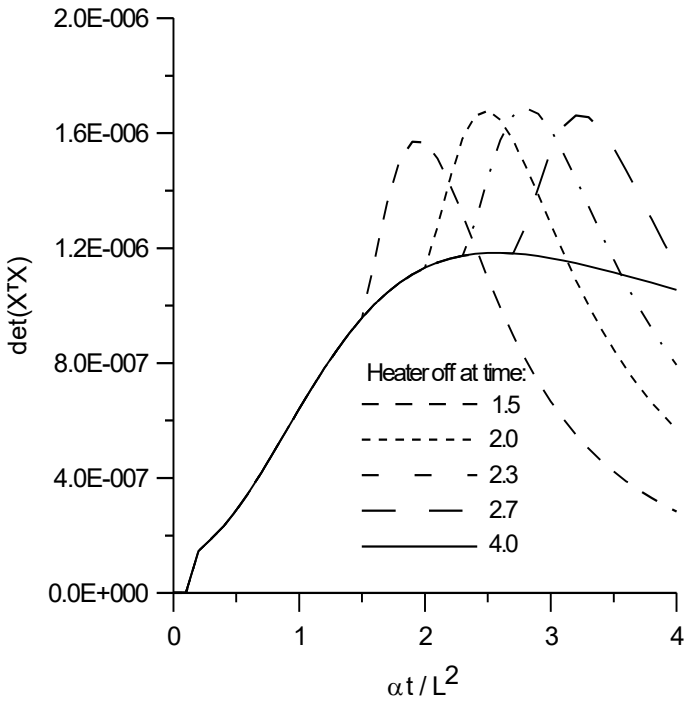


Experiment 2.

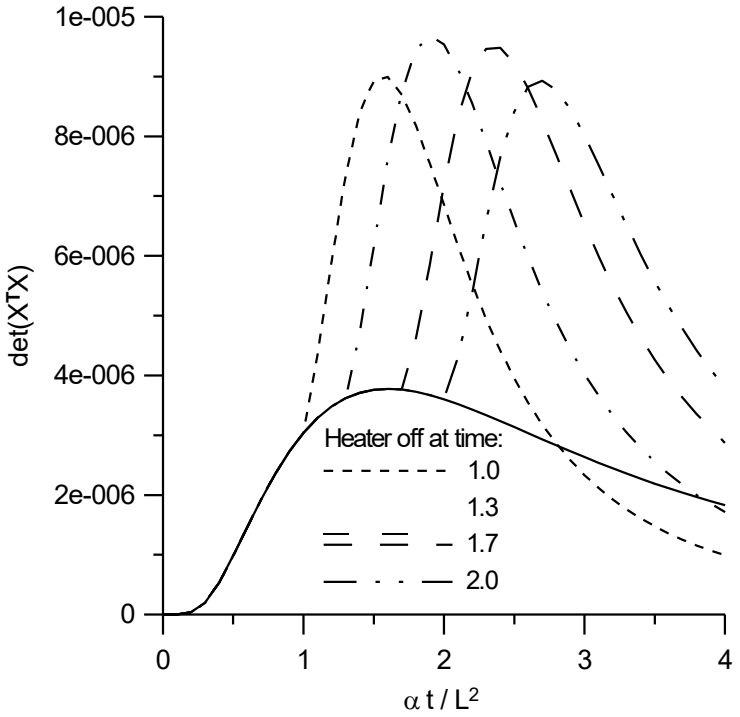


Optimality Criterion (for e = 0.2), at several heating durations.

Experiment 1.
x=0, x = L/4



Experiment 2. Sensors
Two heating events



Optimal Experiments

Experiment Design	e	Heat time	Data time	Max. **D** value
1. Heat x=0, sensors at x=0, L/4.	0.2 1.0 1.8	2.3 1.5 1.5	2.8 1.8 1.7	1.7 E-06 8.7 E-05 1.2 E-03
2. Two heat events, one sensor each.	0.2 1.0 1.8	1.3 1.7 1.3	1.9 2.2 1.5	9.5 E-06 24. E-05 2.2 E-03
3. k = const.	--	2.25	3.0	2.0 E-01

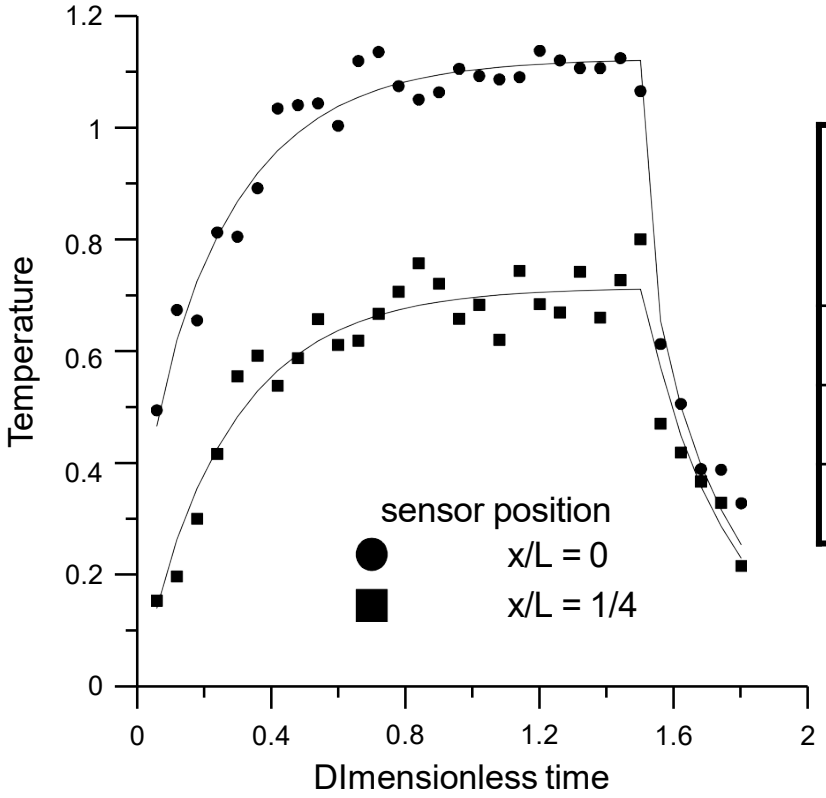
Simulated data analysis

- Compute T_{exact} vs time from simulation of optimal experiment
- Add noise: $T_{data} = T_{exact} + \varepsilon_i$

  ε_i= Zero mean, gaussian, additive error
- Analyze T_{data} to estimate parameters

  k_{av}, C_{av}, e.

Simulate Experiment 1, two sensors, error 5% variance



	Exact values	Curve fit
k_{av}	1.0	1.0148
c_{av}	1.0	1.0080
e	1.0	1.0388

Analysis of optimum experiments (one heat event and two sensors)

slope e	Error variance	% error in k_{av}	% error in C_{av}	% error in e
0.2	1%	0.22	0.92	13.9
1.0	1%	0.41	0.79	0.27
1.8	1%	0.39	0.14	0.14
0.2	5%	2.68	7.13	*
1.0	5%	1.48	0.80	3.88
1.8	5%	0.42	3.00	0.33

* No convergence

Summary, Example 3 Functionally Graded Material

- Best experiment combines two heat events, heat/sensor at x=0 and at x=L. Because no interior sensors are needed, this approach is non-invasive.
- Optimality criterion in D ~ det($\mathbf{X}^T\mathbf{X}$) gives best heating duration and data record length, and gives aid in choosing between two competing experiments.
- Optimal heat duration and data record duration depend somewhat on spatial-variation slope, *e*.
- It is possible to fit three parameters (k_{av}, C_{av}, e) with data from two sensors, for data "not too noisy".
- More accurate parameter estimates are possible for materials with larger x-variation in k (larger *e*); that is, it is easier to "see" larger-*e* values.

Acknowledgements

Functionally graded material example
- National Aeronautics and Space Administration
- Paul Crittenden, University of Florida

Additional Topics

Sequential Estimation over Experiments

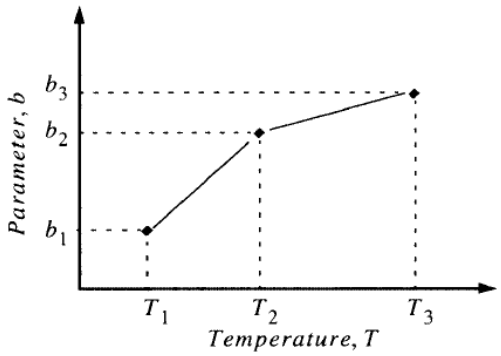
- Typically experiments are analyzed individually

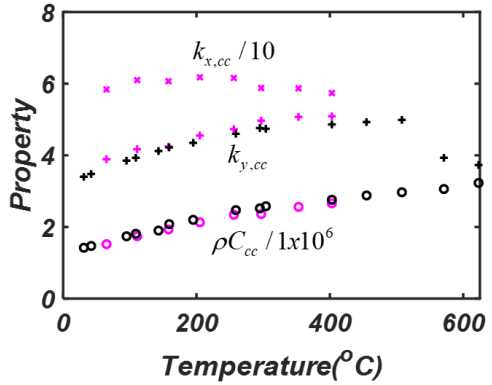
$$S = (Y - \hat{T})^T W (Y - \hat{T})$$

- Expand the analysis to estimate properties that are functions of temperature using a sequential analysis

$$S_n = (Y_n - \hat{T}_n)^T W_n (Y_n - \hat{T}_n) + S_{p_n}$$

- Function cannot be estimated from a single test, but can be estimated through sequential estimation





Estimating Parameters Sequentially

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- Typical sum of squares function for exp n

$$S_n = (\boldsymbol{Y}_n - \hat{\boldsymbol{T}}_n)^T \boldsymbol{W}_n (\boldsymbol{Y}_n - \hat{\boldsymbol{T}}_n) + S_{p_n}$$

- Prior information

$$S_{p_n} = (\boldsymbol{u}_{n-1} - \boldsymbol{b}_n)^T \boldsymbol{U}_{n-1} (\boldsymbol{u}_{n-1} - \boldsymbol{b}_n)$$

$$= \sum_{k=1}^{p} \sum_{l=1}^{p} U_{l,k,n-1} (u_{l,n-1} - b_{l,n})(u_{k,n-1} - b_{k,n})$$

- Estimation algorithm

$$n = 1$$

$$\boldsymbol{U}_1^{(k)} \left[\hat{\boldsymbol{b}}_1^{(k+1)} - \hat{\boldsymbol{b}}_1^{(k)} \right] = \boldsymbol{X}_1^{(k)T} \boldsymbol{W}_1 \left[\boldsymbol{Y}_1 - \hat{\boldsymbol{T}}_1^{(k)} \right] - \boldsymbol{H}^T \boldsymbol{H} \hat{\boldsymbol{b}}_1^{(k)}$$

$$\boldsymbol{U}_1^{(k)} \equiv \boldsymbol{X}_1^{(k)T} \boldsymbol{W}_1 \boldsymbol{X}_1^{(k)} + \boldsymbol{H}^T \boldsymbol{H}$$

Regularization term

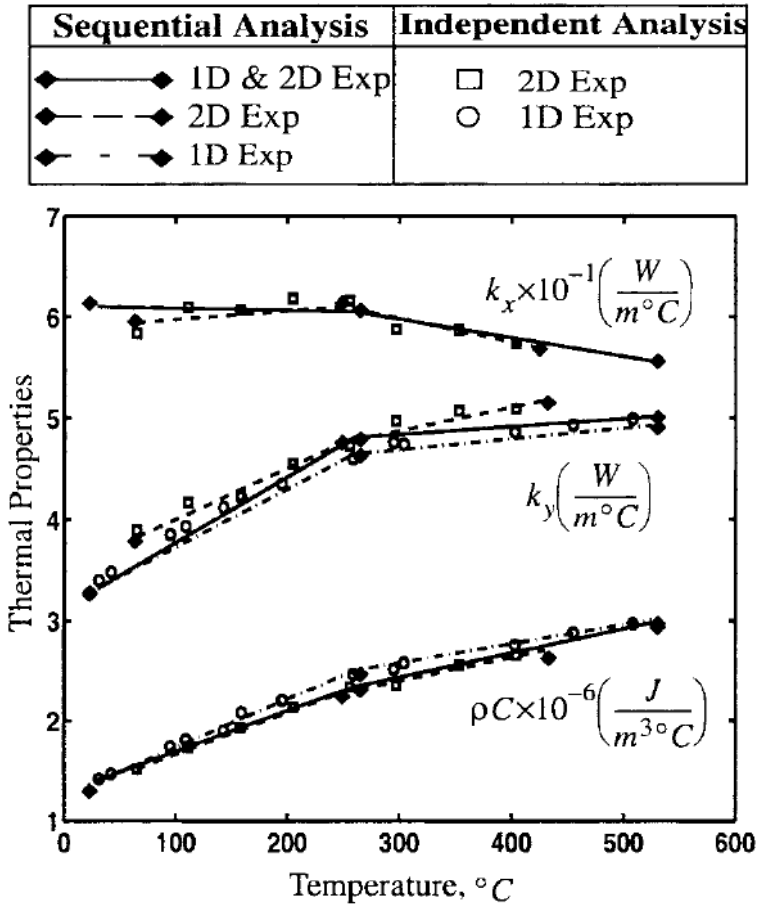
$$n > 1$$

$$\boldsymbol{U}_n^{(k)} \left[\hat{\boldsymbol{b}}_n^{(k+1)} - \hat{\boldsymbol{b}}_n^{(k)} \right] = \boldsymbol{X}_n^{(k)T} \boldsymbol{W}_n \left[\boldsymbol{Y}_n - \hat{\boldsymbol{T}}_n^{(k)} \right] + \boldsymbol{U}_{n-1} \left[\boldsymbol{u}_{n-1} - \hat{\boldsymbol{b}}_n^{(k)} \right]$$

$$\boldsymbol{U}_n^{(k)} \equiv \boldsymbol{X}_n^{(k)T} \boldsymbol{W}_n \boldsymbol{X}_n^{(k)} + \boldsymbol{U}_{n-1}$$

Sequentially estimated temperature dependent properties

- Two linear segments for each thermal property
- Estimated using 1D, 2D, and 1D&2D exps



Temp, °C	ρC $(b_1 - b_3)$, J/m³°C	k_y $(b_4 - b_6)$, W/m°C	k_x $(b_7 - b_9)$, W/m°C
	One-dimensional experiments $(\alpha_1 = \alpha_2 = 0.5E-12), (\alpha_4 = \alpha_5 = 0.25)$		
30	1.41 ± 0.003	3.35 ± 0.013	——
260	2.56 ± 0.006	4.60 ± 0.019	——
525	3.06 ± 0.009	4.85 ± 0.022	——
	Two-dimensional experiments $(\alpha_1 = \alpha_2 = 0.5E-12), (\alpha_4 = \alpha_5 = 1.0), (\alpha_7 = \alpha_8 = 0.05)$		
65	1.52 ± 0.008	3.82 ± 0.078	59.5 ± 0.89
250	2.29 ± 0.008	4.76 ± 0.056	61.2 ± 0.59
430	2.71 ± 0.012	5.17 ± 0.065	56.9 ± 0.68
	One- and two-dimensional experiments $(\alpha_1 = \alpha_2 = 0.5E-12), (\alpha_4 = \alpha_5 = 0.25), (\alpha_7 = \alpha_8 = 0.05)$		
30	1.41 ± 0.004	3.32 ± 0.021	61.0 ± 1.0
260	2.34 ± 0.007	4.81 ± 0.034	60.5 ± 0.57
525	2.98 ± 0.016	5.01 ± 0.052	55.7 ± 1.22

Optimal design of an experiment to estimate temperature varying properties

Study Experimental Design to estimate linearly varying thermal properties

$$\frac{\partial}{\partial x^+}\left\{\left[1+\frac{k_2-k_1}{k_1}\left(\frac{T-T_1}{T_2-T_1}\right)\right]\frac{\partial T}{\partial x^+}\right\}=\left[1+\frac{C_2-C_1}{C_1}\left(\frac{T-T_1}{T_2-T_1}\right)\right]\frac{\partial T}{\partial t^+}$$

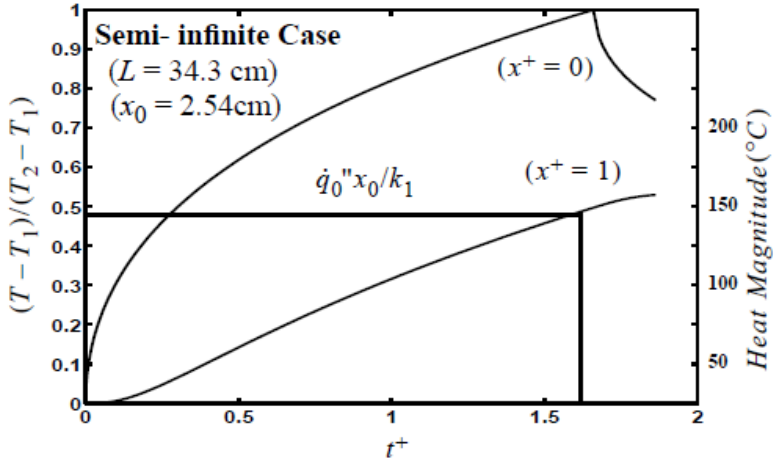
$$\frac{k_2-k_1}{k_1},\ \frac{C_2-C_1}{C_1},\ \frac{T-T_1}{T_2-T_1}.$$

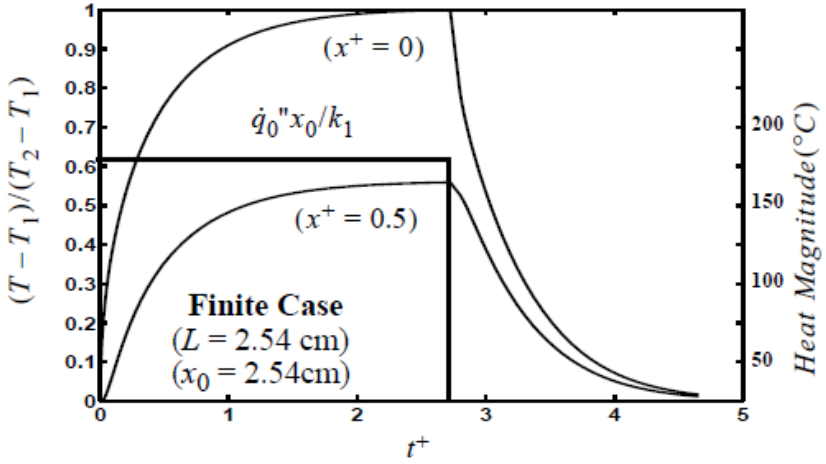
Parameter Groups (0.66, 1.22, 1.0)

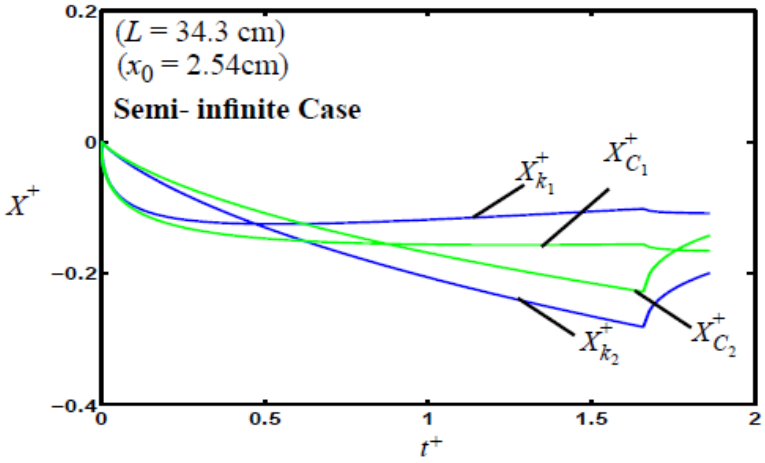
$$\Delta^+ \equiv \left|\frac{(\boldsymbol{X}^+)^T\boldsymbol{X}^+}{(T^+_{max})^2 N_t N_s}\right|.$$

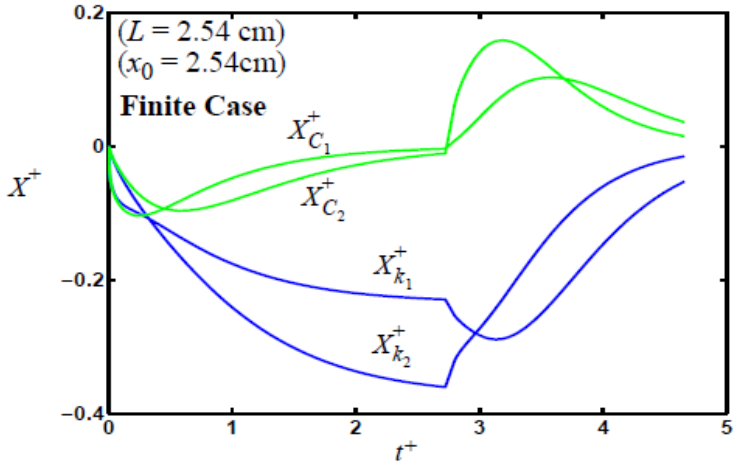
$$(\boldsymbol{X}^+)^T = \left[\frac{\beta_1}{(\dot{q}_0'' x_0/k_1)}\frac{\partial \boldsymbol{T}}{\partial \beta_1}\ \ \frac{\beta_2}{(\dot{q}_0'' x_0/k_1)}\frac{\partial \boldsymbol{T}}{\partial \beta_2}\ \ \cdots\ \ \frac{\beta_p}{(\dot{q}_0'' x_0/k_1)}\frac{\partial \boldsymbol{T}}{\partial \beta_P}\right]$$

Proposed Experimental Approaches and Sensitivity Coefficients

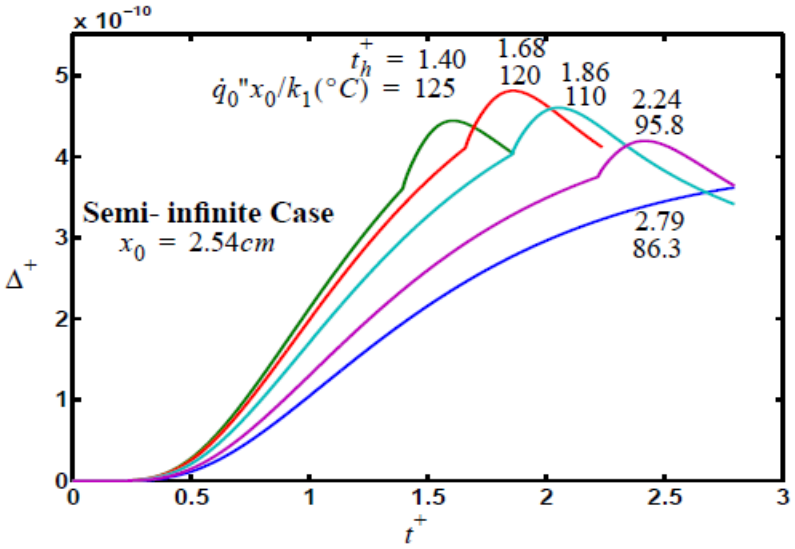


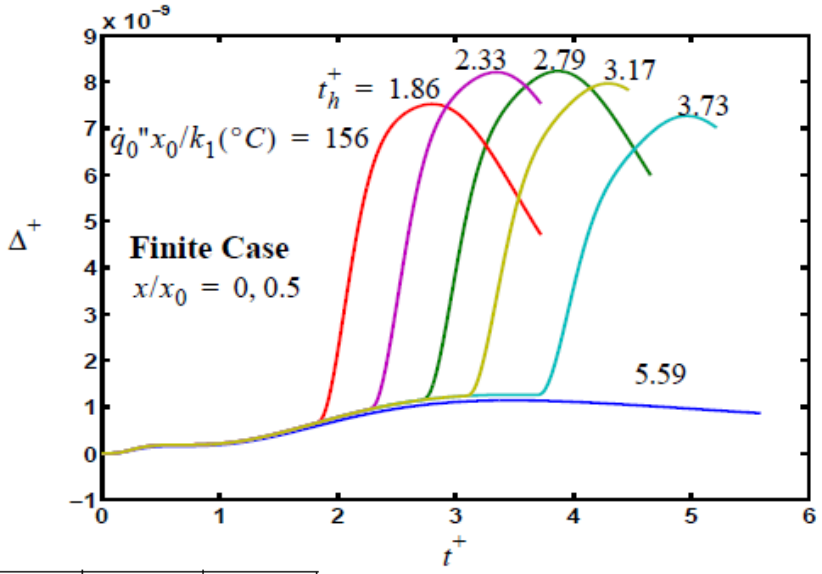






Optimal Experimental Design





x_0 (cm)	Sensor Locations x/x_0	Heating t_h^+	Heating $\dot{q}_0'' x_0/k_1$ (°C)	$\frac{T_{max}-T_1}{T_2-T_1}$	Max Δ^+	Optimal time $t_f^+(\Delta^+)$
Semi-infinite Body						
2.54	0, 1.0	1.68	120	1.0	4.81E-10	1.86
1.27	0, 1.0	1.68	120	0.99	4.45E-10	1.84
3.81	0, 1.0	1.68	115	0.98	4.87 E-10	1.89
Finite Body						
2.54	0, 0.5	2.79	156	0.98	8.23 E-09	3.87
2.54	0, 0.25	2.33	156	0.97	7.91 E-09	3.55
2.54	0, 0.75	2.79	156	0.98	3.95 E-09	3.87
2.54	0, 0.5	2.79	71.9	0.51	1.73 E-09	3.74