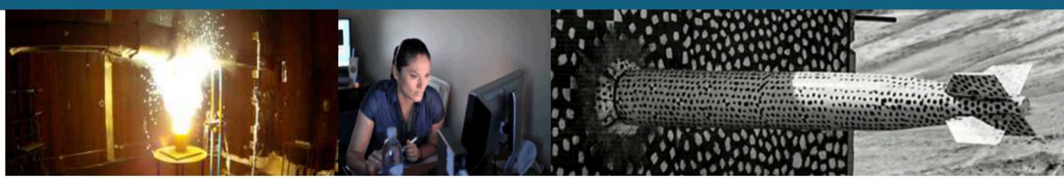
SAND2019-8098C

Tutorial: Computational Methods for Inverse Heat Transfer Problems



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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 – 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

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, conductivity
    - correlation coefficients in a formula:

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

    - Constants related to a property

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

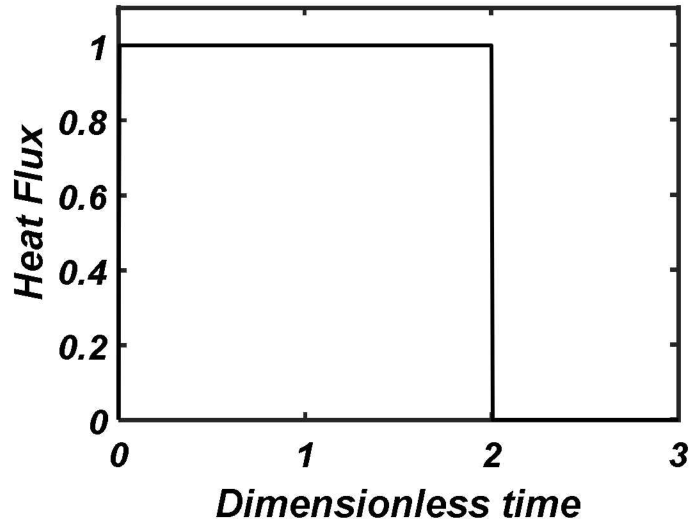
Transient heat conduction experiment:

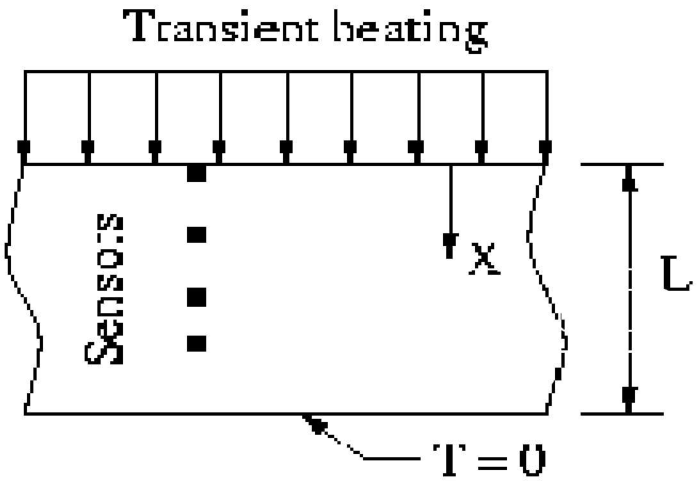
Surface heating:

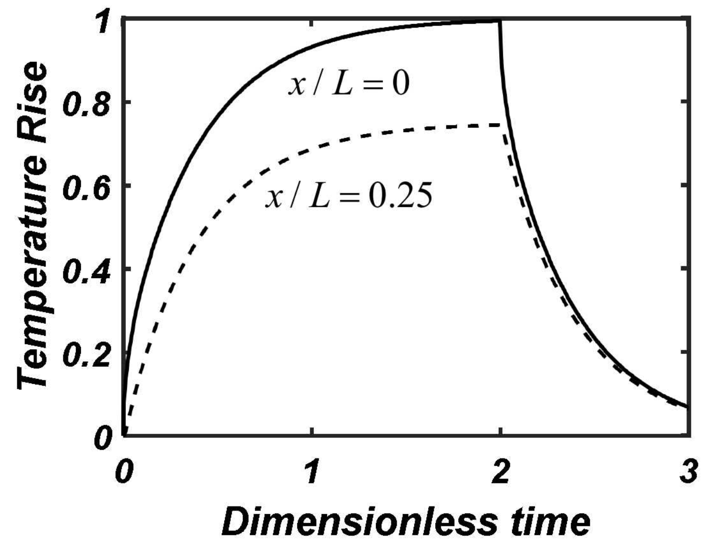
$$q(t) = \begin{cases} q_0 & 0 < t < t_1 \\ 0 & t > t_1 \end{cases}$$

Temperature data

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







Seek thermal properties k, α in model.

Mathematical Model

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

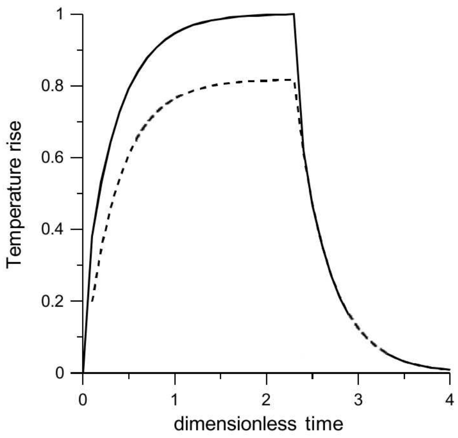
$$k\left.\frac{\partial T}{\partial x}\right|_{x=0} = -q(t)$$

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

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

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 used in this course

- Scaled Sensitivity Coefficients

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

- Scaled sensitivity coefficients will be used as metric for this course
  - Scale factor is the nominal parameter value
- Scaled sensitivity coefficient will have units of the result (Temperature)
  - Will allow for direct comparison of importance of various parameters
  - Compare to measured response

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

350 CHAPTER 7 MINIMIZATION OF SUM OF SQUARES FUNCTIONS

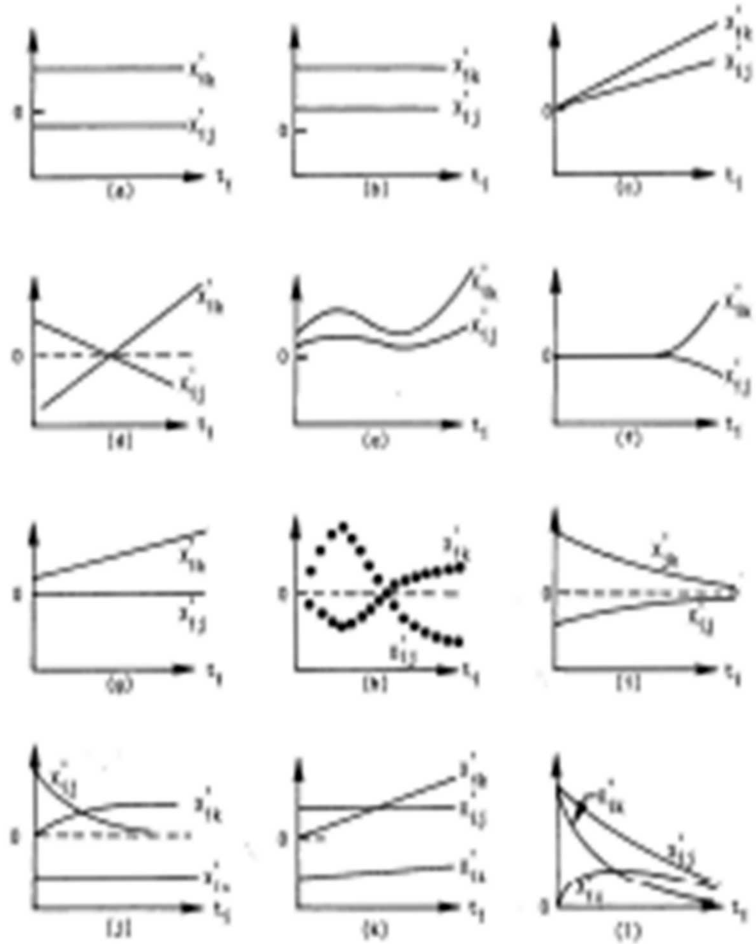


Figure 7.3 Examples of some linearly dependent sensitivity coefficients.

7.5 GAUSS METHOD INVOLVING DIFFERENTIAL EQUATIONS 351

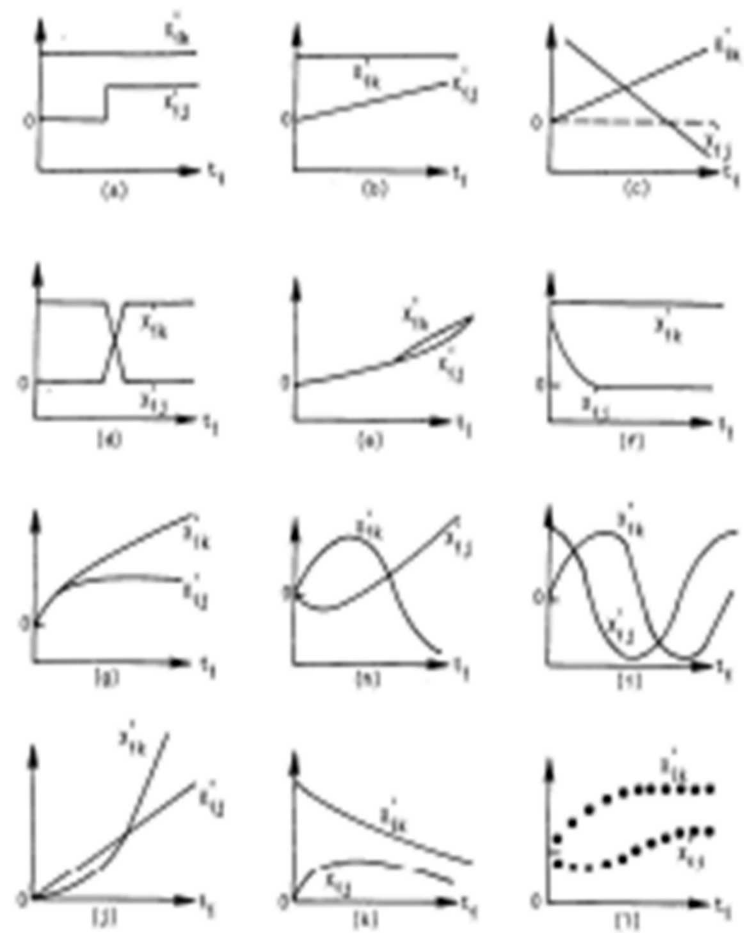


Figure 7.4 Examples of some linearly independent sensitivity coefficients.

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:

$$\det\left|X^T X\right| \neq 0$$

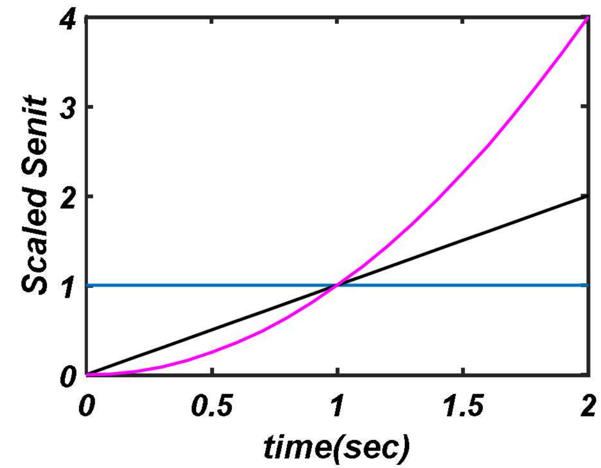
Model linear in parameters

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:

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

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

Model 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:

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

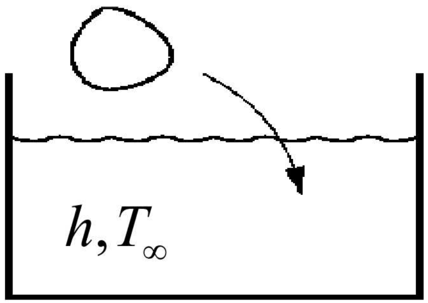
for measurements Y and model η

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

Example 1

Example 1. Quenching problem.

$\rho c V; A_s; T_0$



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

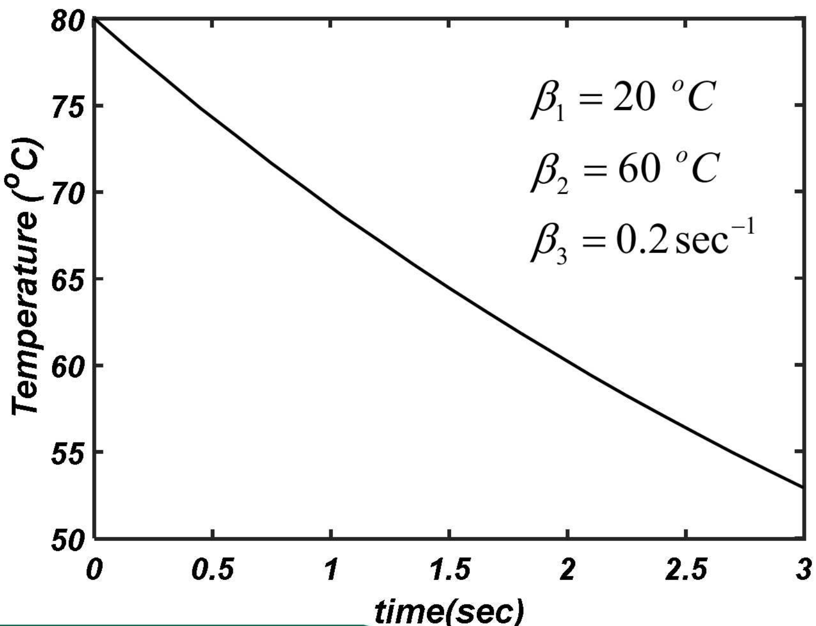
T_0 : Initial Temperature
h : Convection Coefficient
T_∞ : Fluid Temperature

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

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

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

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



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

Example 1. Quenching problem.

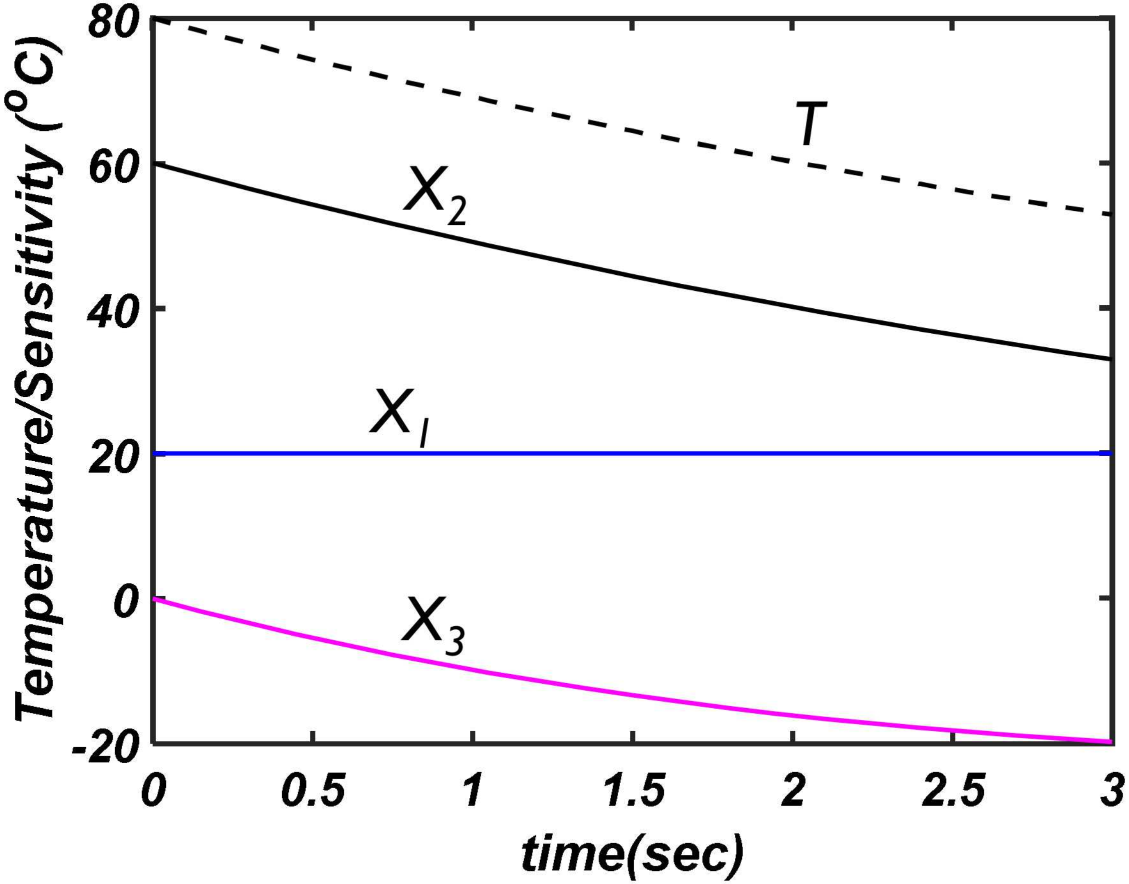
Scaled sensitivity coefficients:

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

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

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

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



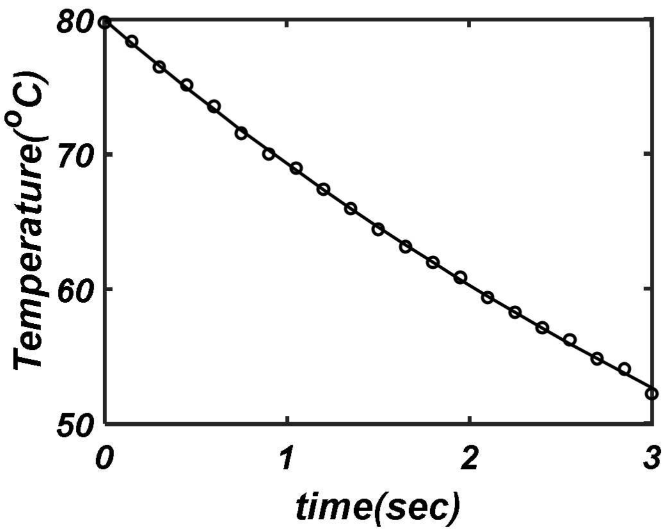
Estimation of parameters from data

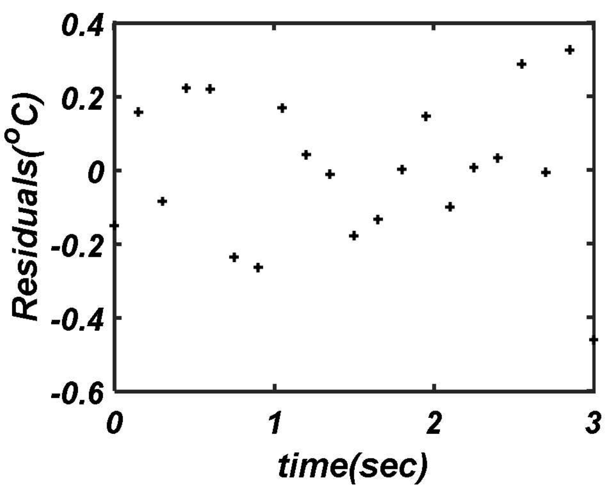
Synthetic data 0<t<3 sec
with $\beta_1 = 20$, $\beta_2 = 60$, $\beta_3 = 0.2$
added error $\sigma = 0.25$ C

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

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

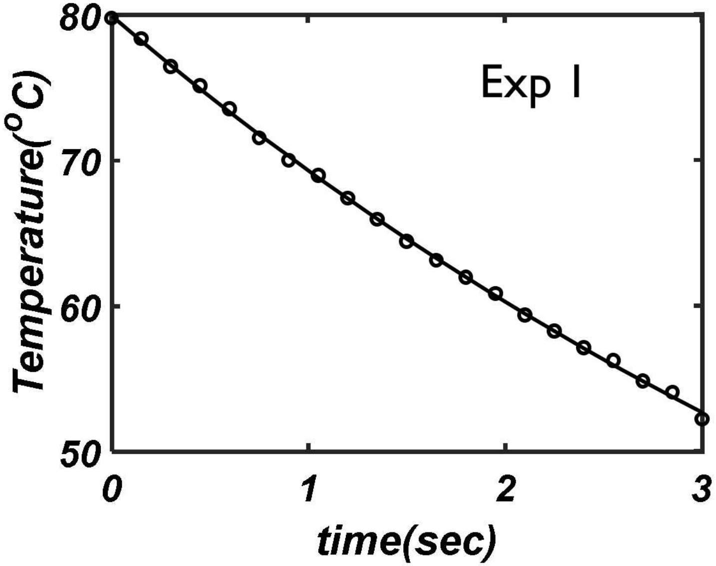
Parameter	Estimates Exp 1	Estimates Exp 2
B_1 (20)	10.8841	26.1172
B_2 (60)	69.0291	54.2988
B_3(0.2)	0.1672	0.2321
$S = \Sigma(Y_i - T_i)^2$	0.7940	0.8353

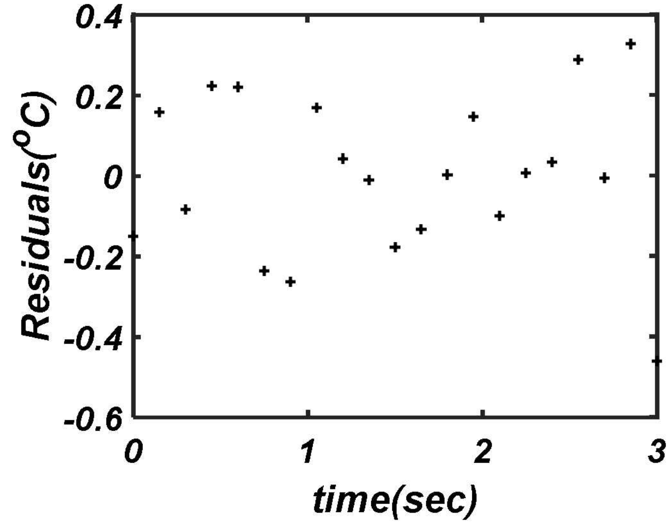


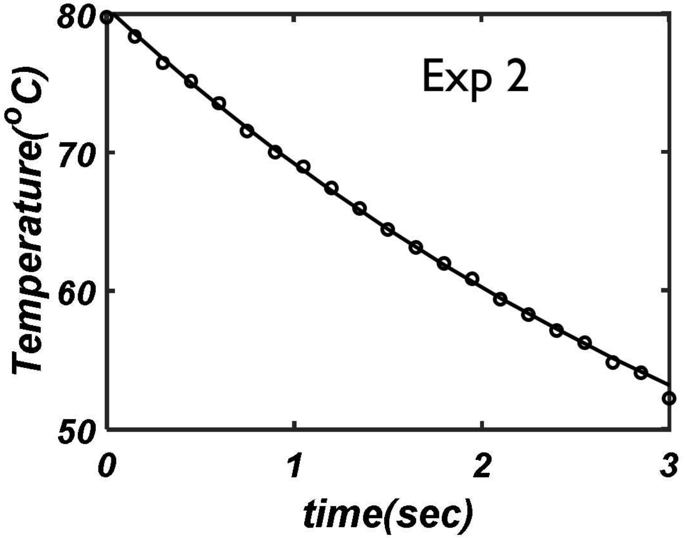


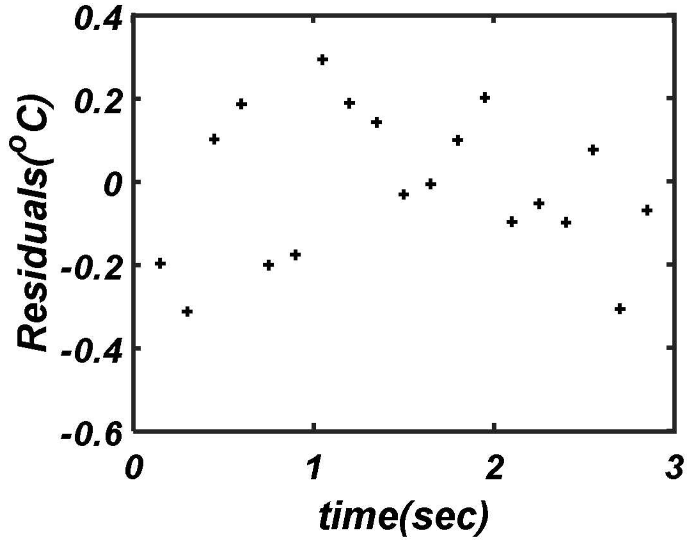
Matlab results using nlinfit

Results for Quenching Example



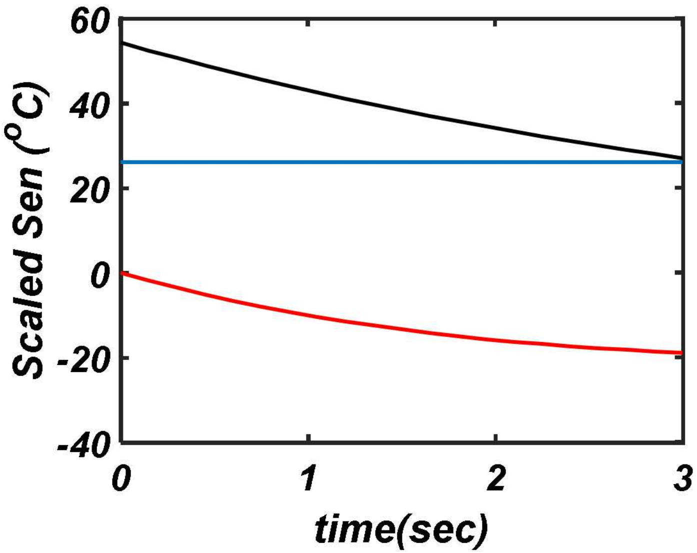




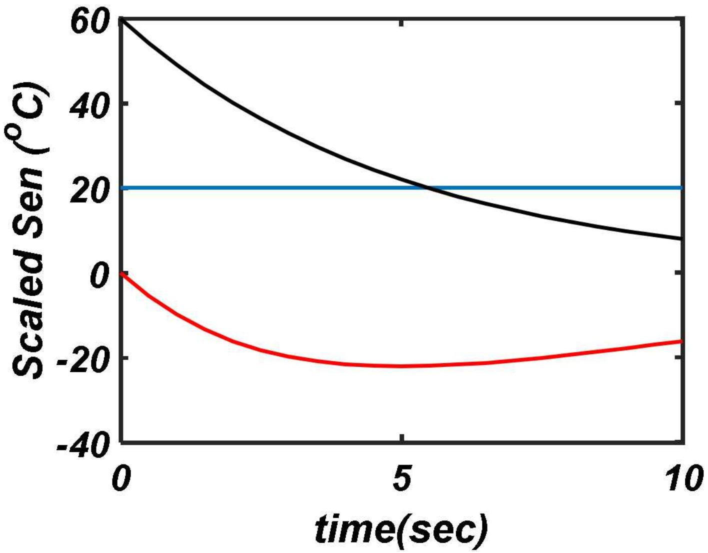


Explain poor fit -- sensitivity coefficients

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

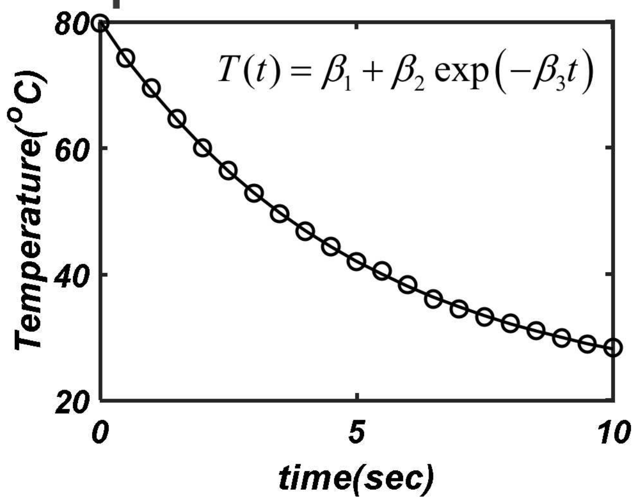


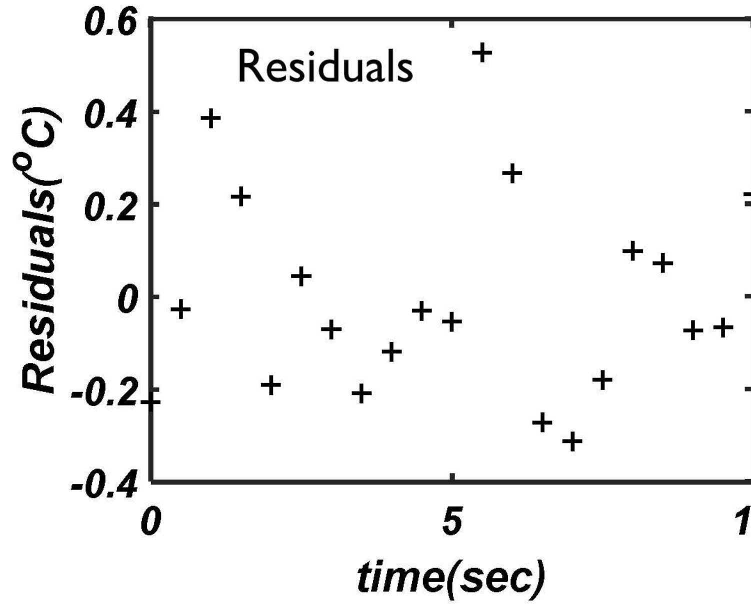
Actual time range 0 < t < 3



Improved time range 0 < t < 10

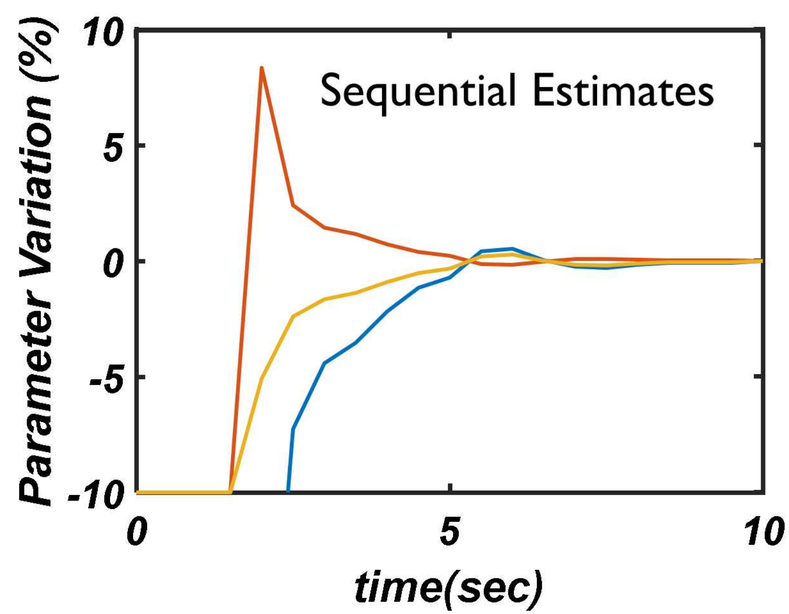
Sequential Estimates





Previous data 0<t<3 . . . too short.
Present data 0<t<10 . . . "right" data.

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



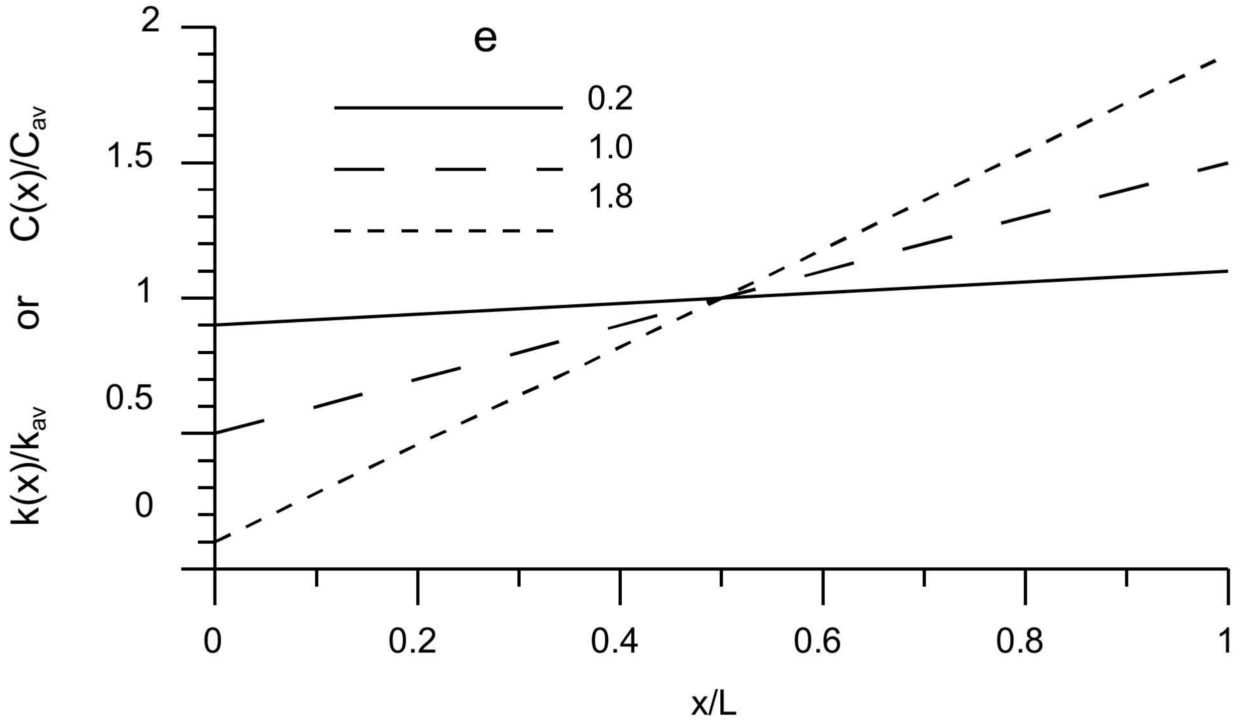
Lessons from quenching example

- 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.
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

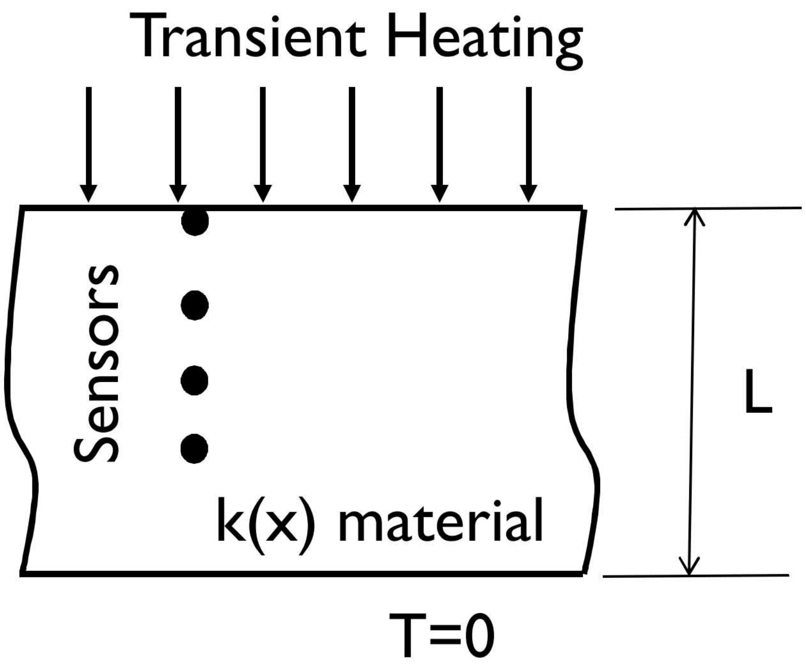
FG Material with conductivity k(x)



- $k(x) = k_{av}\,[1 + e(x/L - 0.5)]$ (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



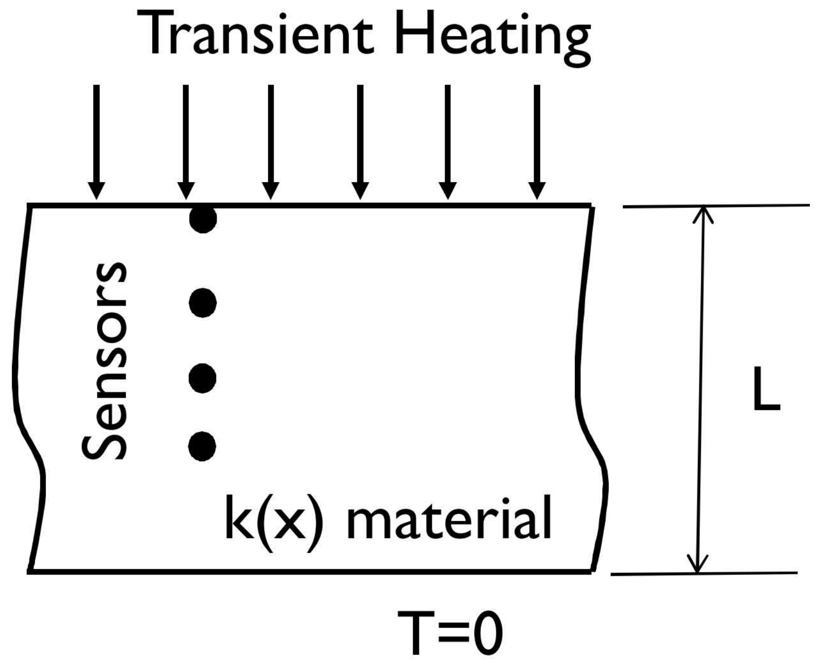
Computational Model (solution method:finite difference)

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

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

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

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



with dimensionless parameters

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

$$x^+=\frac{x}{L};\theta=\frac{k_{av}}{C_{av}}\frac{t}{L^2};T^+=\frac{T-T_0}{q_0L/k_{av}}$$

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

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

- 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 $\mathbf{X}^T\mathbf{X}$:

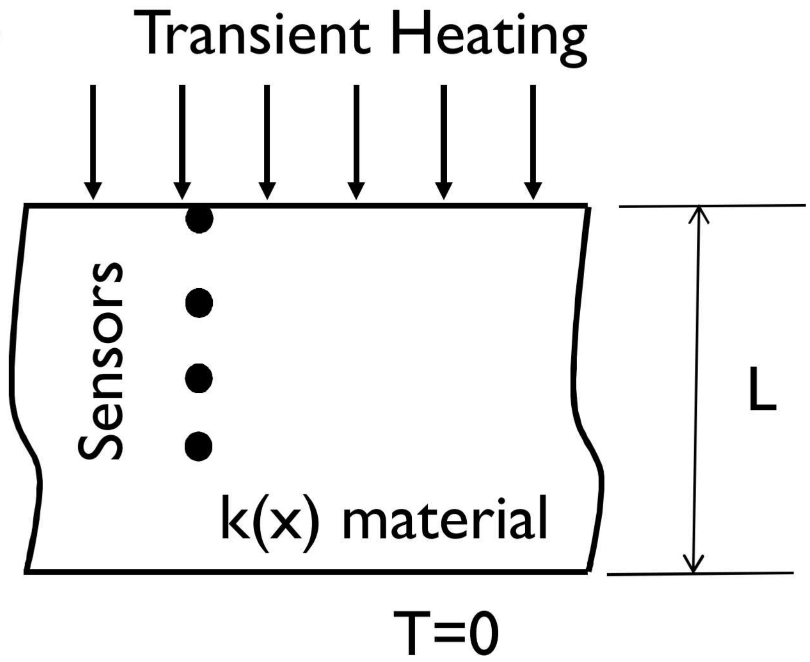
$$D = \frac{1}{sn(T^+_{\max})^2}\det(X^T X)$$

s – number of sensors

n – number of time steps

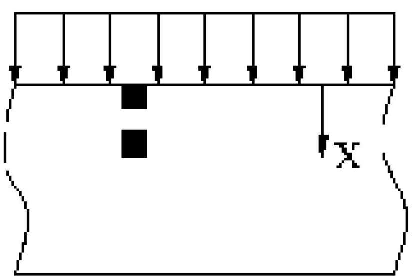
Seek best experiment by varying:

- 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)

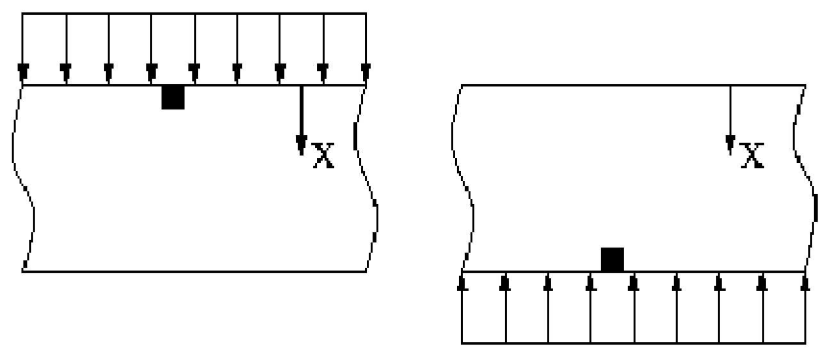


Compare 2 Experimental Designs

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



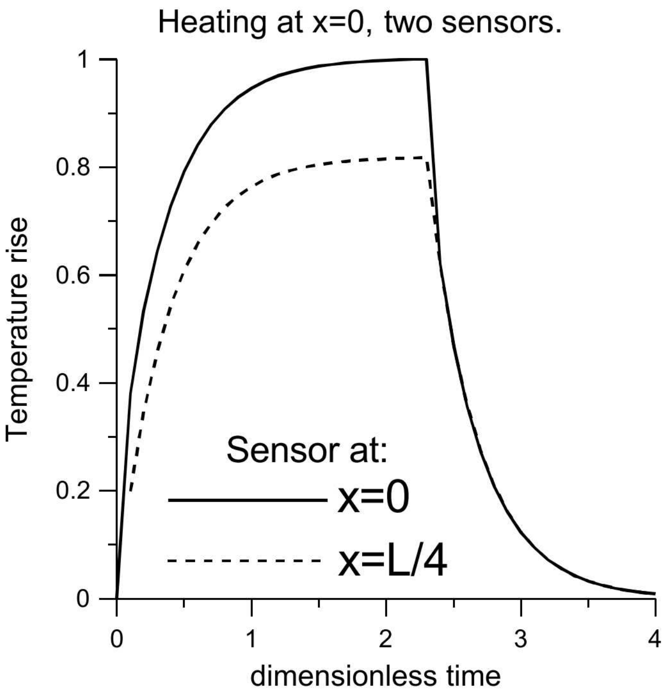
Experiment 2:
Two heating events with
one sensor each:
•Heat/sensor at x=0.
•Heat/sensor at x=L.



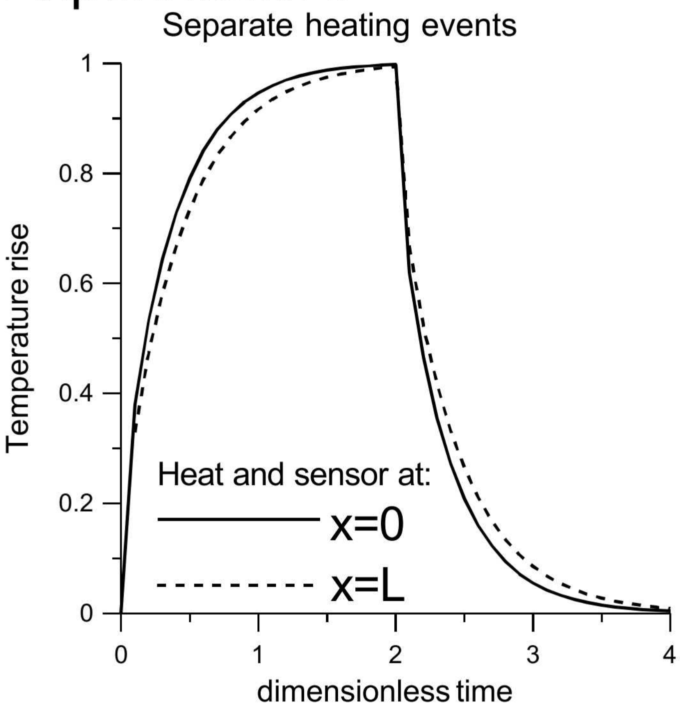
Seek optimum for each experimental design by varying heat duration and data duration, for several values of slope e

Calculated temperatures (e = 0.2)

Experiment 1.

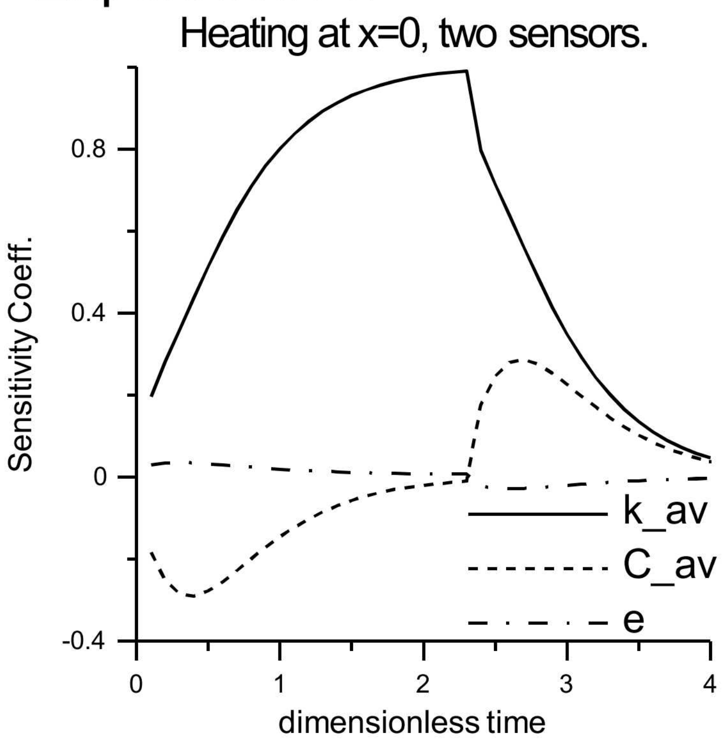


Experiment 2.

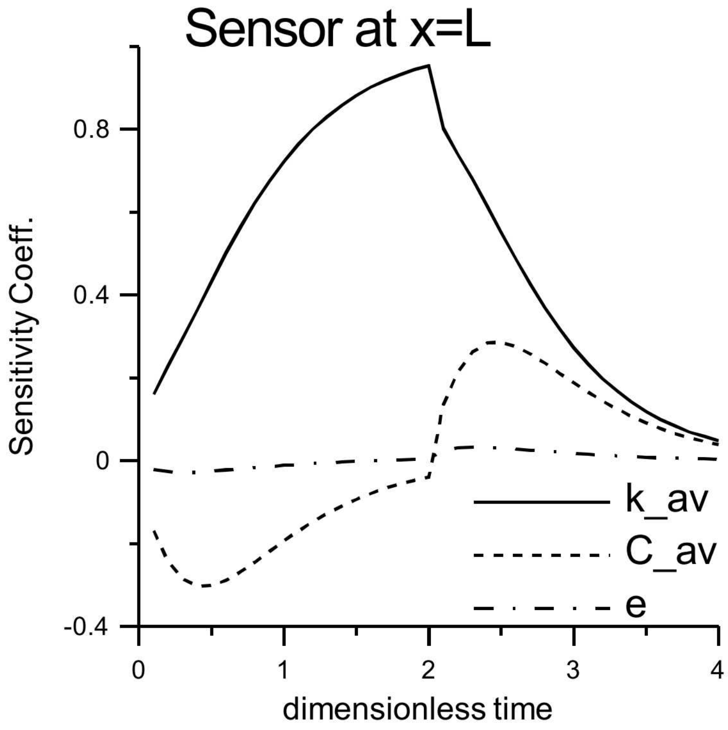


Sensitivity Coefficients (e = 0.2)

Experiment 1.

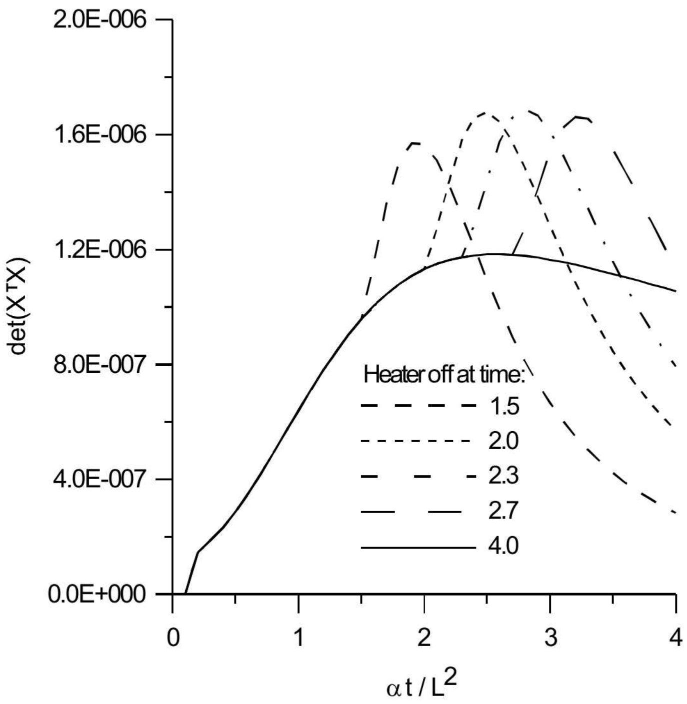


Experiment 2.

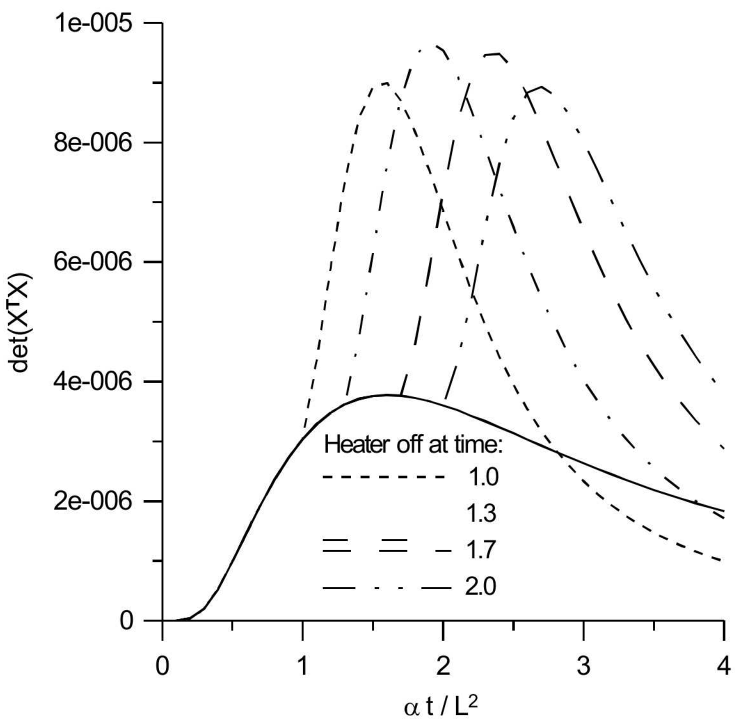


Optimality Criterion (for e = 0.2), at several heating durations.

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

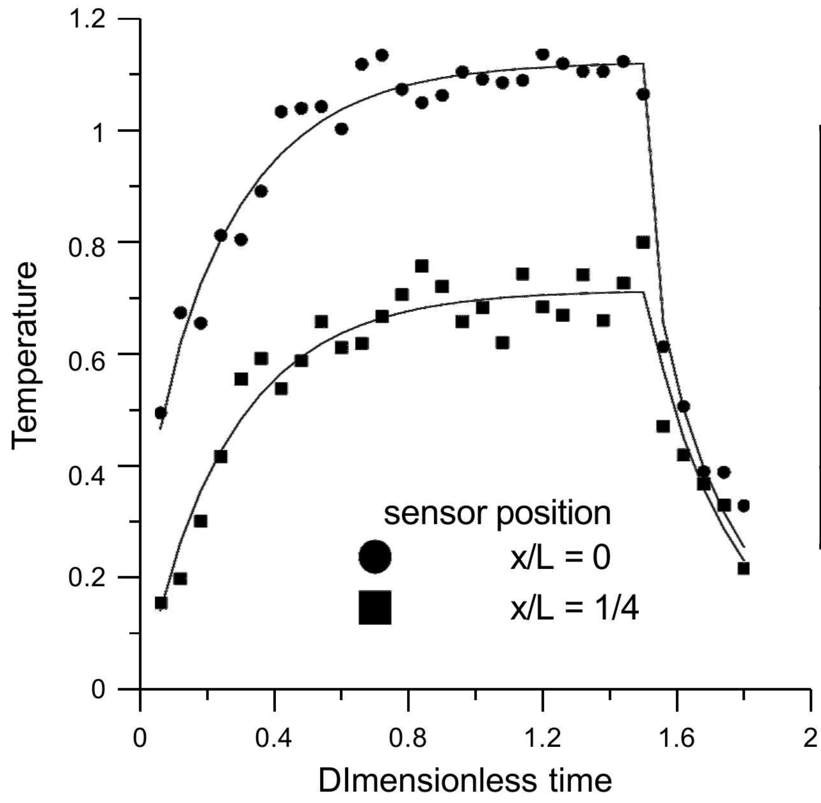
Simulated data analysis

- 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 2 Functionally Graded Material

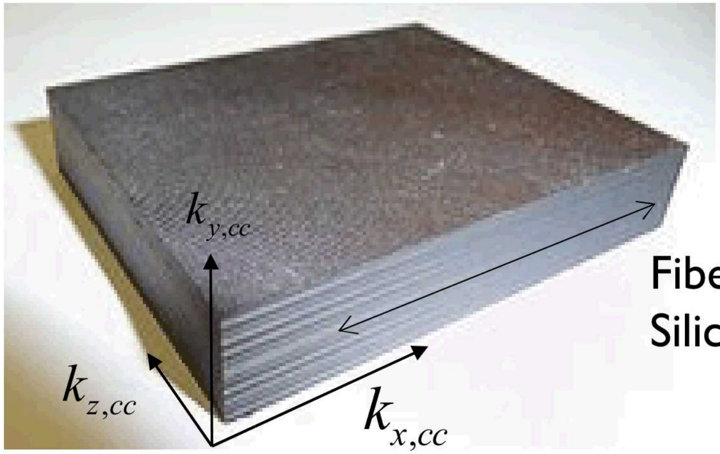
- Best experiment combines two heat events, heat/sensor at x=0 and at x=L. Because no interior sensors are needed, this approach is non-invasive.
- Optimality criterion in D ~ det($\mathbf{X}^T\mathbf{X}$) gives best heating duration and data record length, and gives aid in choosing between two competing 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.

Example 3

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 ^oC



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

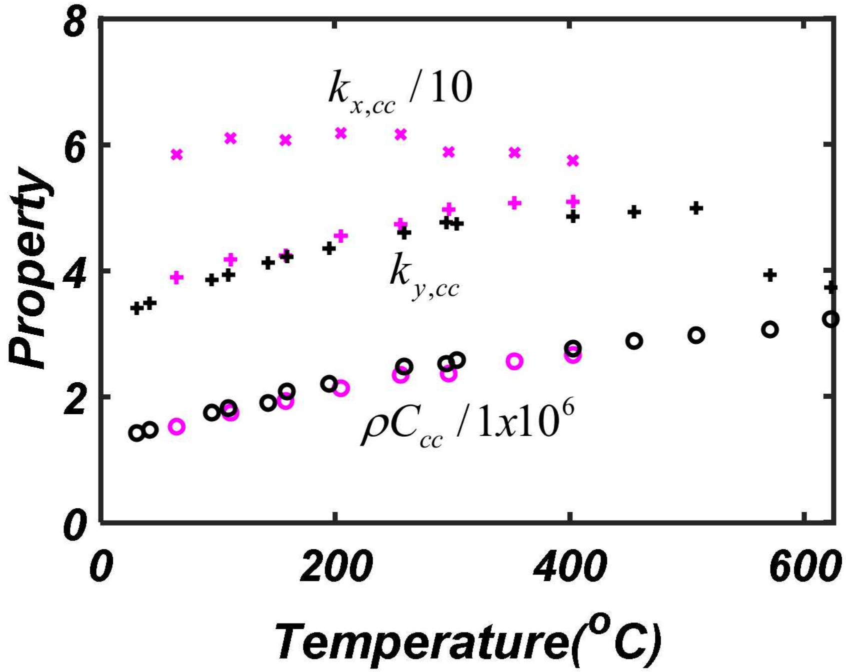
Temperature Dependent Properties

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

$25^o C$ to $600^o C$

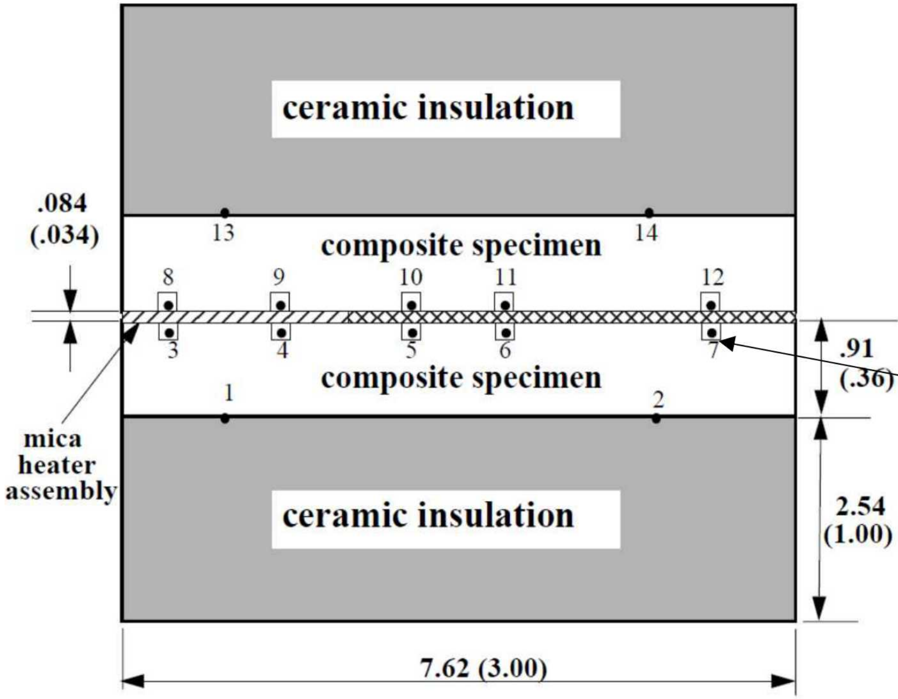
2D Experiments $(k_{y,cc}, k_{y,cc}, \rho C_{cc})$

$25^o C$ to $400^o C$



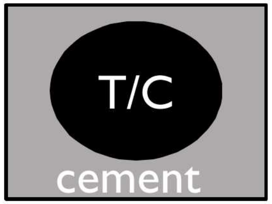
- Experimental Discussion
- 1D Approach and Results
- 2D Approach and Results

Experimental apparatus designed to estimate properties of anisotropic carbon-carbon



Sensor number	Location x (cm)	Location y (cm)
3, 8	0.89	0
4, 9	1.91	0
5, 10	3.18	0
6, 11	4.45	0
7, 12	6.73	0
1, 13	1.27	0.91(L_y)
2, 14	6.35	0.91(L_y)

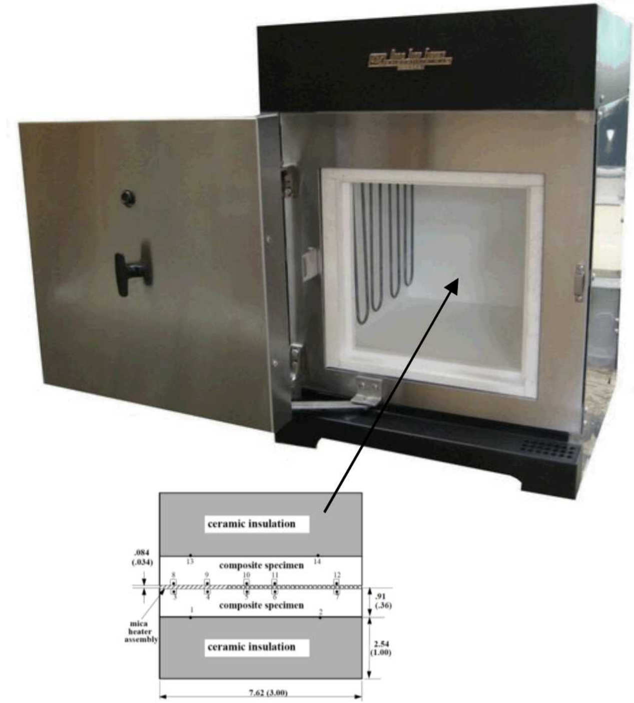
Thermocouples attached to CC Specimen (dia 0.01 in)



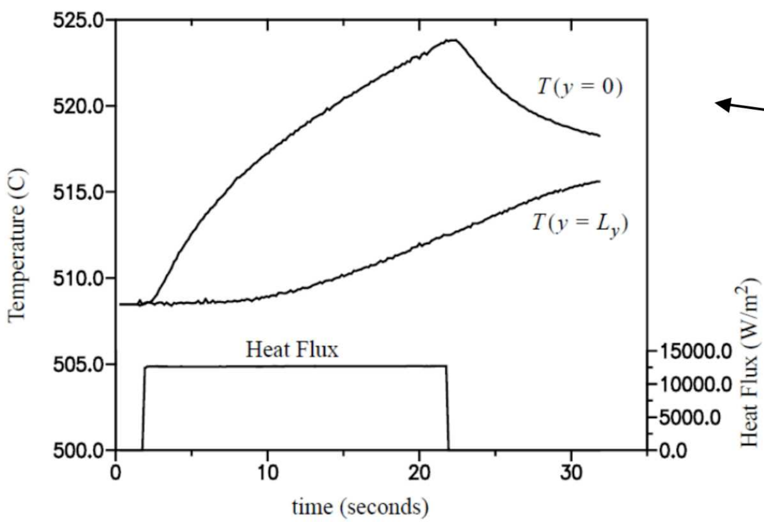
- Design allowed for 1D and 2D heat conduction within the composite sample
  - 3 independently controlled electric heaters (1/3 used for 2D)
- Thermocouples located along heater/composite interface and composite/insulation interface
  - Symmetric implementation
- Designed to estimate properties of a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

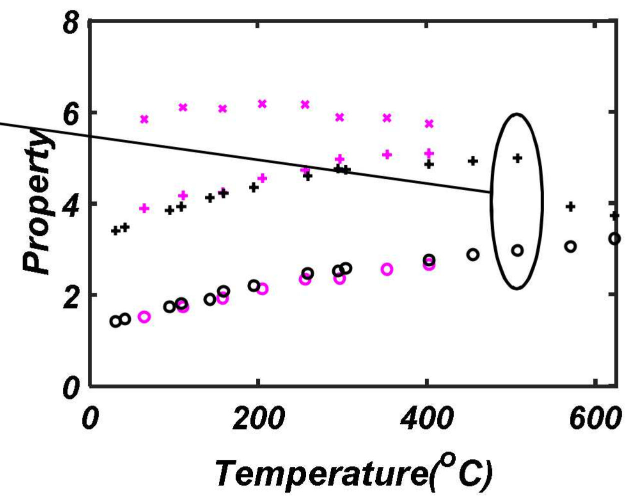
Series of experiments conducted to cover the temperature range

- 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

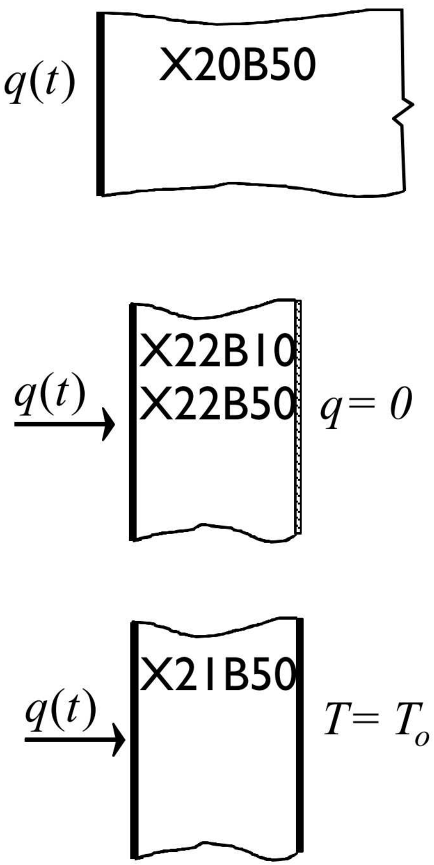


Typical Experiment ΔT = 15-20 °C

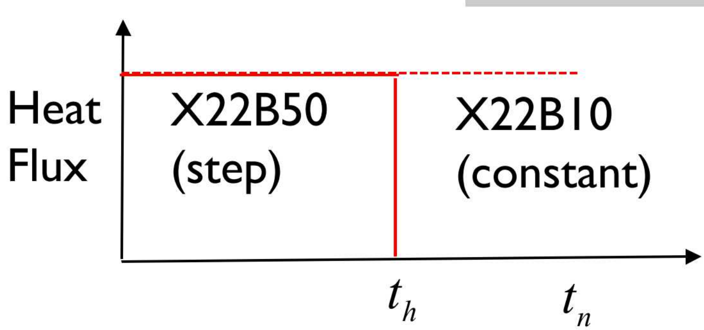




Can maximize the available information with Experimental Design



Geometry	BCs	Sensor	Max D	Opt (t_h)	Opt (t_n)
Semi-Infinite (Beck and Arnold)	(X20B1T0)	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)	(X22B10T0)	Heated Surface	0.00098	1.2	1.2
Finite (Beck and Arnold)	(X22B10T0)	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

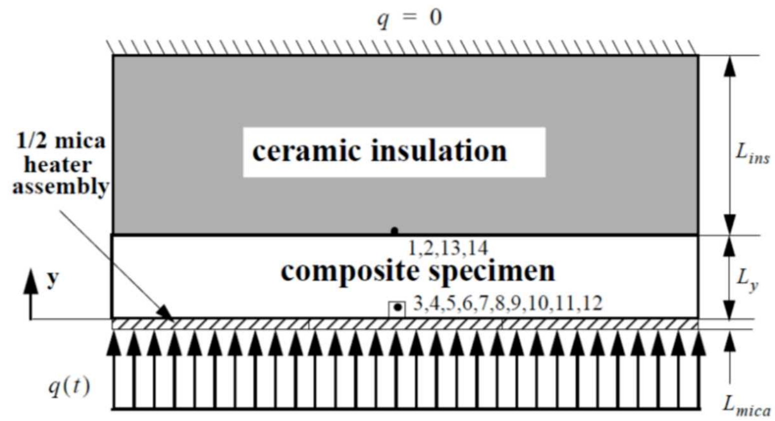
PROP1D (Beck Engineering Consultants)

- Finite difference numerical solution
- Integrated with a Gauss method to estimate parameters

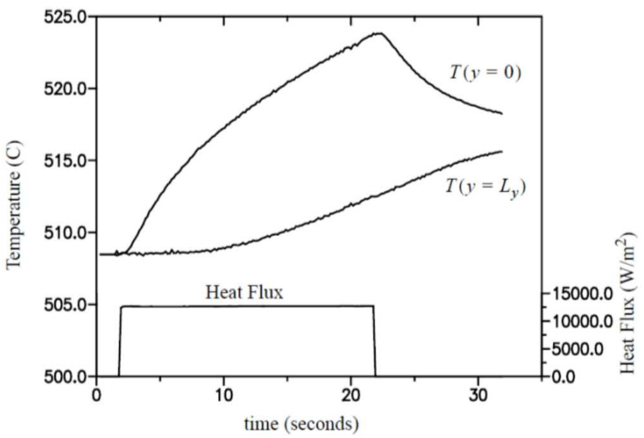
$$b^{k+1} = b^k + P\left[X^T W\left(Y - \hat{T}\right) + U\left(u - b^{(k)}\right)\right]$$

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

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



Thermal Model - $\hat{T}$

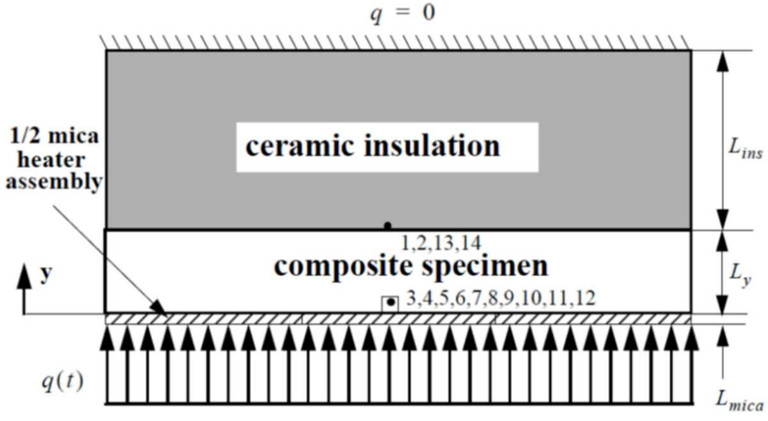


Exp Measurements - Y

Thermal model includes ancillary materials that will affect the estimated parameters

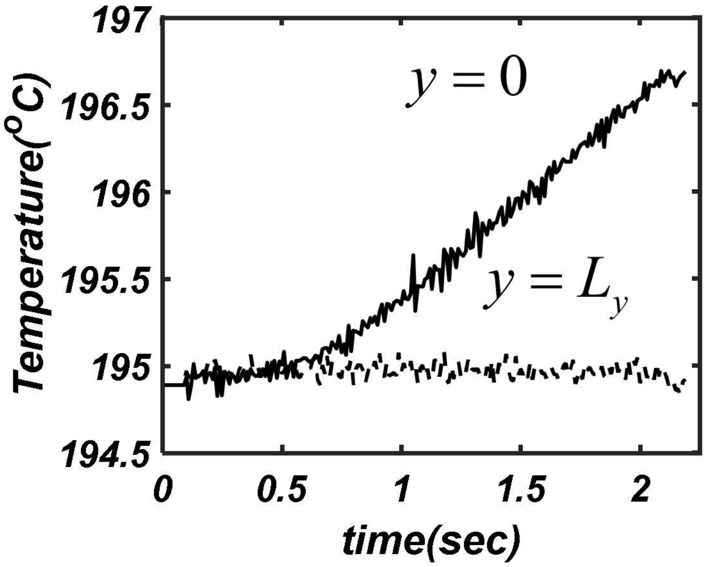
Heater Assembly

- 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

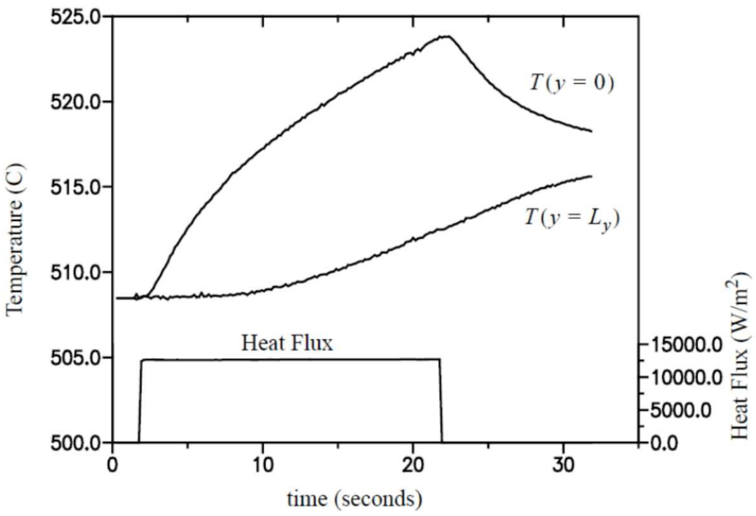
- Experiments conducted with composite replaced by insulation
  - Estimated for 2 temperatures (40 and 175 ^oC)
  - 50% difference from values provided by the manufacture



One-dimensional experiment

Typical experiment (T = 508 °C)

Exp Measurements - Y

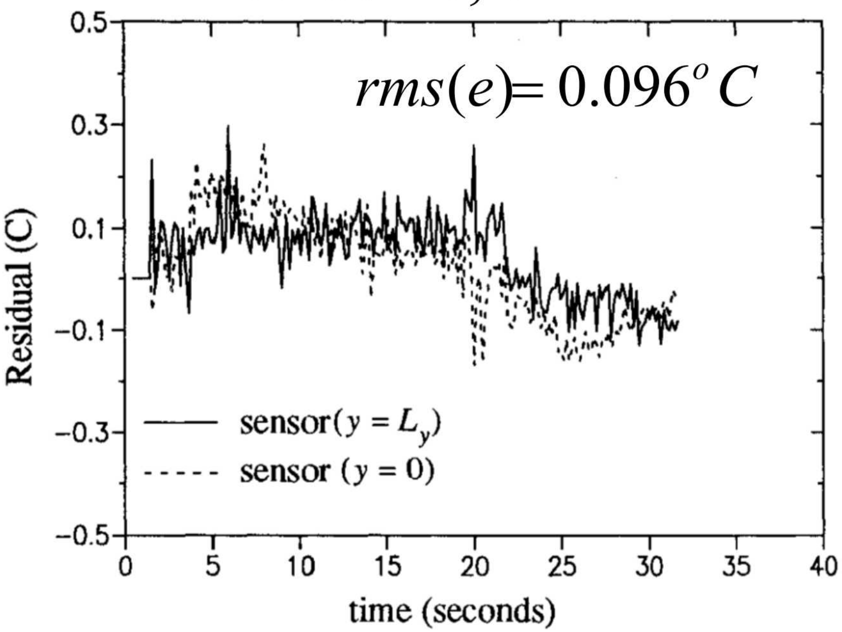


Estimated Parameters

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

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

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



Confidence Intervals

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

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

Standard Statistical Assumptions

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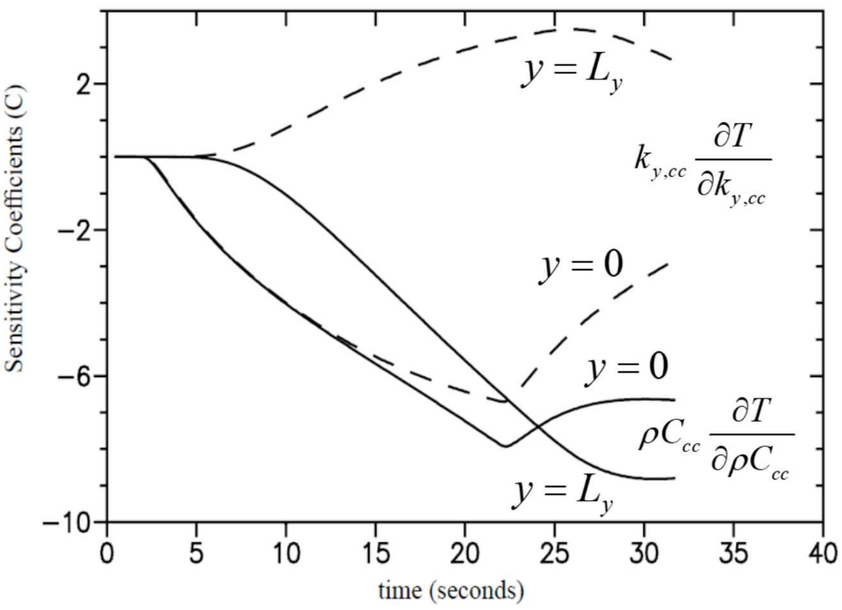
Standard Statistical Assumptions for the measurement errors

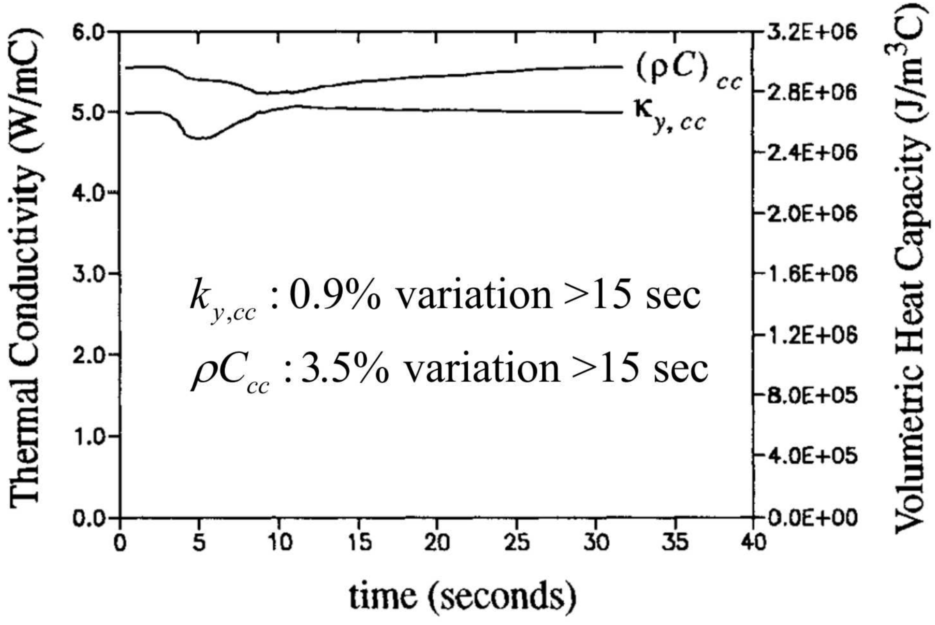
1. Additive measurement errors
2. Zero mean measurement error
3. Constant variance measurement error
4. Uncorrelated measurement error
5. Measurement error is normal
6. Known statistical parameters for measurement error
7. Errorless independent variables
8. Constant parameters

Sensitivity Coefficients and Sequential Parameter Estimates

Scaled Sensitvity Coefficients

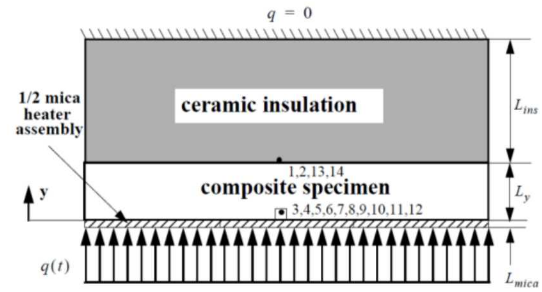


Sequential Estimates



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/(m³ C)	W/(m C)	(%)	(%)
q	125 W/m²	0.033	0.049	0.162	0.345
L_y	0.05 mm	0.016	0.027	0.038	0.105
y_I	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		



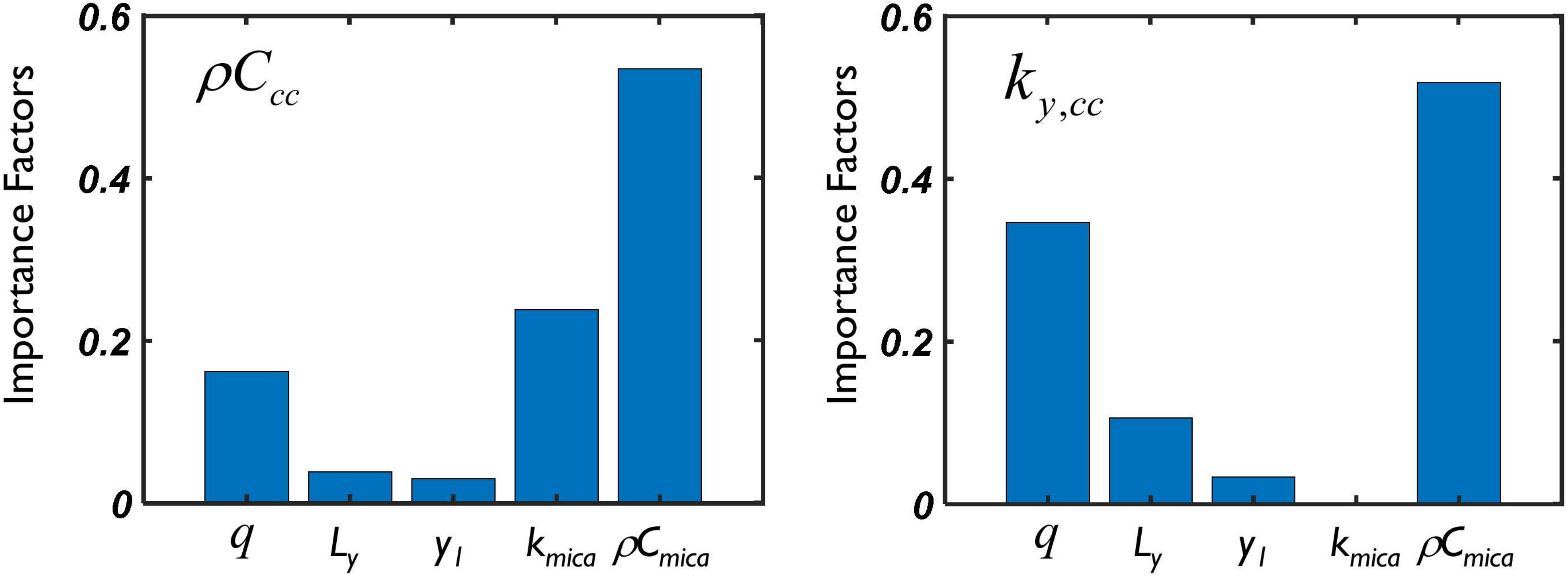
$$\Delta_{\hat{b}}^2 = \sum_{i=1}^{N}\left(\frac{\partial \hat{b}}{\partial z_i}\Delta_z\right)^2$$

Uncertainty due to measurement error

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

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

Experimental Uncertainty Analysis (1D)

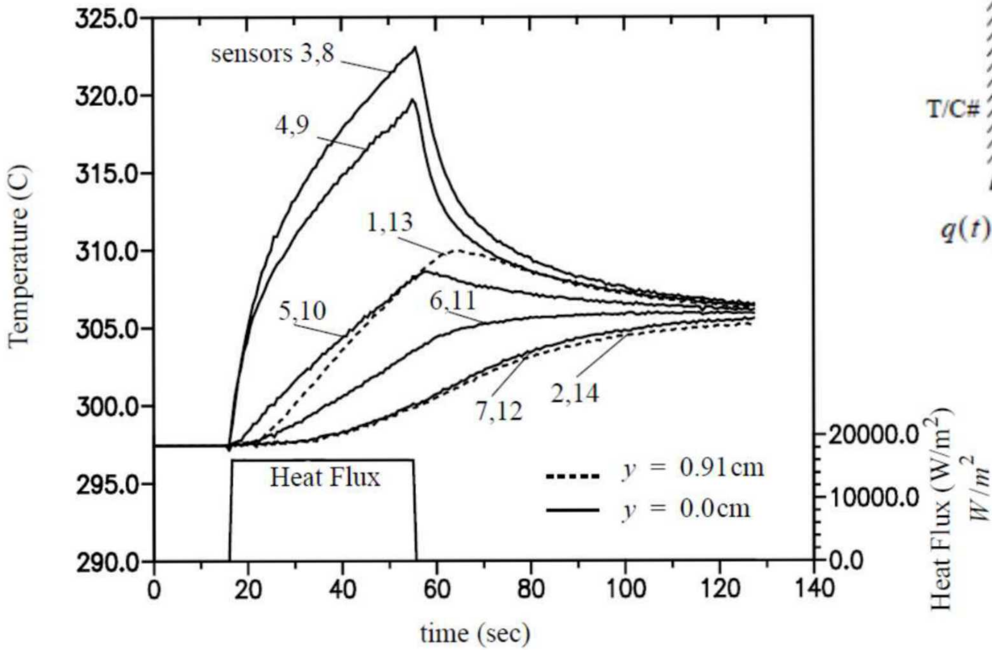


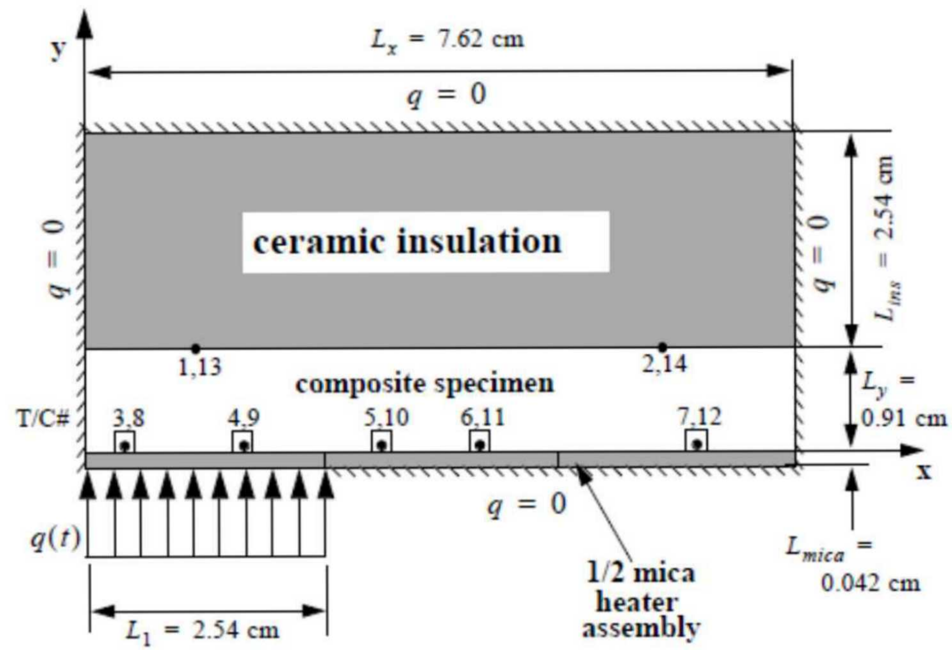
$$IF_i = \left(\frac{\partial \hat{b}}{\partial z_i} \Delta_z \right)^2 / \sum_{i=1}^{N} \left(\frac{\partial \hat{b}}{\partial z_i} \Delta_z \right)^2$$

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

Analysis of 2D Experiments

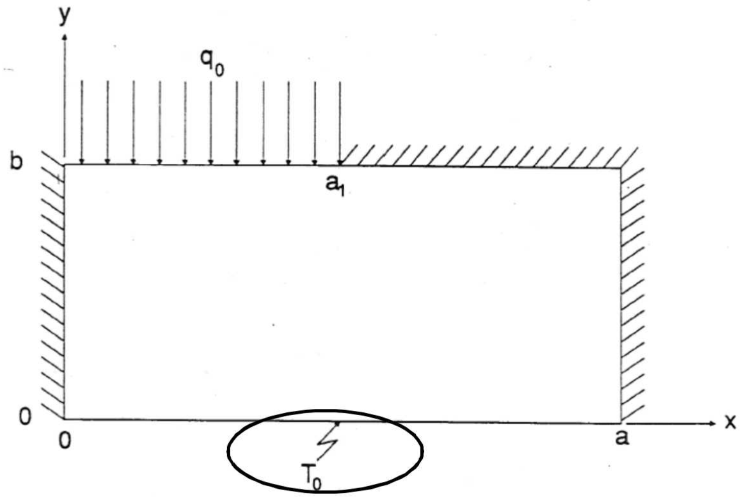
- Need a 2D heat conduction solver
- Estimate three parameters for each experiment





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

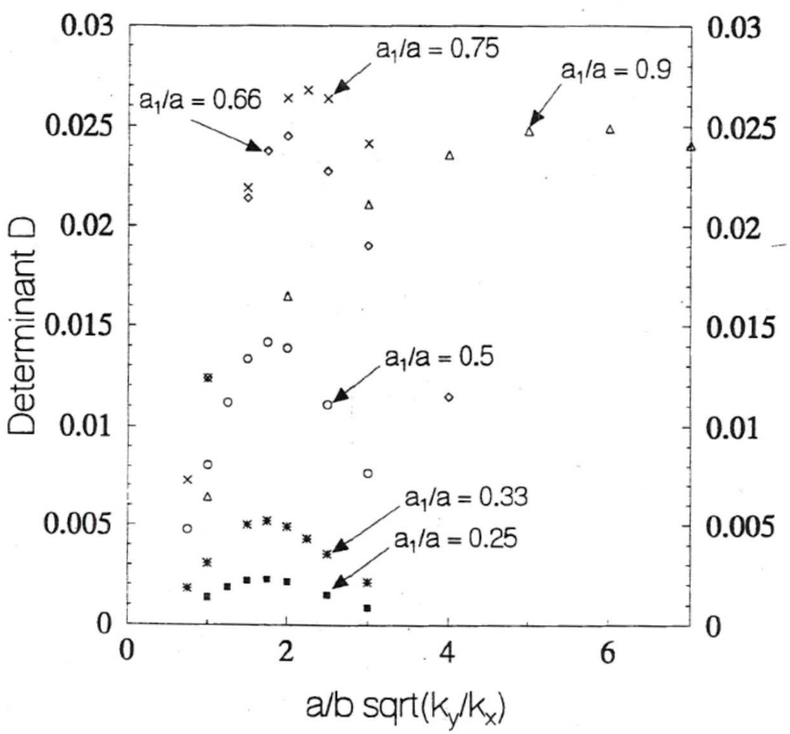
Design of Experiments (Taktak, 1992)

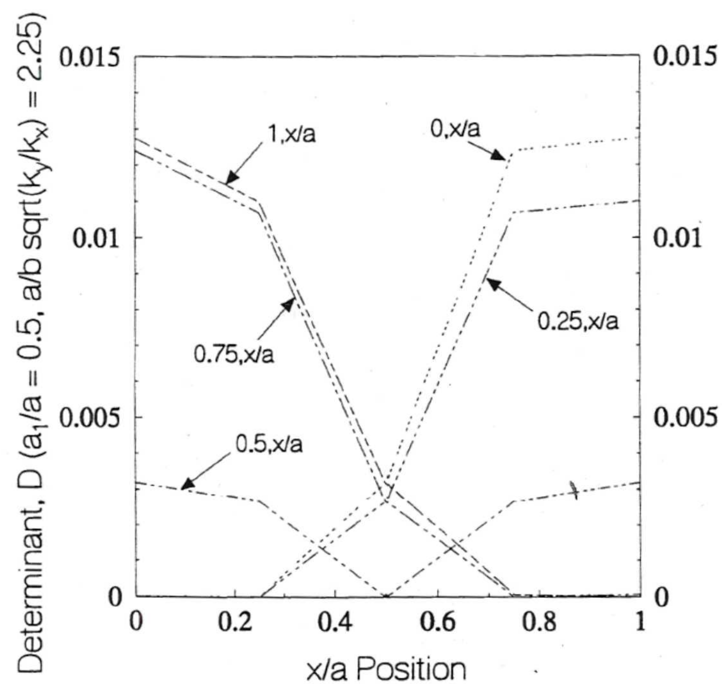


$$T_t^+(x^+,y^+,t^+) = 2a_1^+\sum_{n=1}^{\infty}\frac{(-1)^n}{\lambda_n^2}\sin(\lambda_n y^+)e^{-\lambda_n^2 t^+} + \frac{4}{\pi} *$$

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

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





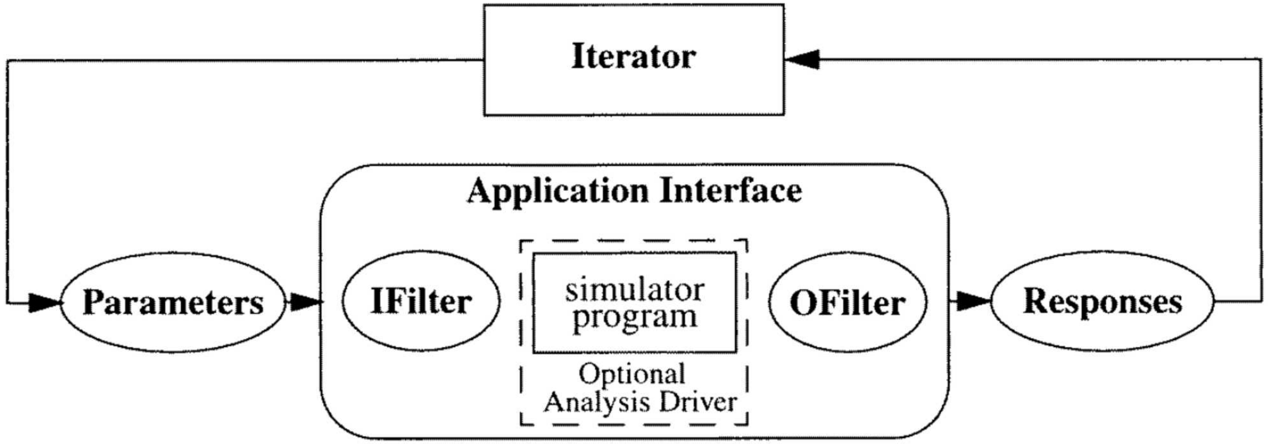
Analysis code for 2D parameter estimation

PROP2D (Developed at Michigan State in 1990s)

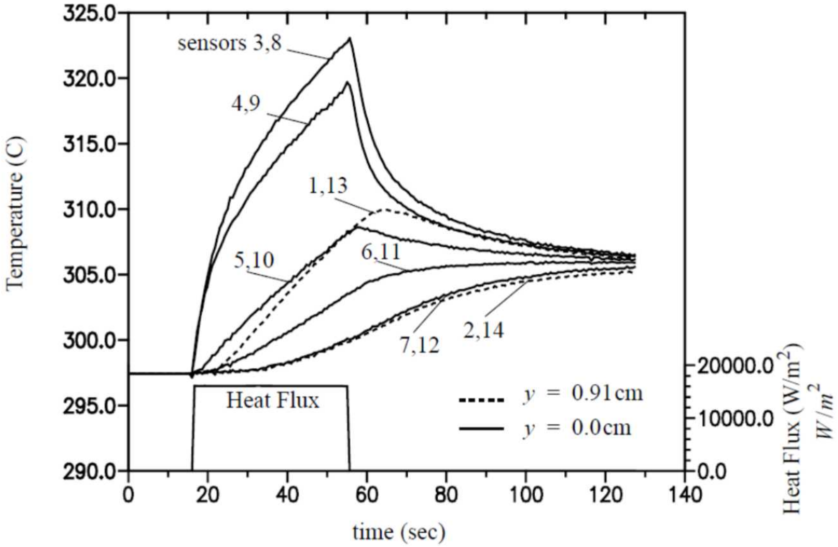
- Finite element solution (Topaz2D, LLNL)
- Converted to a subroutine and merged with a least-squares solver

Dakota

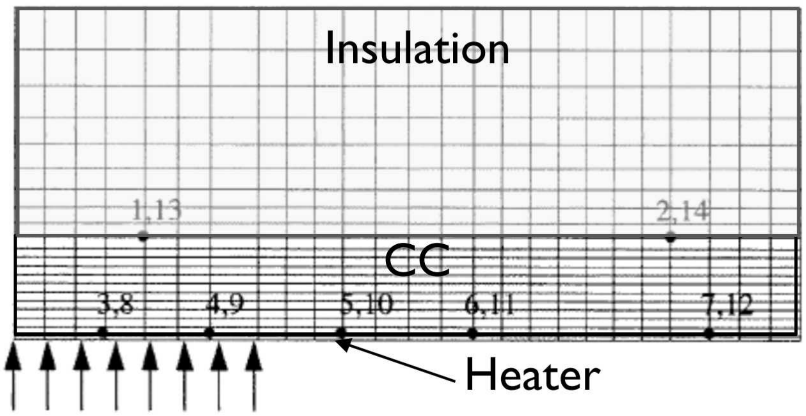
- Implements algorithms for optimization, uncertainty, and least-squares
- Leverages existing direct simulation programs



Exp Measurements - Y



Thermal Model - $\hat{T}$



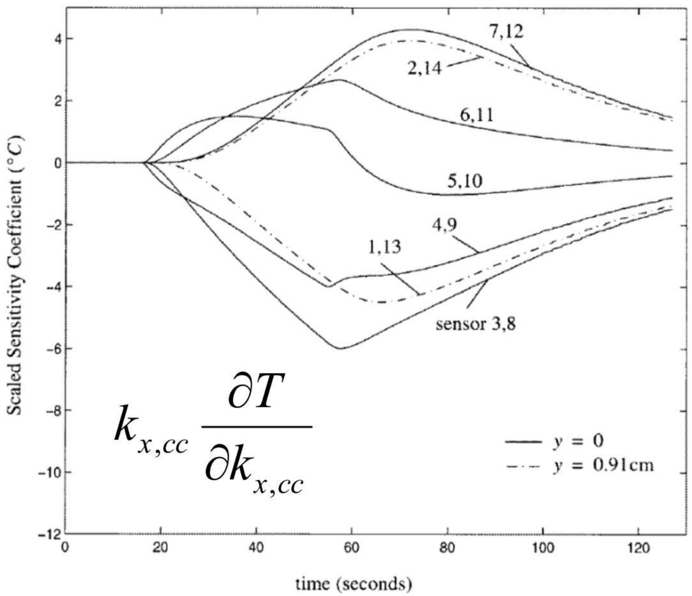
Estimated Parameters

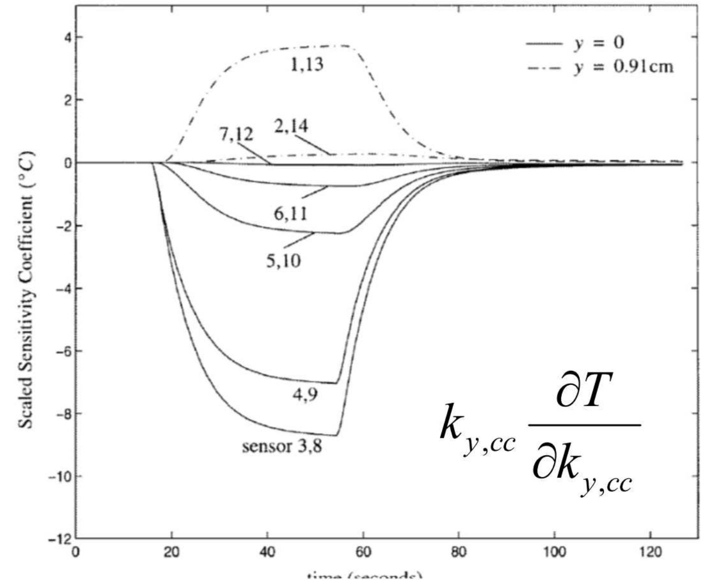
$$k_{x,cc} = 58.8 \pm 0.38 \;\; W / m^{o}C$$

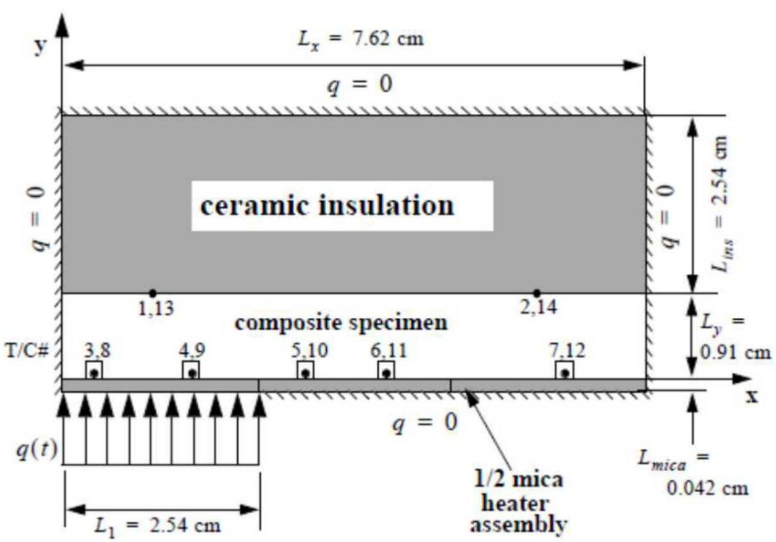
$$k_{y,cc} = 4.97 \pm 0.06 \;\; W / m^{o}C$$

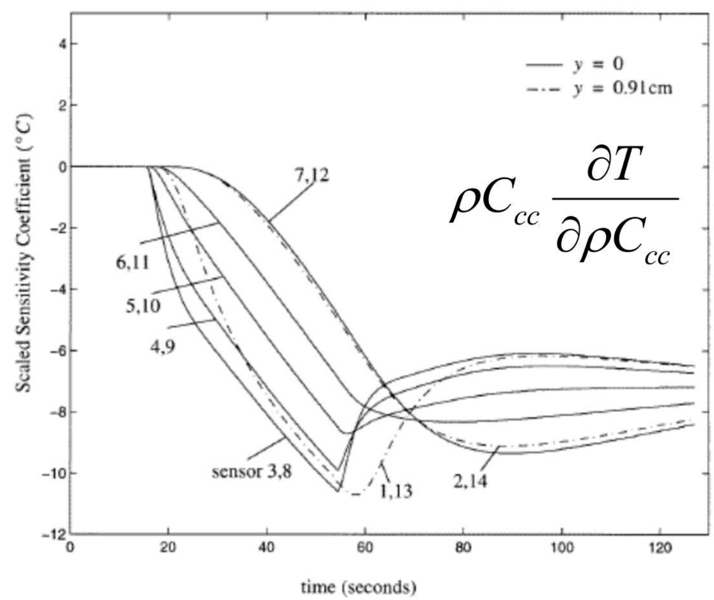
$$\rho C_{cc} = 2.36x10^{6} \pm 0.007 \;\; J / m^{3o}C$$

Scaled Sensitivity Coefficients

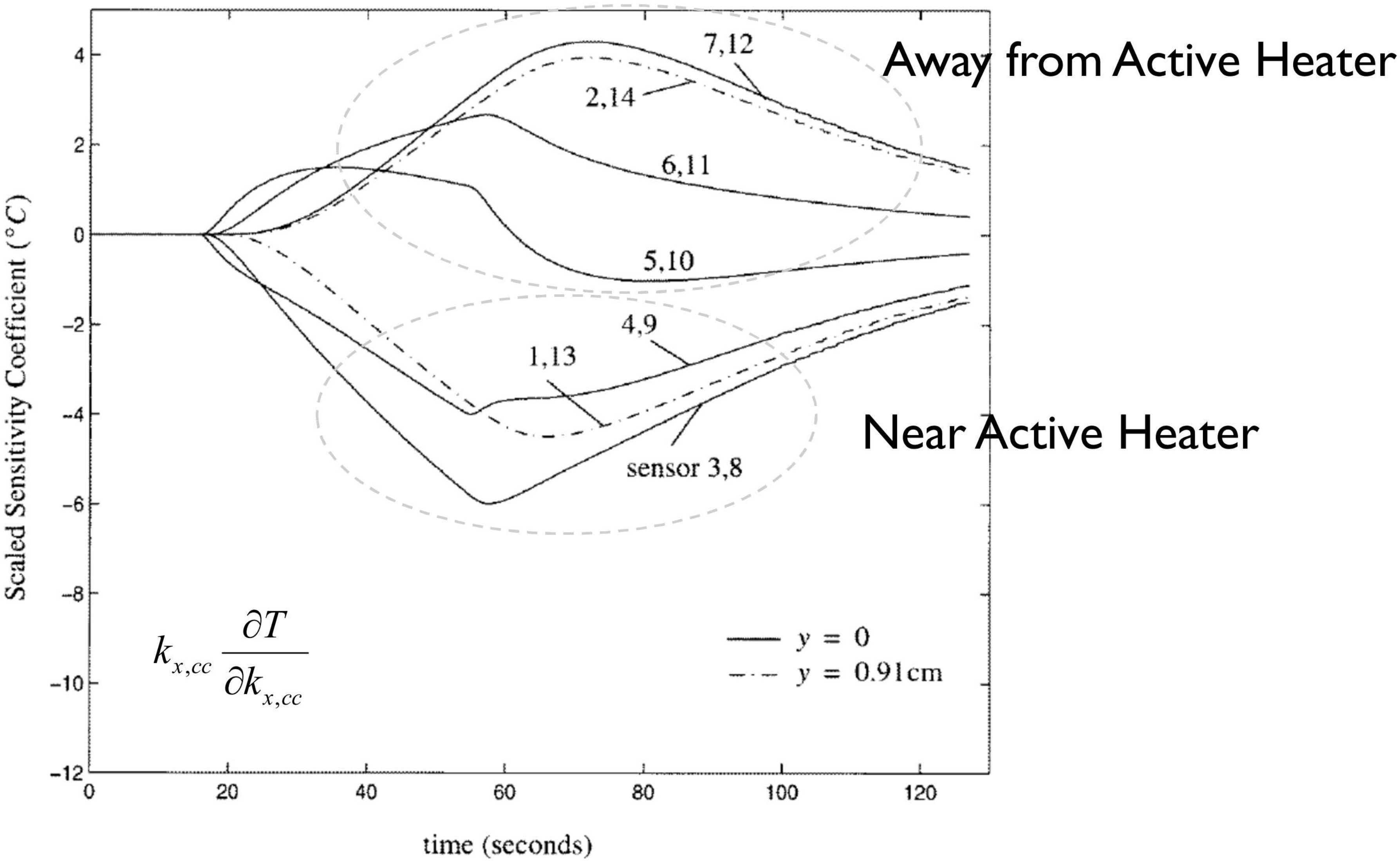




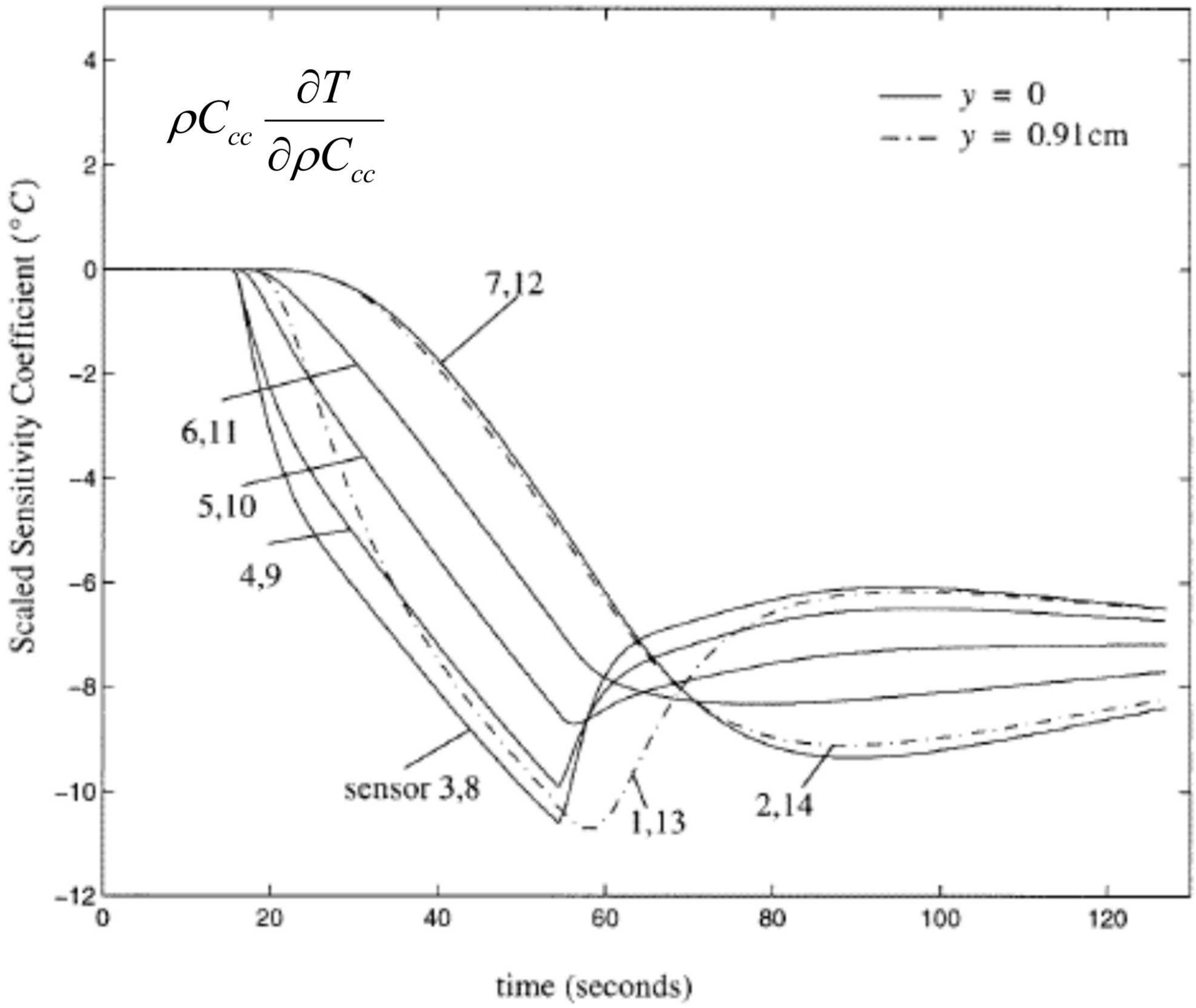




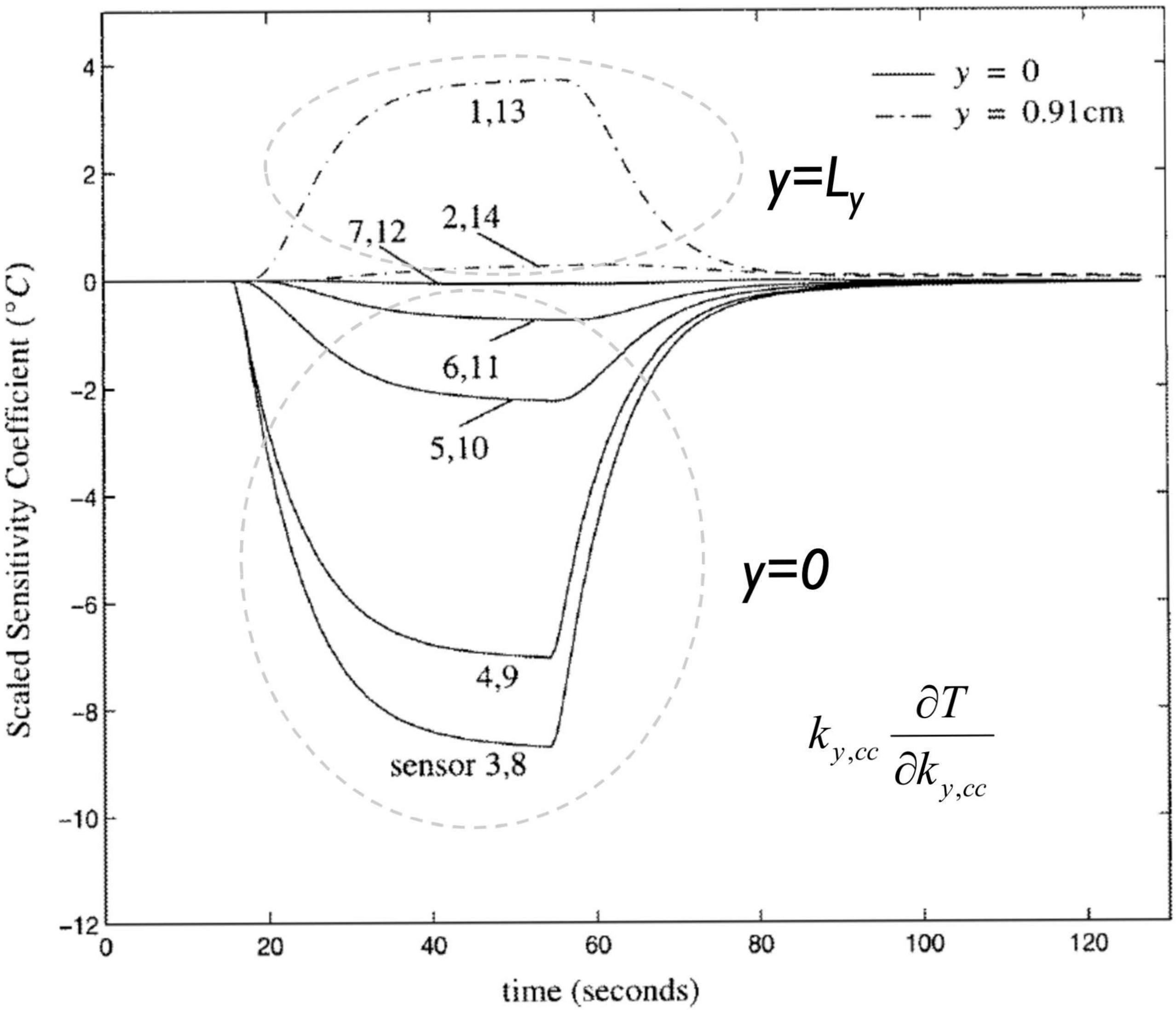
Scaled Sensitivity, $k_{x,cc}\dfrac{\partial T}{\partial k_{x,cc}}$



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

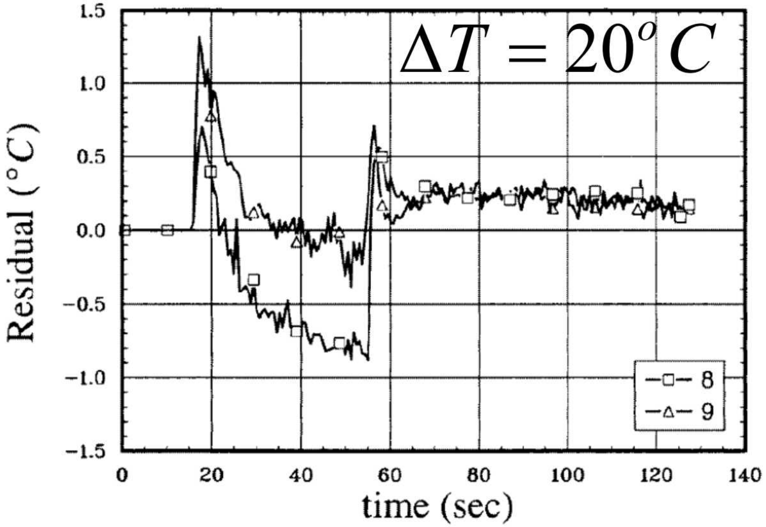


Scaled Sensitivity, $k_{y,cc} \dfrac{\partial T}{\partial k_{y,cc}}$

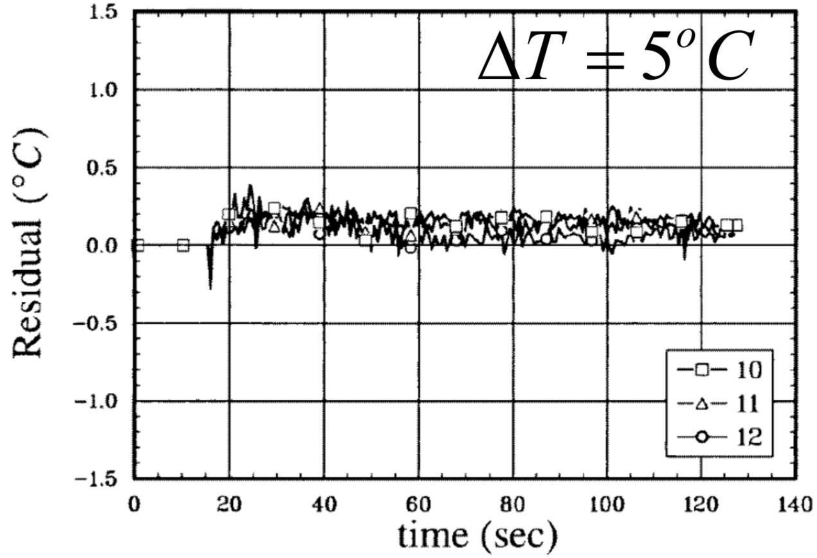


Residuals demonstrate signatures

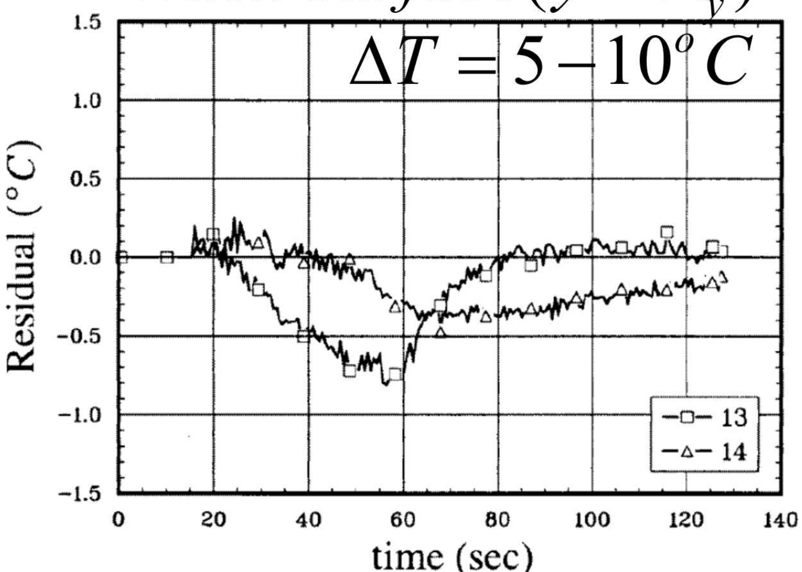
$Active\ Heater(y=0)$



$Inactive\ Heater(y=0)$



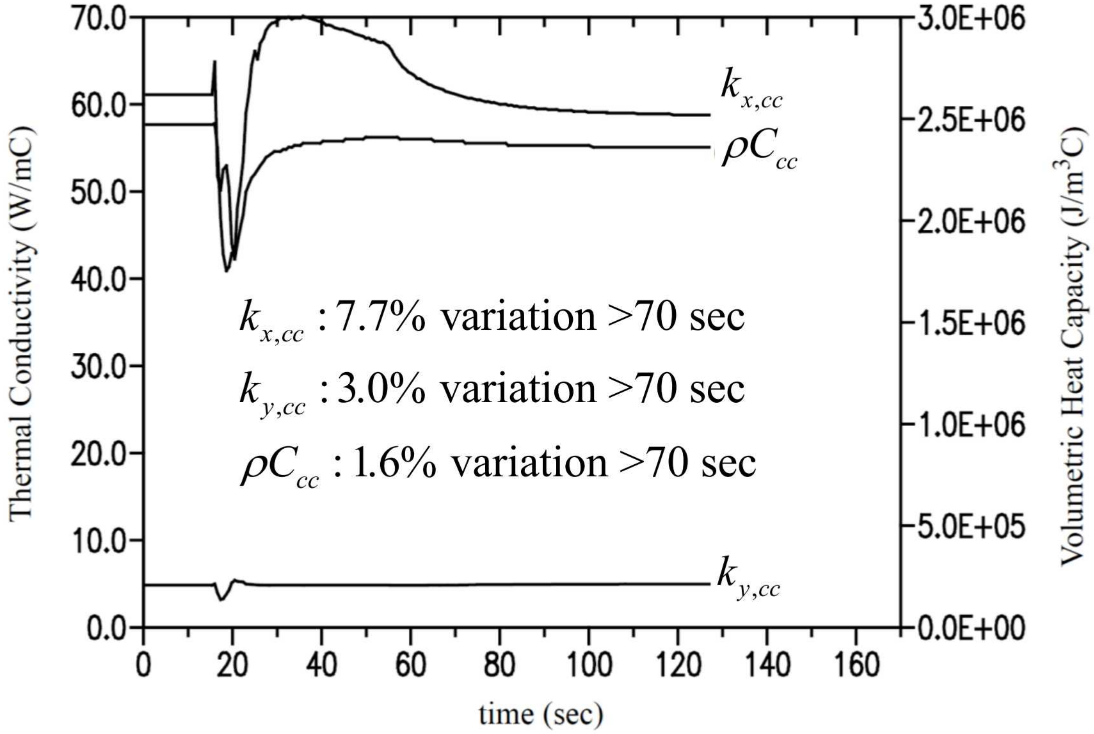
$Back\ surface(y=L_y)$



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

$rms = 0.30^o C$

Sequential Estimates



Uncertainty analysis (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			

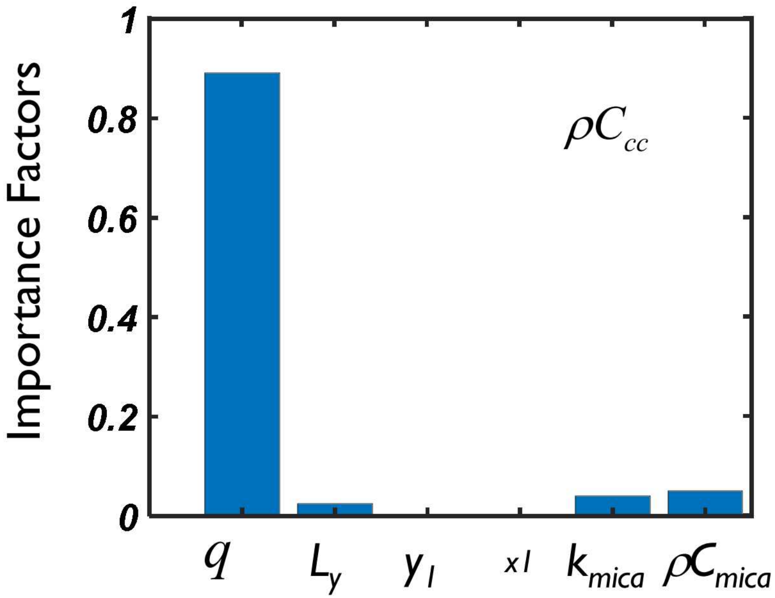
$$\Delta_{\hat{b}}^2 = \sum_{i=1}^{N}\left(\frac{\partial \hat{b}}{\partial z_i}\Delta_z\right)^2$$

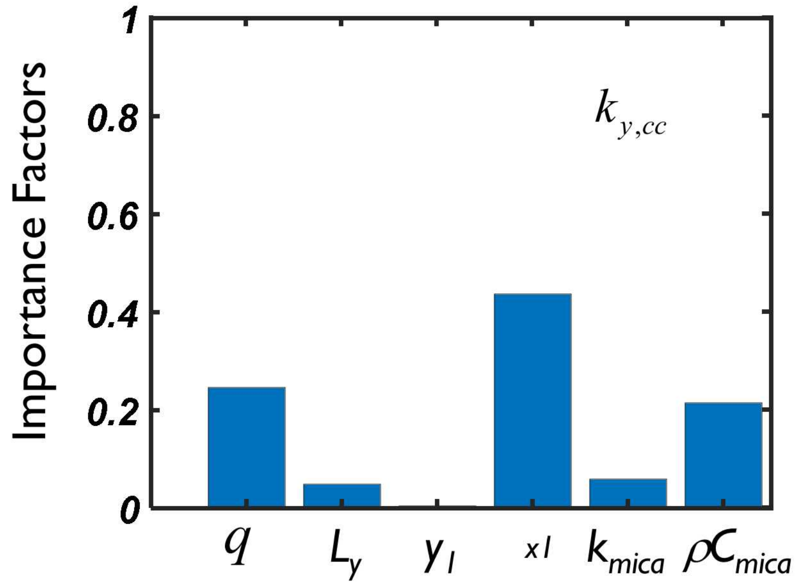
$$\rho C_{cc} = 2.36x10^6 \pm 0.007 \quad J/m^{3o}C$$

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

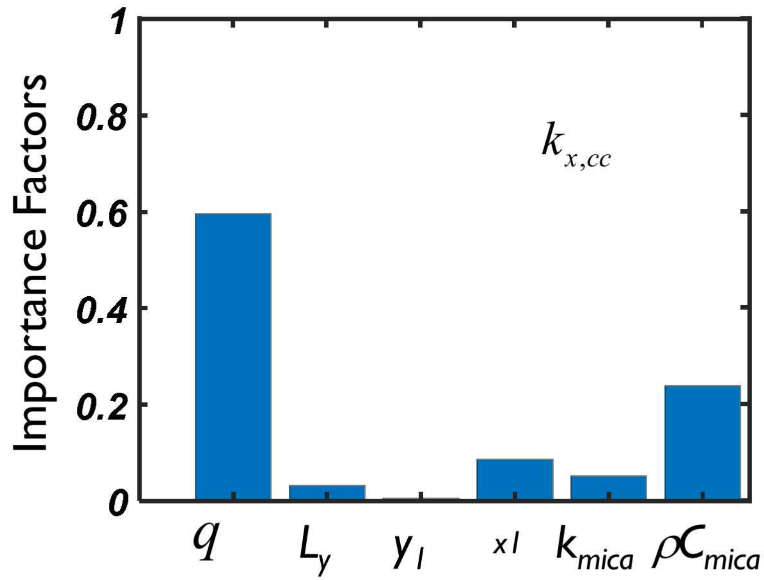
$$k_{y,cc} = 4.97 \pm 0.06 \quad W/m^oC$$

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 for Example 3

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.

Sequential Estimation over Experiments

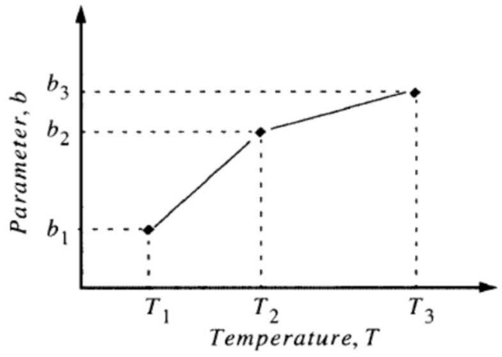
- Typically experiments are analyzed individually

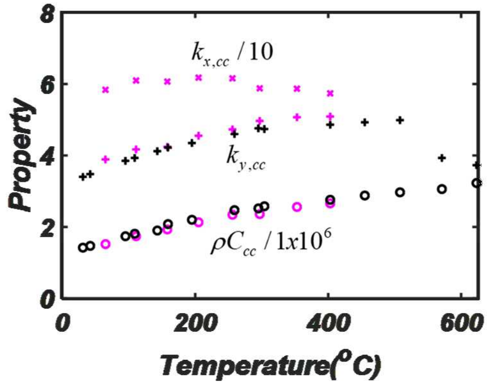
$$S = (Y - \hat{T})^T W (Y - \hat{T})$$

- 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

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

- Prior information

$$S_{pn} = (u_{n-1} - b_n)^T U_{n-1} (u_{n-1} - b_n)$$

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

- Estimation algorithm

$$n = 1$$

$$U_1^{(k)} \left[\hat{b}_1^{(k+1)} - \hat{b}_1^{(k)} \right] = X_1^{(k)T} W_1 \left[Y_1 - \hat{T}_1^{(k)} \right] - H^T H \hat{b}_1^{(k)}$$

$$U_1^{(k)} \equiv X_1^{(k)T} W_1 X_1^{(k)} + H^T H$$

Regularization term

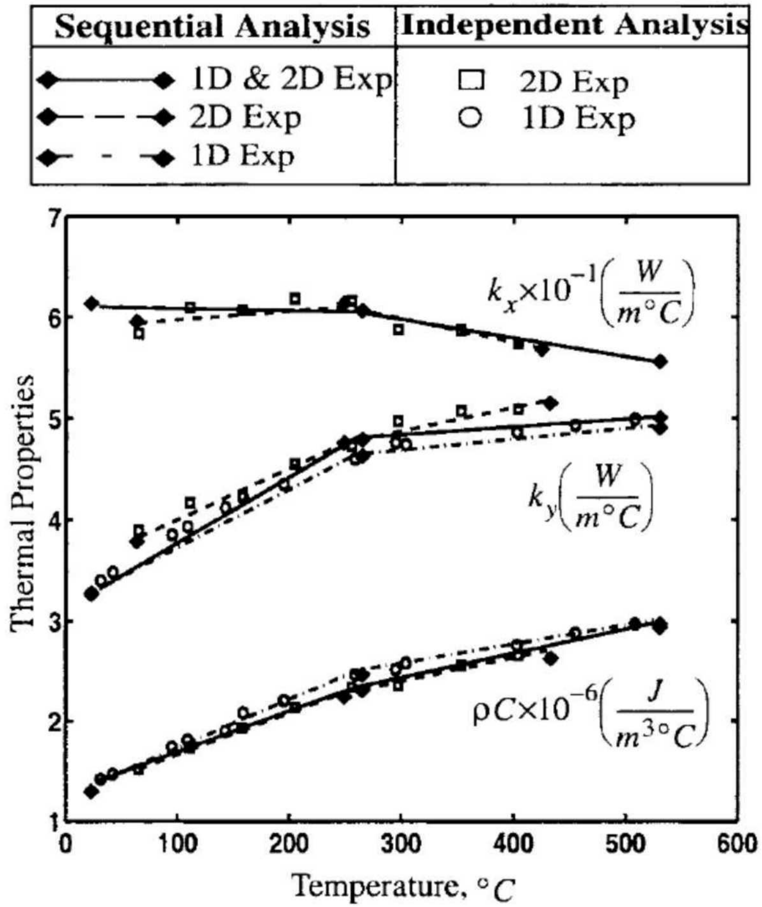
$$n > 1$$

$$U_n^{(k)} \left[\hat{b}_n^{(k+1)} - \hat{b}_n^{(k)} \right] = X_n^{(k)T} W_n \left[Y_n - \hat{T}_n^{(k)} \right] + U_{n-1} \left[u_{n-1} - \hat{b}_n^{(k)} \right]$$

$$U_n^{(k)} \equiv X_n^{(k)T} W_n X_n^{(k)} + U_{n-1}$$

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/m$^{3\circ}$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

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

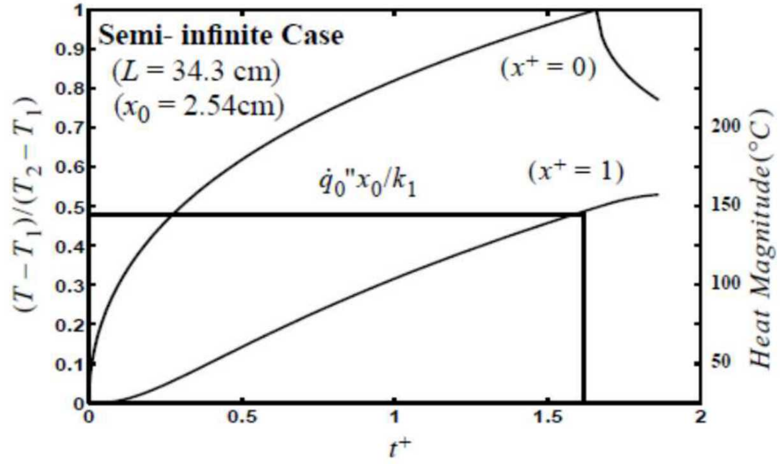
$$\frac{k_2-k_1}{k_1}, \frac{C_2-C_1}{C_1}, \frac{T-T_1}{T_2-T_1}.$$

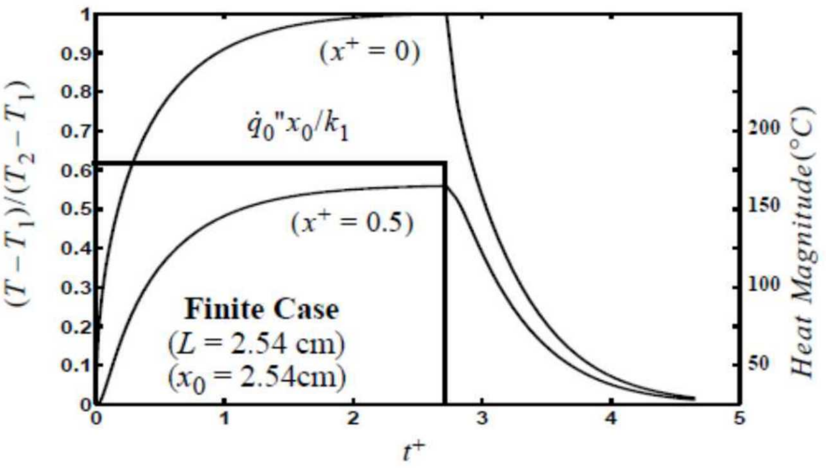
Parameter Groups (0.66, 1.22, 1.0)

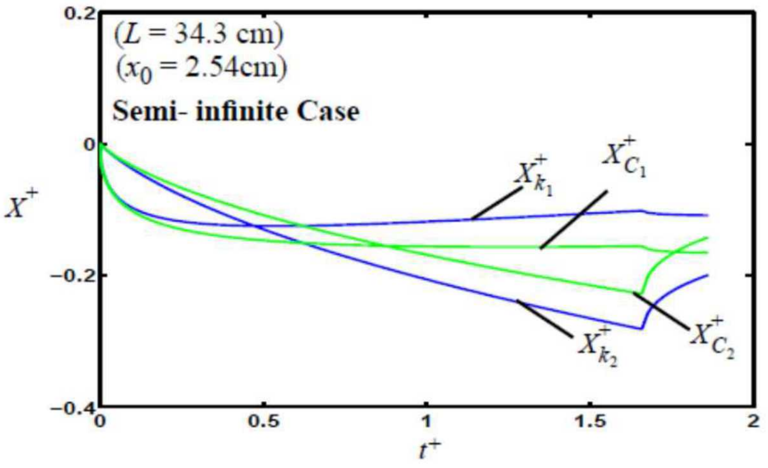
$$\Delta^+ \equiv \left|\frac{(X^+)^T X^+}{(T^+_{max})^2 N_t N_s}\right|.$$

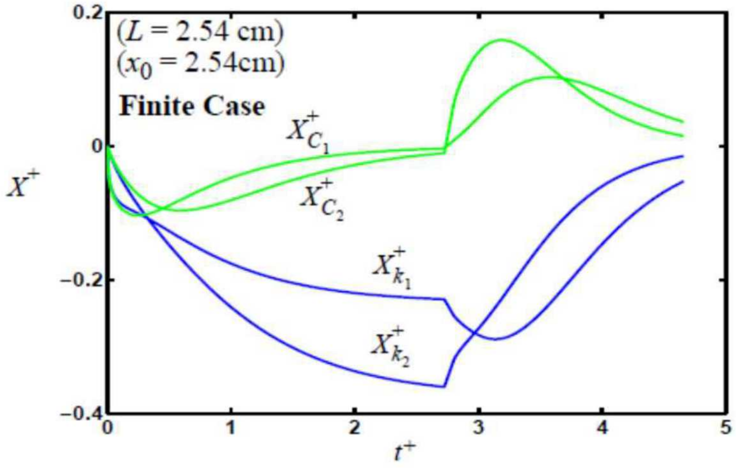
$$(X^+)^T = \left[\frac{\beta_1}{(\dot{q}_0"x_0/k_1)}\frac{\partial T}{\partial \beta_1} \quad \frac{\beta_2}{(\dot{q}_0"x_0/k_1)}\frac{\partial T}{\partial \beta_2} \quad \cdots \quad \frac{\beta_p}{(\dot{q}_0"x_0/k_1)}\frac{\partial T}{\partial \beta_p}\right]$$

Proposed Experimental Approaches and Sensitivity Coefficients

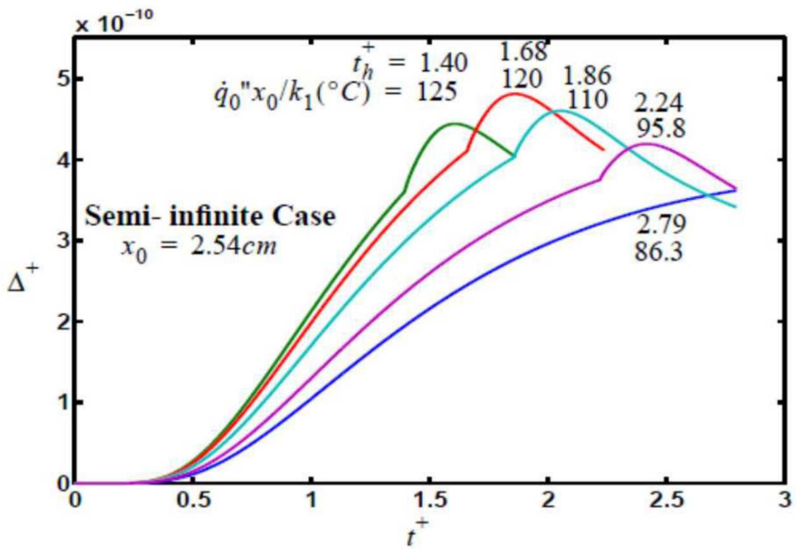


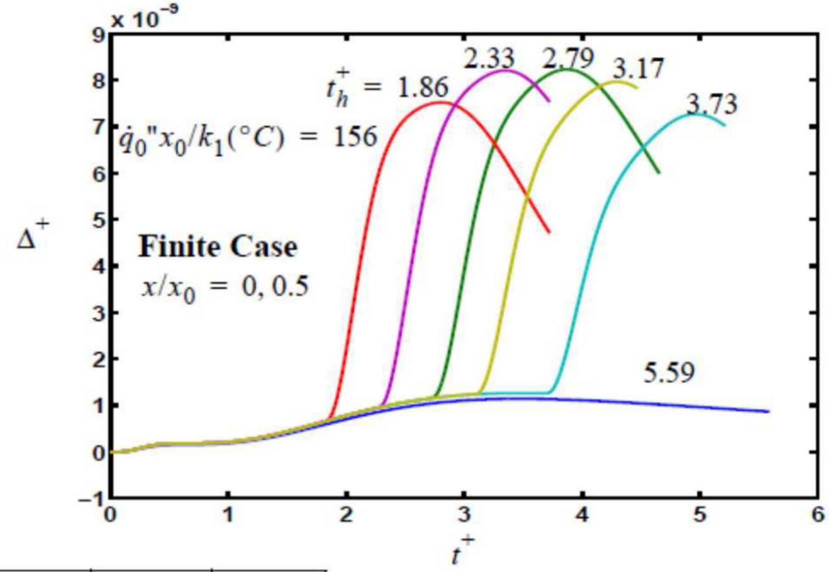






Optimal Experimental Design





x_0 (cm)	Sensor Locations x/x_0	Heating t_h^+	$\dot{q}_0''x_0/k_1$ (°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

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Taktak, R., 1992, "Design and Validation of Optimal Experiments for Estimating Thermal Properties of Composite Materials," Ph.D thesis, Michigan State University, East Lansing, Michigan.

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Tutorial Overview

Inverse Heat Conduction

- Basic concepts
- Damping and lagging
- Solution methods and examples

Inverse Heat Conduction Problem

- What is the Inverse Heat Conduction Problem (IHCP)?
- Stolz Method
- Damping and Lagging $\rightarrow$ ill-posed
- Future Times (Function Specification) Method
- Tikhonov Regularization Method
- Singular Value Decomposition Method
- Summary

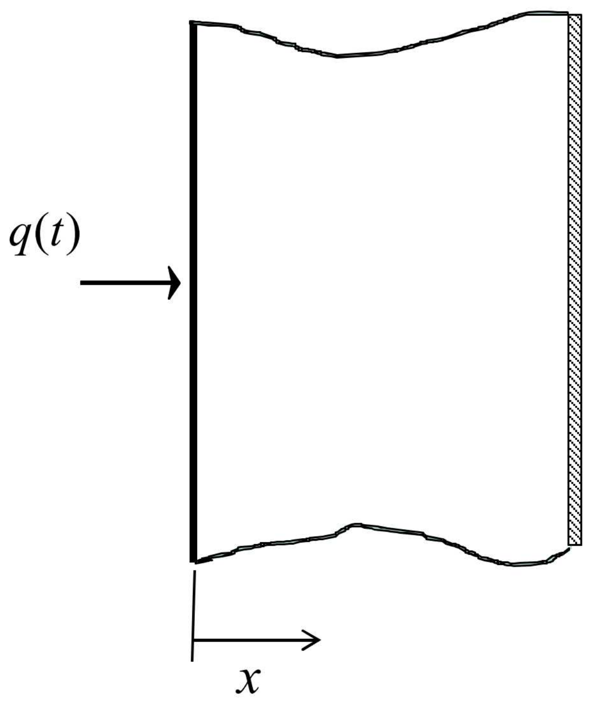
Dimensionless Variables

$$x = \frac{x_d}{L}$$

$$t = \frac{\alpha t_d}{L^2}$$

$$q = \frac{q_d}{q_{ref}}$$

$$T = \frac{T_d - T_{ref}}{\left(q_{ref} L / k\right)}$$



What is the IHCP?

- "Usual" or forward heat conduction problem:

Given:

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

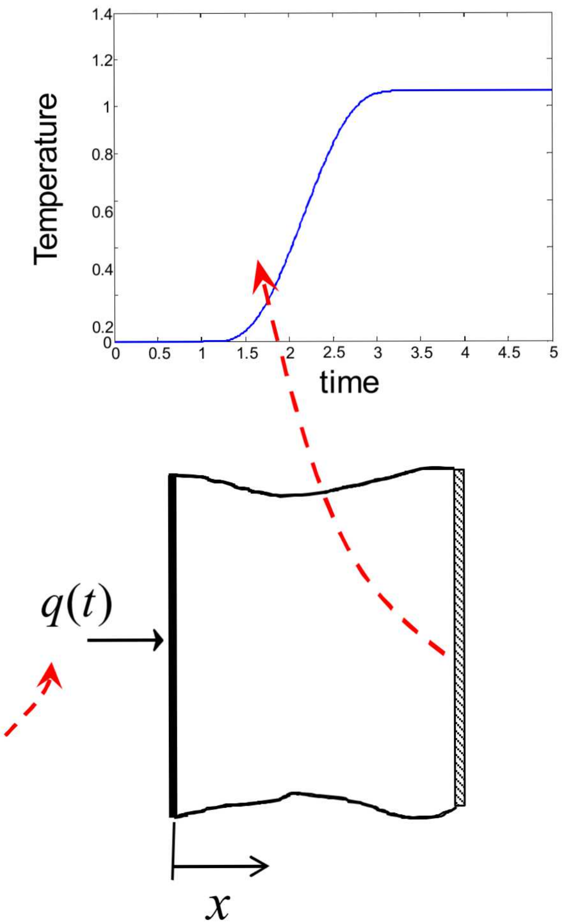
$$\left.\frac{\partial T}{\partial x}\right|_{x=0} = q(t)$$

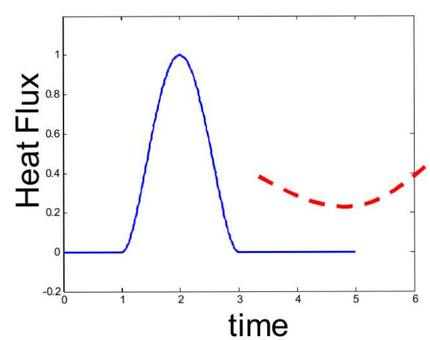
$$\left.\frac{\partial T}{\partial x}\right|_{x=1} = 1$$

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

Find:

$$T(x_i, t)$$



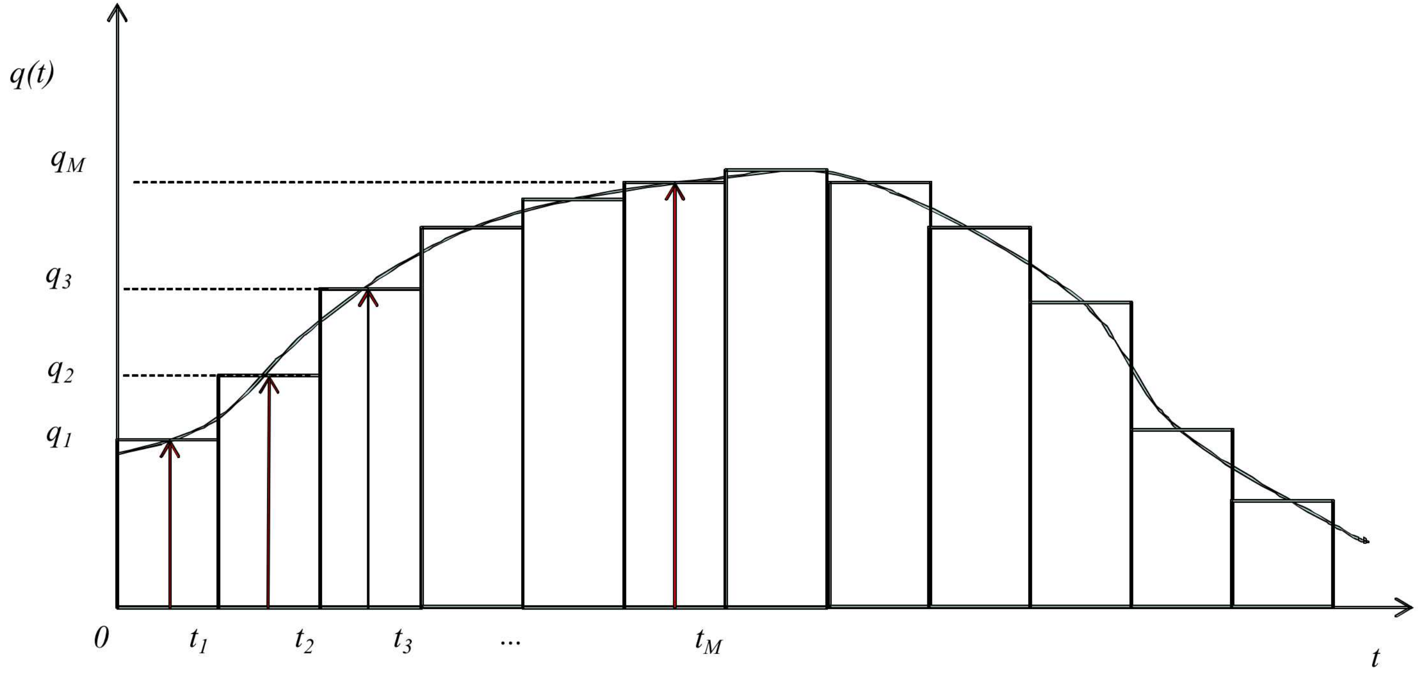


Nature of Boundary IHCP

- This is a ***function estimation*** problem
  - – Requires estimation of a “large” number of unknown parameters $q(t_j)$
- The problem is ***ill-posed*** in the sense of Hadamard
  - – Solution may not exist or may not be unique
  - – Solution does not depend continuously on the data $(T(x_i, t_j))$
    - Noise in data is amplified in the solution

Piecewise Constant Heat Flux

- Consider a piecewise-constant representation of the boundary heat flux
  – Note fluxes are "centered" at the "t-1/2" times



Forward Problem Solution

- For the piece-wise constant heat flux representation, the solution for the linear forward heat conduction problem can be written as

$$\mathbf{T} = \mathbf{X}\mathbf{q}$$

where

$$\mathbf{X} = \left[\left. \frac{\partial T}{\partial q_j} \right|_{t=t_i} \right] = \left[X_{ij} \right]$$

Forward Problem – Property 1

- Due to the parabolic nature of the heat conduction process, the **X** matrix is lower triangular

$$\begin{bmatrix} X_{11} & 0 & 0 & \cdots & 0 & 0 \\ X_{21} & X_{22} & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \ddots & 0 & \vdots \\ X_{M1} & \cdots & X_{MM-1} & X_{MM} & 0 & 0 \\ \vdots & & & & \ddots & \\ X_{N1} & X_{N2} & \cdots & X_{NN-2} & X_{NN-1} & X_{NN} \end{bmatrix}$$

  – Physically, this means the current temperature only depends on all the *past and current* heat flux components

Forward Problem – Property 2

- A further property of the **X** matrix is that each column is the same – only shifted down one position
  This makes values along each band the same (this is called a *Toeplitz* matrix)

$$
\begin{bmatrix}
X_1 & 0 & 0 & \cdots & 0 & 0 \\
X_2 & X_1 & 0 & \cdots & 0 & 0 \\
\vdots & \vdots & \ddots & \ddots & 0 & \vdots \\
X_M & \cdots & X_2 & X_1 & 0 & 0 \\
\vdots & & & & \ddots & \\
X_N & X_{N-1} & \cdots & X_3 & X_2 & X_1
\end{bmatrix}
$$

Stolz Method for IHCP (1960)

- Stolz realized, with the lower-triangular form of the **X** matrix, that the model values **T = Xq** can be written sequentially:

$$
\begin{aligned}
T_1 &= X_1\hat{q}_1 \\
T_2 &= X_2\hat{q}_1 + X_1\hat{q}_2 \\
T_3 &= X_3\hat{q}_1 + X_2\hat{q}_2 + X_1\hat{q}_3 \\
&\vdots \\
T_M &= \sum_{j=1}^{M-1} X_{M+j-1}\hat{q}_j + X_1\hat{q}_M
\end{aligned}
$$

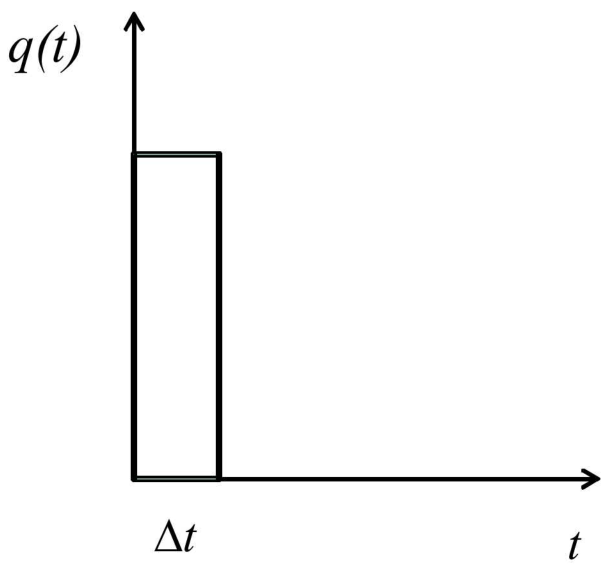
- Then the heat fluxes can be found sequentially by exactly matching the model to the data, **Y = T**:

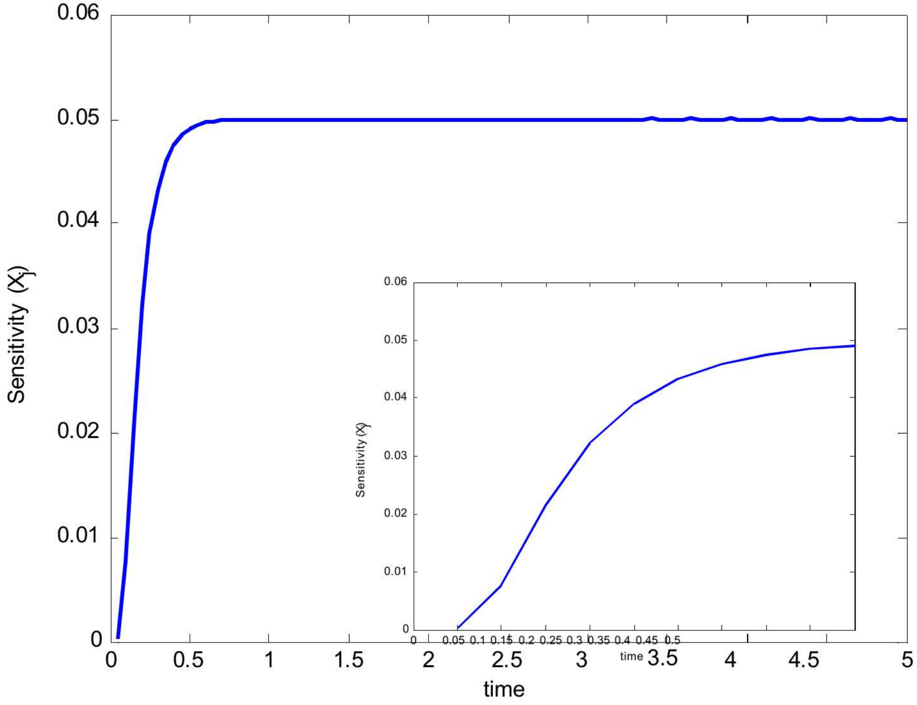
$$
\begin{aligned}
\hat{q}_1 &= \frac{Y_1}{X_1} \\
\hat{q}_2 &= \frac{Y_2 - X_2\hat{q}_1}{X_1} \\
\hat{q}_3 &= \frac{Y_3 - X_3\hat{q}_1 - X_2\hat{q}_2}{X_1} \\
&\vdots
\end{aligned}
$$

$$
\boxed{\hat{q}_M = \frac{Y_M - \sum_{j=1}^{M-1} X_{M-j+1}\hat{q}_j + X_1\hat{q}_j}{X_1}}
$$

Sensitivity Coefficients

- The first column of the **X** matrix is the solution of the forward problem to a unit heat flux pulse of width Δt

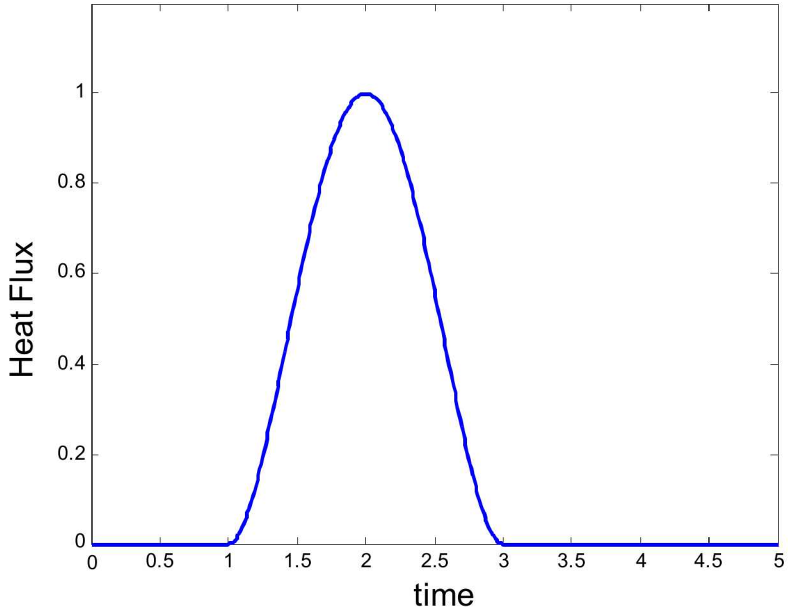


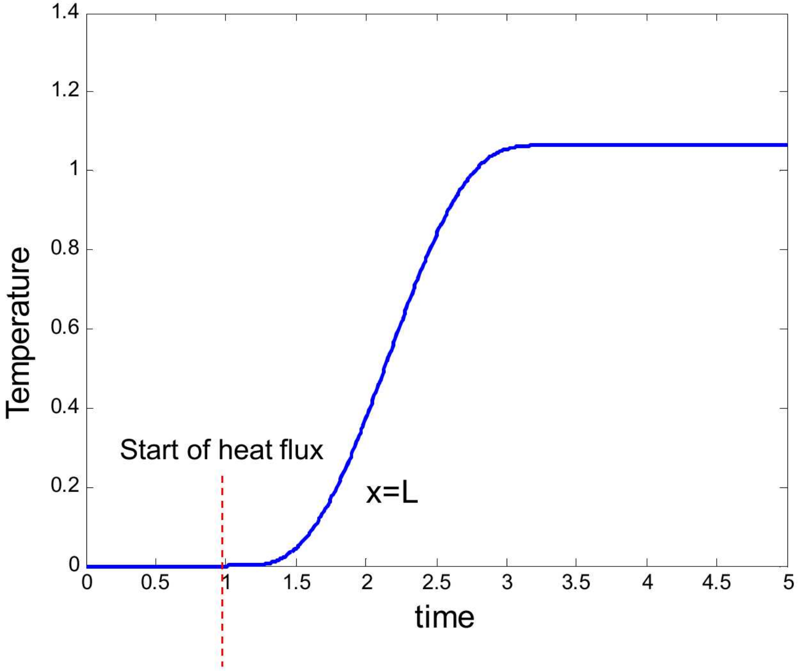


Example

- Consider heat flux that is quartic in time:

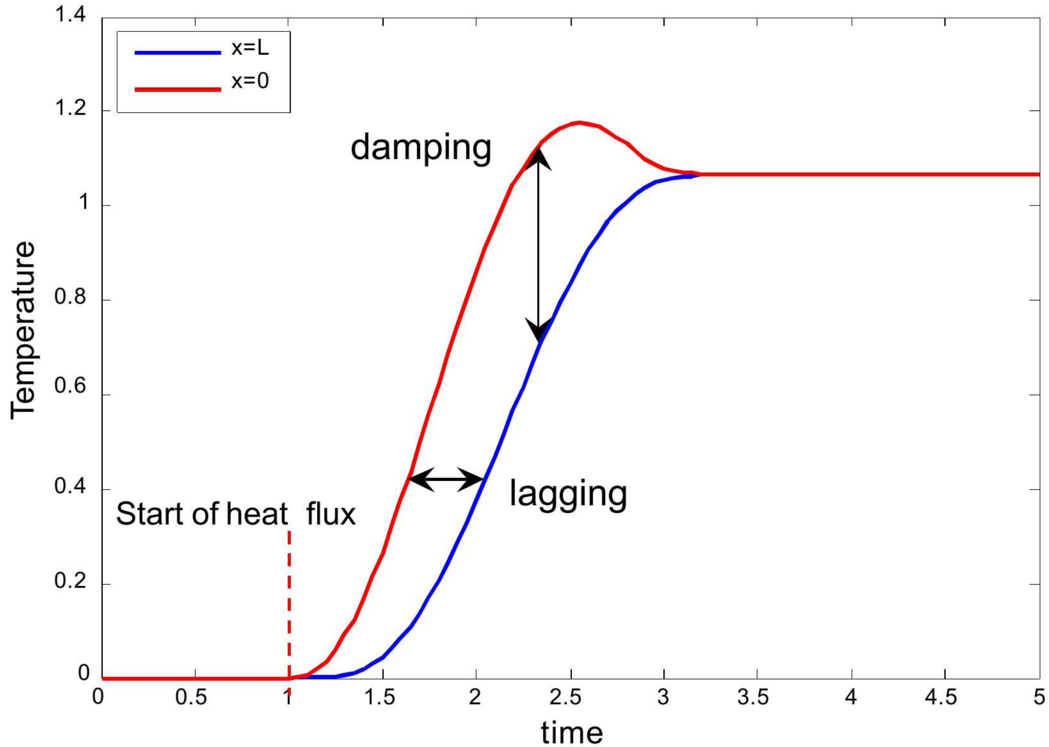
$$q(t) = \begin{cases} t^4 - 4t^3 + 4t^2 & t_{start} < t < t_{stop} \\ 0 & \text{otherwise} \end{cases}$$



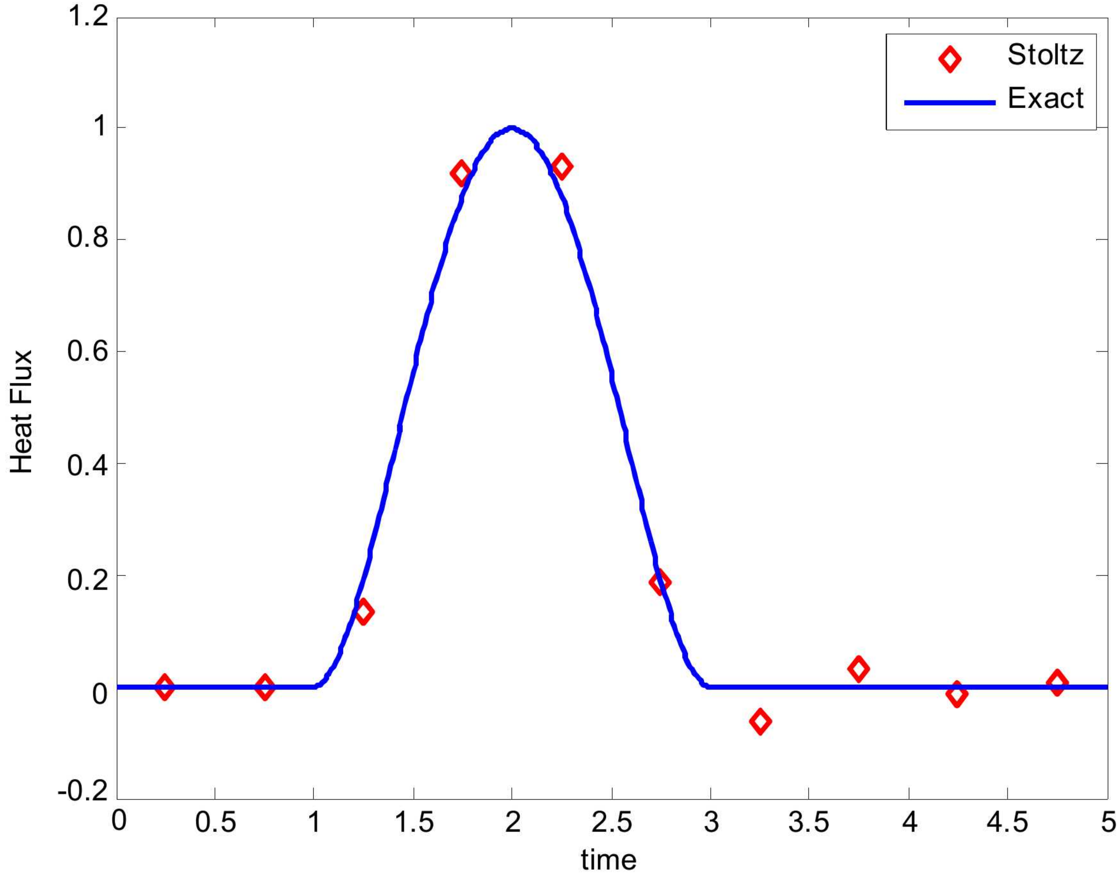


Damping and Lagging

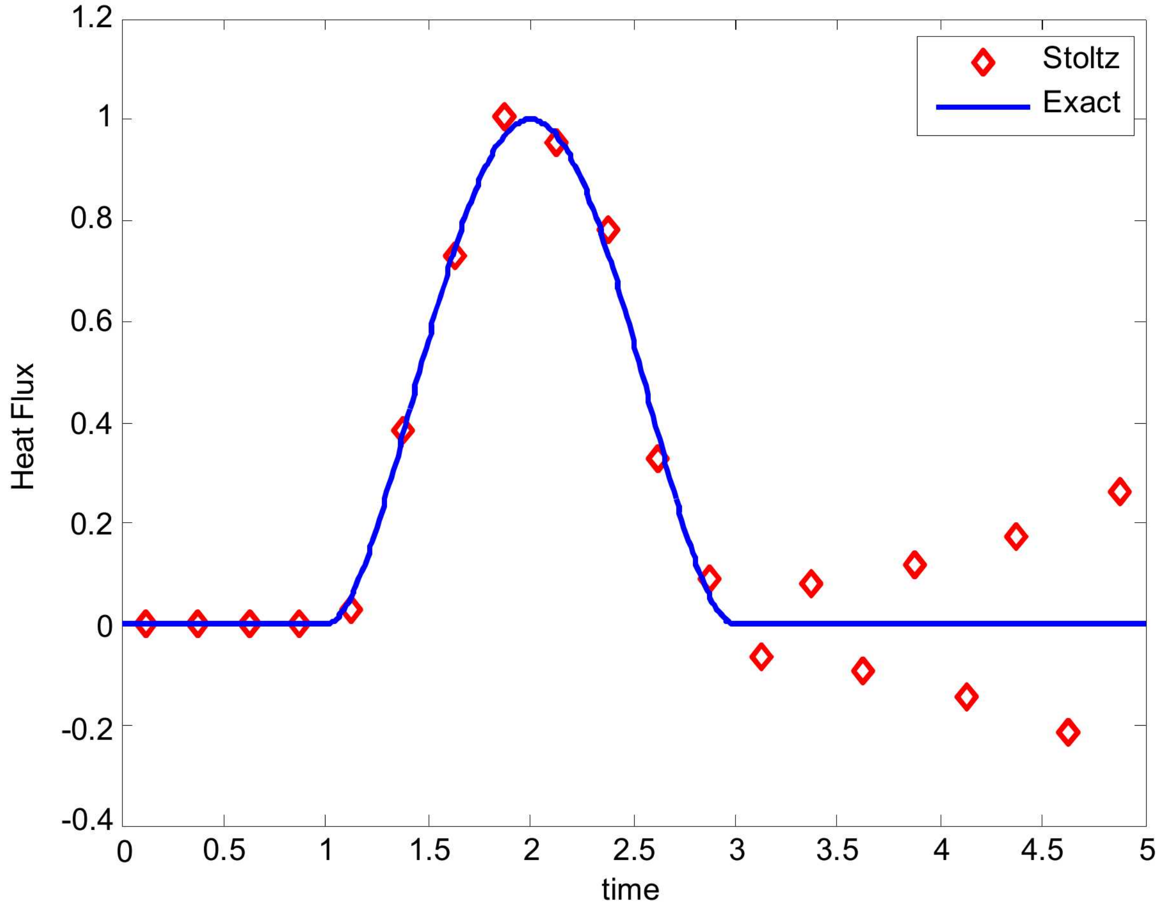
- Temperature at an interior point are both damped and lagged with respect to the surface response



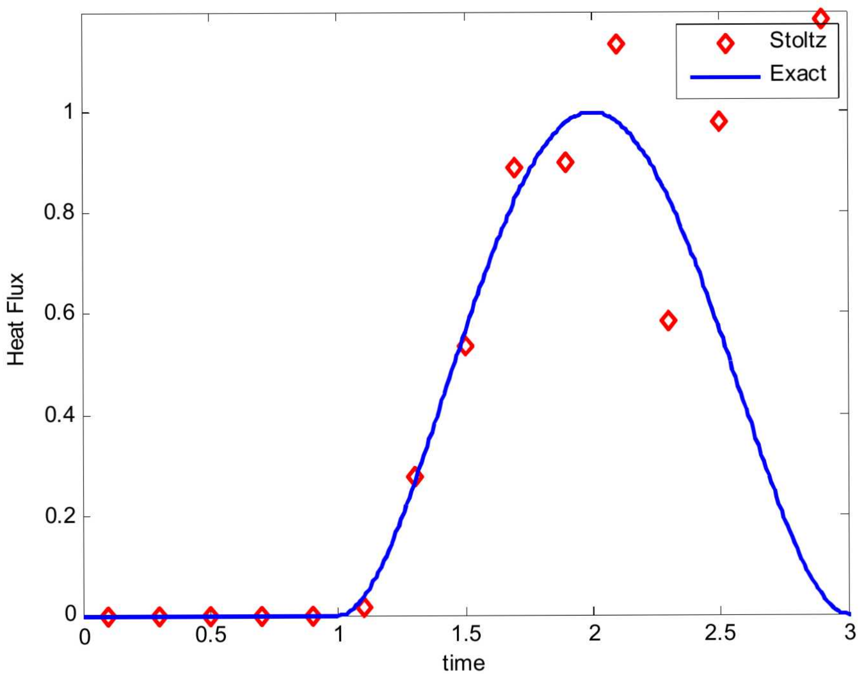
Stoltz Method - $\Delta t = 0.5$

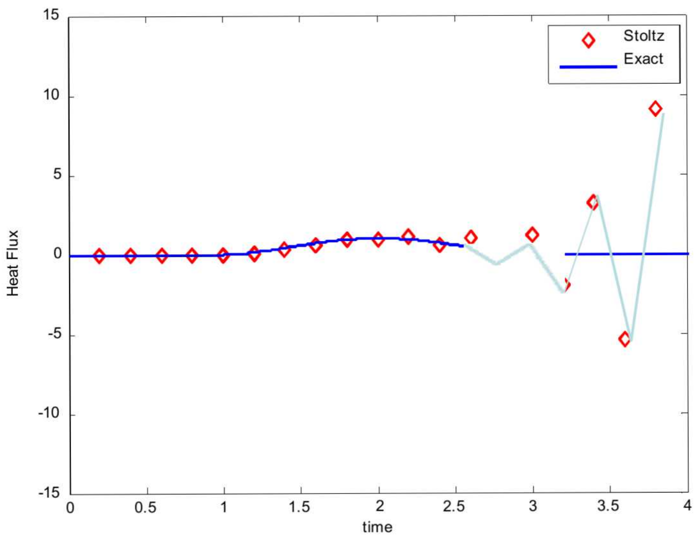


Stolz Method - $\Delta t = 0.25$



Stolz Method - Δt = 0.20

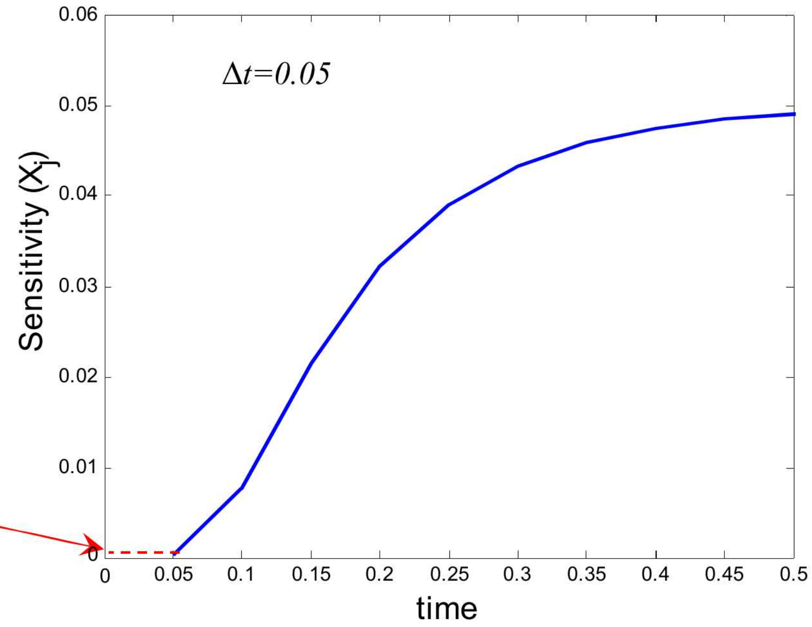




Ill-posed problem

- As time steps get ***smaller***, the inverse solution becomes more unstable
  - This is apparent from the Stolz algorithm and consideration of the X_1 term

$$\hat{q}_M = \frac{Y_M - \sum_{j=1}^{M-1} X_{M-j+1}\hat{q}_j + X_1\hat{q}_j}{X_1}$$



Function Specification Method

- To combat ill-posedness resulting from exact matching while retaining a sequential method, Beck developed the Function Specification Method
  - Assume a defining form for the unknown heat flux (piece-wise constant, piece-wise linear, etc)
  - Minimize sum of squared error between model-computed temperature and measurement
  - Consider limited subset of available data (say r time steps) beginning at current time t_M
  - Invoke temporary assumption that current variation of heat flux does not change

Function Specification Method(2)

- Assume simplest (piece-wise constant) q(t)
- Partition T(q) assuming q_1, …, q_{M-1} are known

$$
\begin{Bmatrix} T_1 \\ T_2 \\ \vdots \\ T_M \\ \vdots \\ T_{M+r-1} \end{Bmatrix}
=
\begin{bmatrix}
X_1 & 0 & 0 & \cdots & 0 & 0 \\
X_2 & X_1 & 0 & \cdots & 0 & 0 \\
\vdots & \vdots & \ddots & \ddots & 0 & \vdots \\
X_M & \cdots & X_2 & X_1 & 0 & 0 \\
\vdots & & & & \ddots & \\
X_N & X_{N-1} & \cdots & X_3 & X_2 & X_1
\end{bmatrix}
\begin{Bmatrix} q_1 \\ q_2 \\ \vdots \\ q_M \\ \vdots \\ q_{M+r-1} \end{Bmatrix}
$$

Function Specification Method (3)

$$
\begin{Bmatrix} T_M \\ T_{M+1} \\ \vdots \\ T_{M+r-1} \end{Bmatrix} = \begin{bmatrix} X_M & \cdots & X_3 & X_2 \\ X_{M+1} & \cdots & X_4 & X_3 \\ \vdots & & \vdots & \vdots \\ X_{M+r-1} & \cdots & X_{r+2} & X_{r+1} \end{bmatrix}_{rx(M-1)} \begin{Bmatrix} \hat{q}_1 \\ \hat{q}_2 \\ \vdots \\ \hat{q}_{M+r-1} \end{Bmatrix}_{1x(M-1)}
$$

Known components

$$
+ \begin{bmatrix} X_1 & 0 & 0 & 0 \\ X_2 & X_1 & 0 & 0 \\ \vdots & \vdots & \ddots & 0 \\ X_r & \cdots & X_2 & X_1 \end{bmatrix}_{rxr} \begin{Bmatrix} \hat{q}_M \\ \hat{q}_{M+1} \\ \vdots \\ \hat{q}_{M+r-1} \end{Bmatrix}_{rx1}
$$

Unknown components

$$
\mathbf{T}_{M \to M+r-1} = \mathbf{X}_{rxr} \hat{\mathbf{q}}_{M \to M+r-1} + \hat{\mathbf{T}}_{\hat{q}_1 \ldots \hat{q}_{M-1}}
$$

Function Specification (4)

- Final assumption is the *temporary* assumption that the assumed heat flux variation is unchanged over the next *r* time steps
- For the piece-wise constant assumption:

$$\hat{q}_M = \hat{q}_{M+1} = \cdots = \hat{q}_{M+r-1}$$

$$\hat{\mathbf{q}}_{M \to M+r-1} = [1 \quad 1 \quad \cdots \quad 1]_{rx1}^T \, \hat{q}_M$$

- So the model equation becomes

$$\mathbf{T}_{M \to M+r-1} = \mathbf{X}_{rxr}[1 \quad 1 \quad \cdots \quad 1]_{rx1}^T \, \hat{q}_M + \hat{\mathbf{T}}_{\hat{q}_1 \ldots \hat{q}_{M-1}}$$

Function Specification (5)

- Note

$$\mathbf{X}_{rxr}[1 \quad 1 \quad \cdots \quad 1]^T_{rx1} = \begin{Bmatrix} X_1 \\ X_1 + X_2 \\ \vdots \\ \sum_{i=1}^{M+r-1} X_i \end{Bmatrix} \equiv \mathbf{X}_r$$

- Now minimize the sum of squared errors:

$$S = \left(\mathbf{Y}_r - \mathbf{X}_r \hat{q}_M + \hat{T}\Big|_{\hat{q}_1 \cdots \hat{q}_{M-1}} \right)^T \left(\mathbf{Y}_r - \mathbf{X}_r \hat{q}_M + \hat{T}\Big|_{\hat{q}_1 \cdots \hat{q}_{M-1}} \right)$$

$$\frac{dS}{d\hat{q}_M} = 2\mathbf{X}_r^T \left(\mathbf{Y}_r - \mathbf{X}_r \hat{q}_M + \hat{T}\Big|_{\hat{q}_1 \cdots \hat{q}_{M-1}} \right) = 0$$

Function Specification (6)

- Finally, the estimation equation is obtained

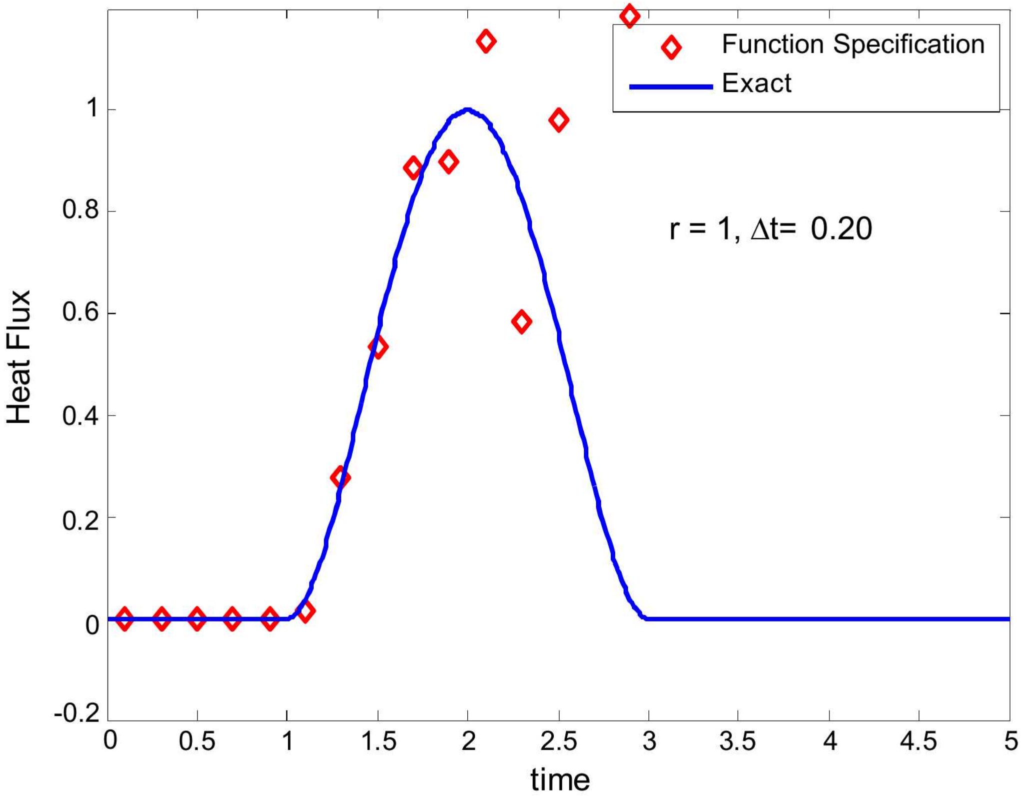
$$\mathbf{X}_r^T \left(\mathbf{Y}_r - \mathbf{X}_r \hat{q}_M + \hat{\mathbf{T}} \Big|_{\hat{q}_1 \cdots \hat{q}_{M-1}} \right) = 0$$

$$\hat{q}_M = \left(\mathbf{X}_r^T \mathbf{X}_r \right)^{-1} \left(\mathbf{X}_r^T \left(\mathbf{Y}_r - \hat{\mathbf{T}} \Big|_{\hat{q}_1 \cdots \hat{q}_{M-1}} \right) \right)$$

$$\hat{q}_M = \frac{\sum_{k=1}^{r} \left[\left(\sum_{i=1}^{k} X_i \right) \left(Y_{M+k-1} - \sum_{j=1}^{M-1} \hat{q}_j X_{M-j+k} \right) \right]}{\sum_{k=1}^{r} \left(\sum_{i=1}^{k} X_i \right)^2}$$

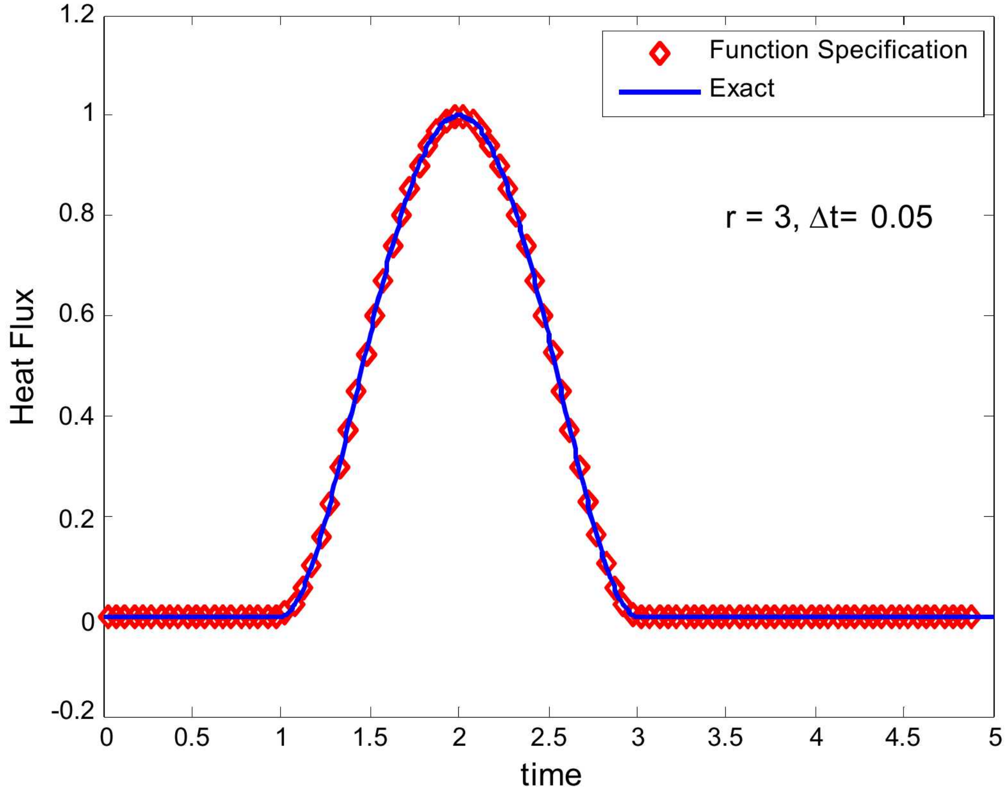
Example – Function Specification

- With r=1, this is the same as Stolz method:



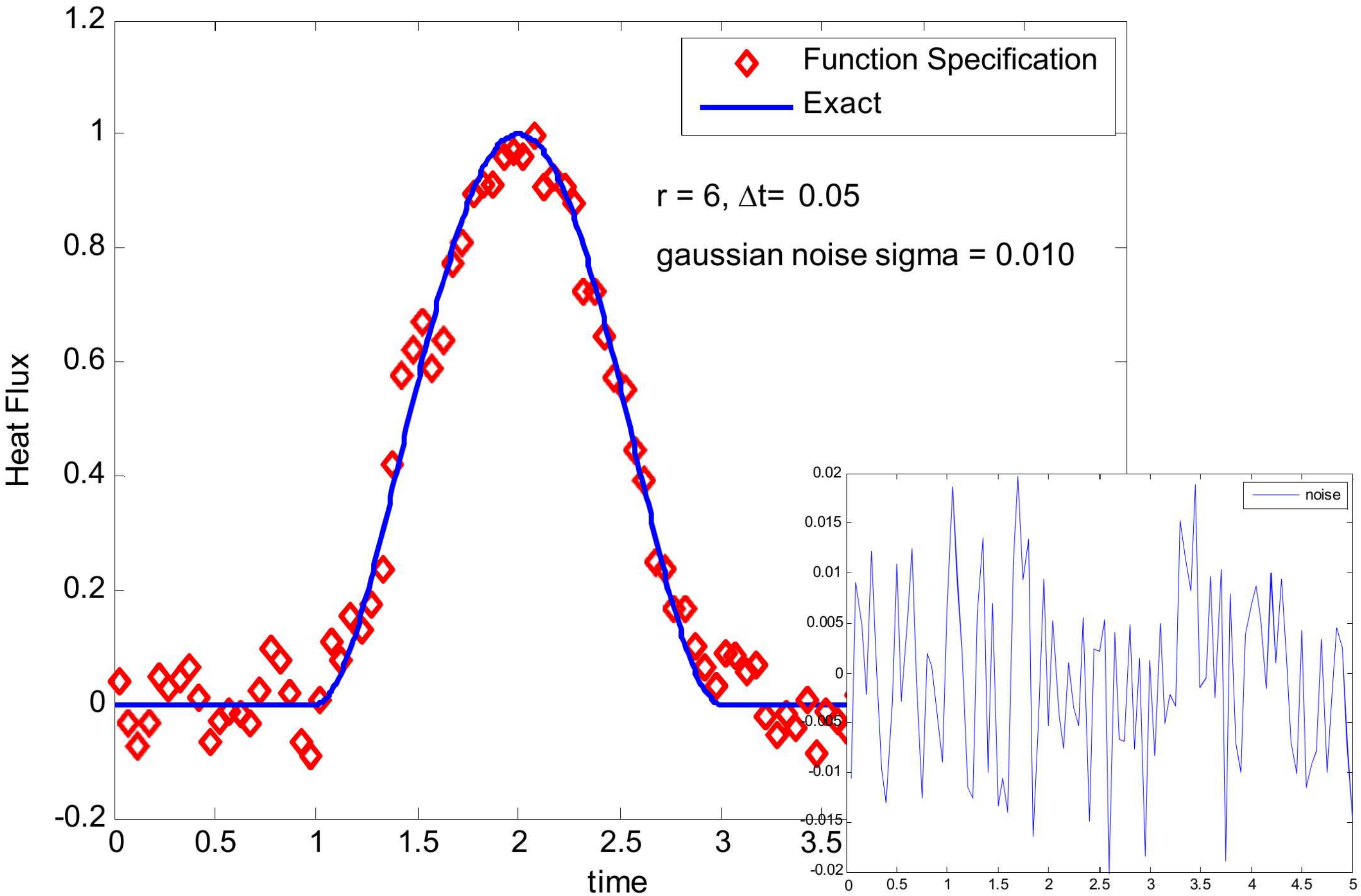
Example – Function Specification

- With r=3, dt can be much smaller:



Example – Function Specification

- With noisy data and r=6:



Tikhonov Regularization (1)

- Is a “batch processing” or whole time domain method
  - Contrasted with the sequential nature of Stolz or Function Specification Method
- Stabilizes the solution by penalizing unwanted variations in the solution for **q**
  - Zeroth order – penalizes function value
  - First order – penalizes function time derivative
  - Etc.

Tikhonov Regularization (2)

- Zeroth order (TR0) $S = (\mathbf{Y}-\mathbf{T})^T(\mathbf{Y}-\mathbf{T}) + \alpha_0 \mathbf{q}^T\mathbf{q}$
- First order (TR1) $S = (\mathbf{Y}-\mathbf{T})^T(\mathbf{Y}-\mathbf{T}) + \alpha_1 \mathbf{q}^T\mathbf{H}^T\mathbf{H}\mathbf{q}$

where ***H*** is a matrix operator the approximates the first time derivative, e.g.

$$\left(\frac{\partial q}{\partial t}\right) = \frac{1}{\Delta t}\begin{bmatrix} -1 & 1 & 0 & \cdots & 0 \\ 0 & -1 & 1 & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & 0 & \cdots & -1 & 1 \\ 0 & \cdots & 0 & 0 & 0 \end{bmatrix}\mathbf{q} \equiv \frac{1}{\Delta t}\mathbf{H}\mathbf{q}$$

– Note the $1/\Delta t$ is generally absorbed into the α_1

Tikhonov Regularization (3)

- Now minimizing the sum of squares with respect to the unknown *vector* **q**.

- For TR1:

$$\frac{dS}{d\mathbf{q}} = -2\mathbf{X}^T\left(\mathbf{Y} - \mathbf{Xq}\right)^T + 2\alpha_1\mathbf{H}^T\mathbf{Hq} = 0$$

$$2\mathbf{X}^T\left(\mathbf{Xq} - \mathbf{Y}\right) + 2\alpha_1\mathbf{H}^T\mathbf{Hq} = 0$$

$$\left(\mathbf{X}^T\mathbf{X} + \alpha_1\mathbf{H}^T\mathbf{H}\right)\mathbf{q} - \mathbf{X}^T\mathbf{Y} = 0$$

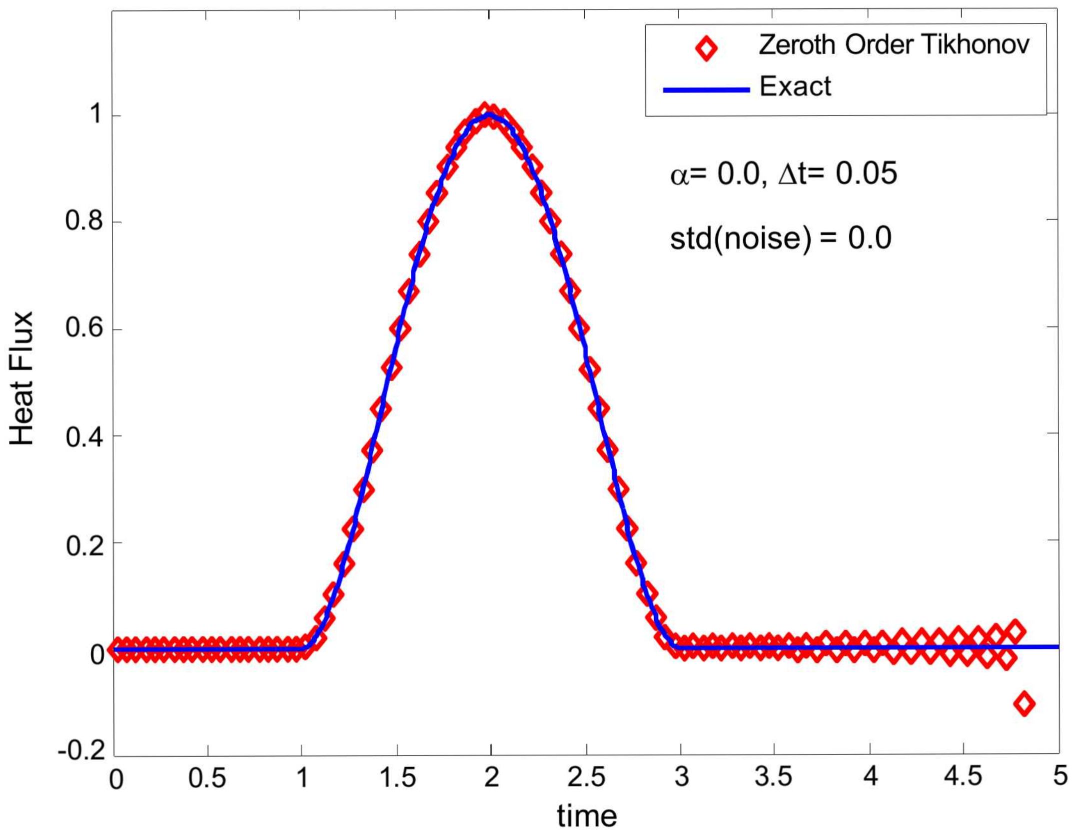
$$\hat{\mathbf{q}} = \left(\mathbf{X}^T\mathbf{X} + \alpha_1\mathbf{H}^T\mathbf{H}\right)^{-1}\mathbf{X}^T\mathbf{Y}$$

- For TR0:

$$\hat{\mathbf{q}} = \left(\mathbf{X}^T\mathbf{X} + \alpha_0\mathbf{I}\right)^{-1}\mathbf{X}^T\mathbf{Y}$$

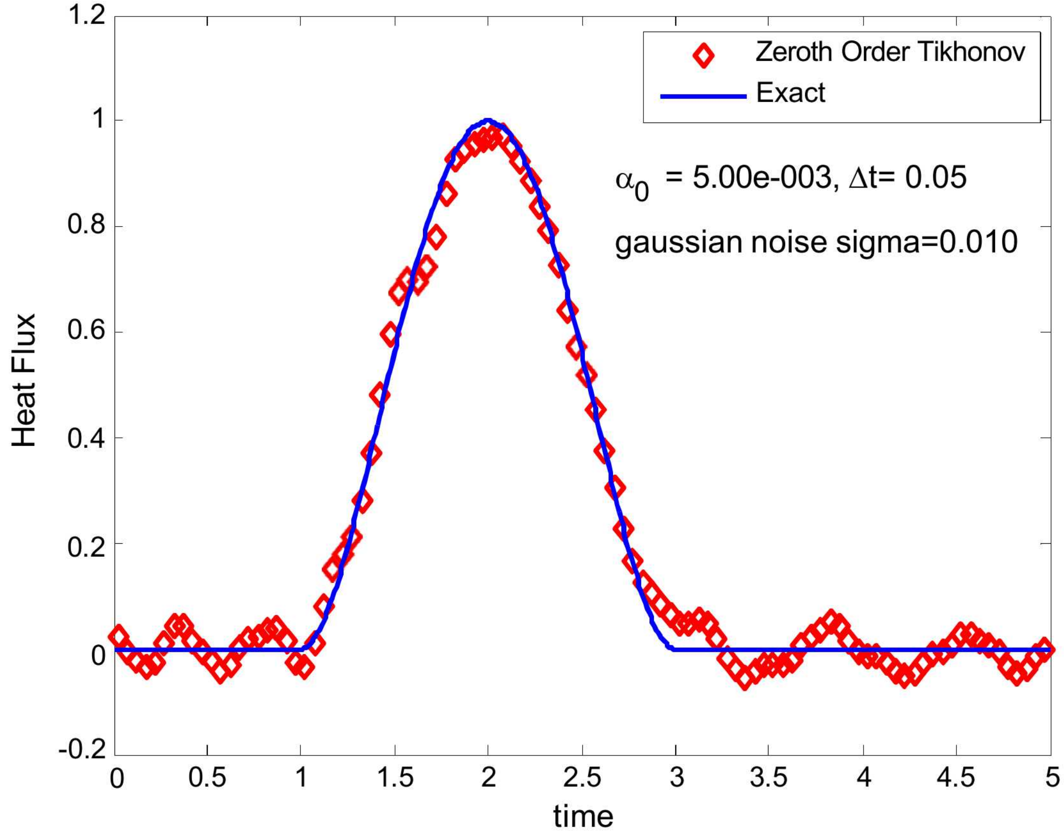
Tikhonov Regularization (4)

- Example – TR0 with no noise in data



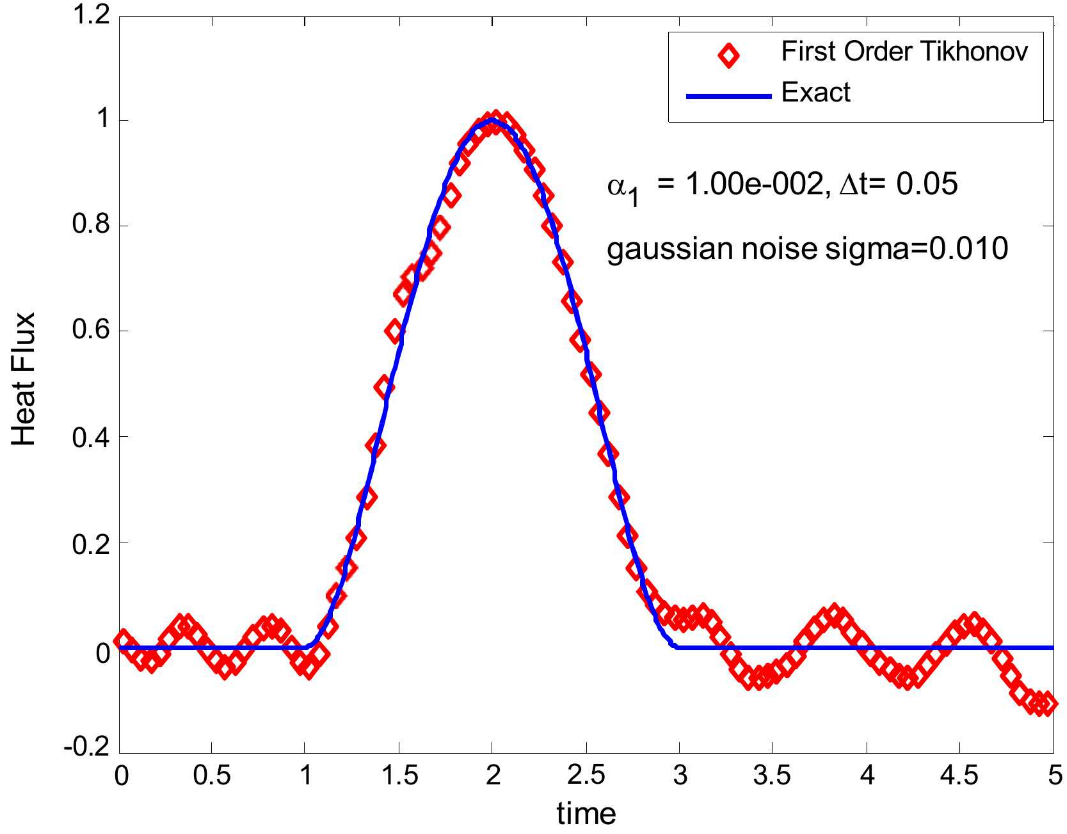
Tikhonov Regularization (5)

- Example – TR0 WITH noise in data



Tikhonov Regularization (6)

- Example – TR1 WITH noise in data



Singular Value Decomposition (SVD)

- Method is ostensibly a batch or whole time domain method
- Based on numerical decomposition of the coefficient matrix by standard techniques
- Regularization afforded by discarding near-zero entries in the coefficient matrix that causes the near singularity

SVD Method (1)

- Based on direct matching of the model equation to the data:

$$\mathbf{Y} = \mathbf{X}\mathbf{q}$$

- This is inverted directly to yield the estimates:

$$\hat{\mathbf{q}} = \mathbf{X}^{-1}\mathbf{Y}$$

- However, the entries of **X** can be small, leading to a near-singular matrix, which is a manifestation of the ill-posed nature of the inverse problem

SVD Method (2)

- To address the instability, the matrix **X** is first decomposed (or factored) using the singular value decomposition method into

$$X = \mathbf{UWV}^T$$

  - **U** is a column orthogonal matrix
  - **W** is a diagonal matrix of the *singular values*
  - **V** is another orthogonal matrix
- This decomposition is a built-in function call in MatLab:

$$\left[\mathbf{U},\mathbf{W},\mathbf{V}\right] = svd(X)$$

SVD Method (3)

- One benefit of SVD is that the inverse of the matrix is easily computed:

$$X^{-1} = \mathbf{V}\mathbf{W}^{-1}\mathbf{U}^{T}$$

  - Note that $\mathbf{W}^{-1}$ is easily computed since **W** is a diagonal matrix

$$\mathbf{W}^{-1} = \begin{bmatrix} 1/w_1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & 1/w_n \end{bmatrix}$$

SVD Method (4)

- Regularization in the SVD method is introduced by simply eliminating the *near-zero* (singular) values of the **W** matrix.
  - The singular values are ordered, largest to smallest, along the diagonal of **W** as a result of the SVD operation
- The corresponding columns of the **U** and **V** matrices are also discarded

SVD Method (5)

- If the first n_{eigen} values are retained

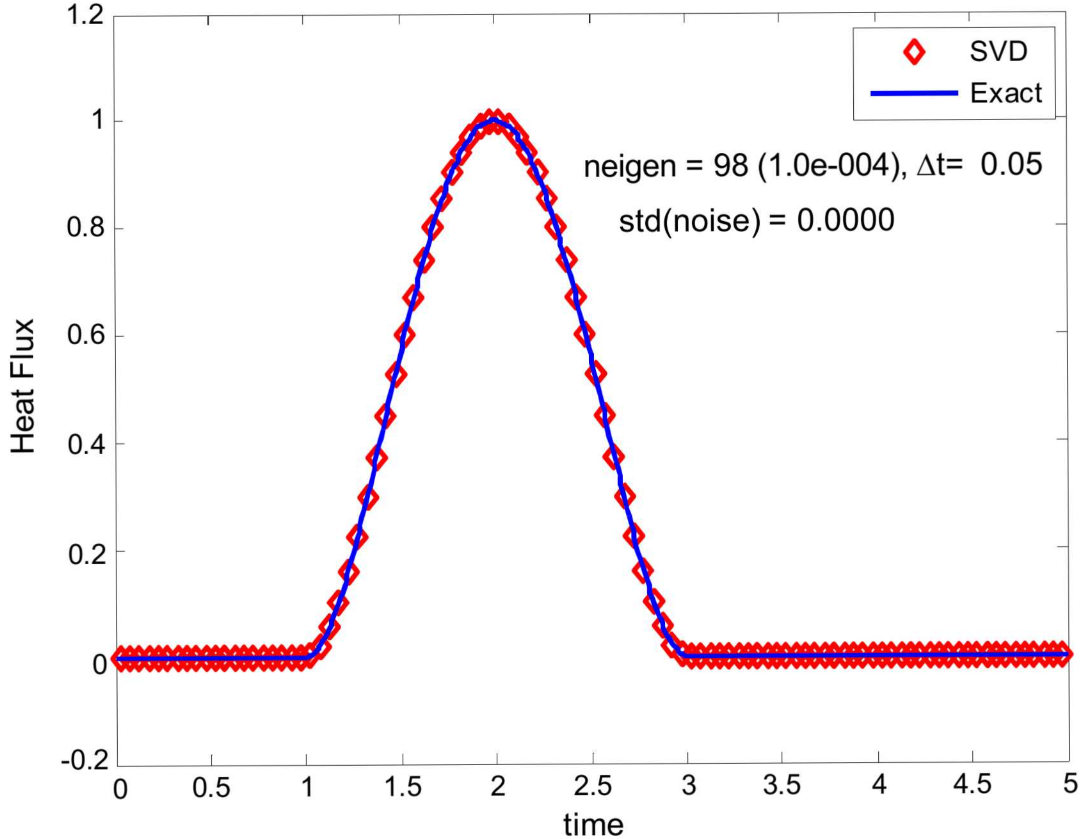
$$\mathbf{X}^{-1} \approx (\mathbf{V})_{Nxn_{eigen}} \left(\mathbf{W}^{-1}\right)_{n_{eigen}xn_{eigen}} \left(\mathbf{U}^{T}\right)_{n_{eigen}xN}$$

- Then the heat fluxes are estimated as

$$\hat{\mathbf{q}} \approx \left(\mathbf{V}_{Nxn_{eigen}}\right)\left(\mathbf{W}_{n_{eigen}xn_{eigen}}\right)^{-1}\left(\mathbf{U}_{n_{eigen}xN}\right)^{T}$$

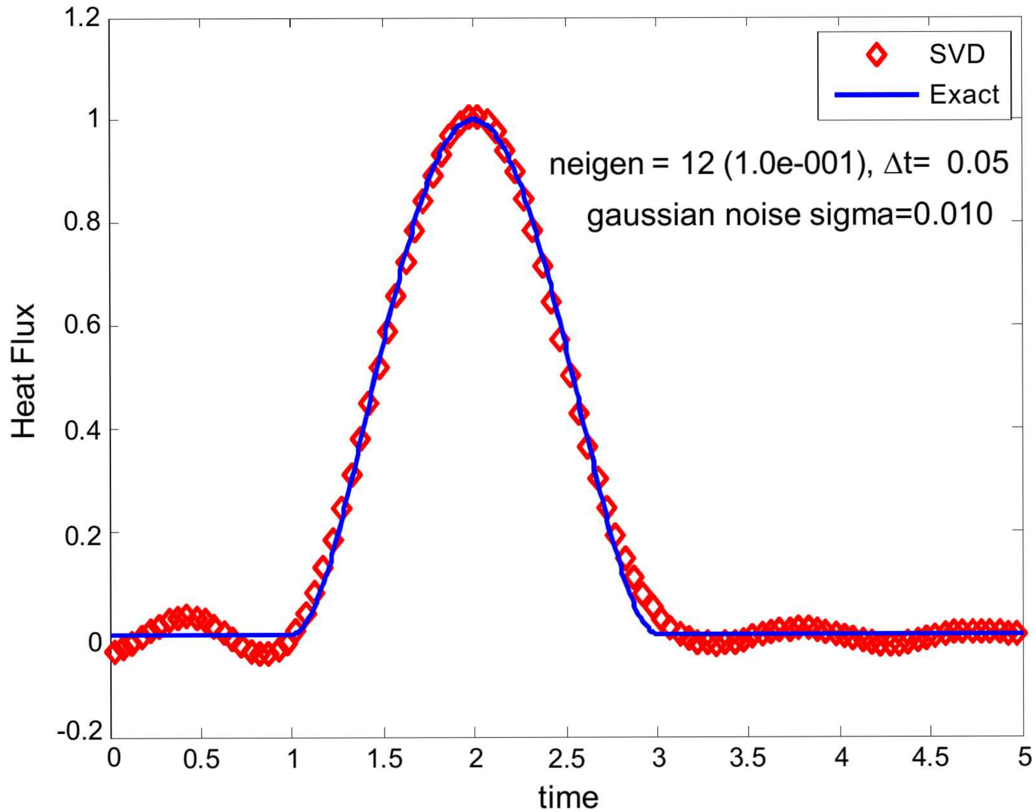
SVD Method (6)

- SVD with no noise in data



SVD Method (7)

- SVD with noise in data



Summary of Inverse Heat Conduction

- Inverse heat conduction is ill-posed
  - Solution is not unique (or may not exist)
  - Noise in data is amplified in solution
  - Exact matching (Stolz) goes unstable for *small* time steps
- All IHCP methods have an adjustable parameter to tame the instability:
  - Specify the functional form of q with future times (Beck)
  - Limit variation in q or dq/dt (Tikhonov)
  - Throw out eigenvalues that allow rapid variation in q-values (singular value decomposition)
- Parameter estimation perspective on IHCP:
  - Seek many parameters q_i -- tends to make **X** dependent
  - Thus $\mathbf{X}^T\mathbf{X}$ (or **X**) has a badly behaved inverse
  - IHCP methods improve $(\mathbf{X}^T\mathbf{X})^{-1}$ (or $\mathbf{X}^{-1}$) in some way

Acknowledgements

Functionally graded material example

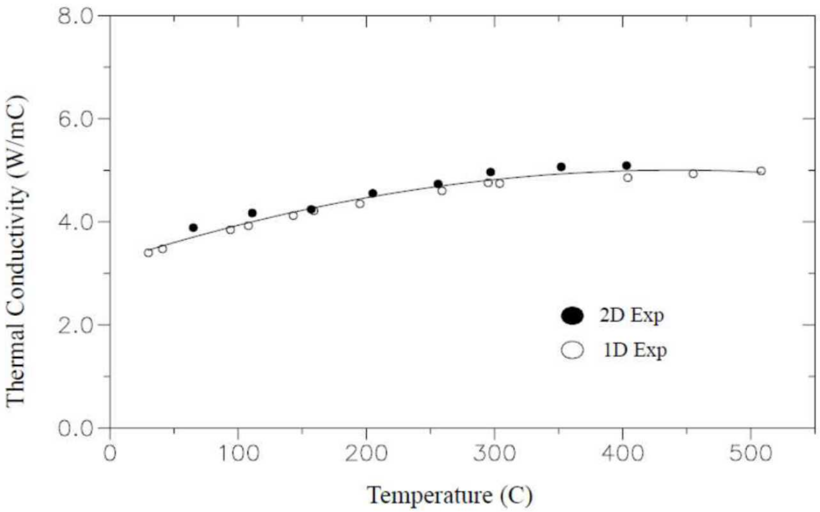
- National Aeronautics and Space Administration
- Paul Crittenden, University of Florida

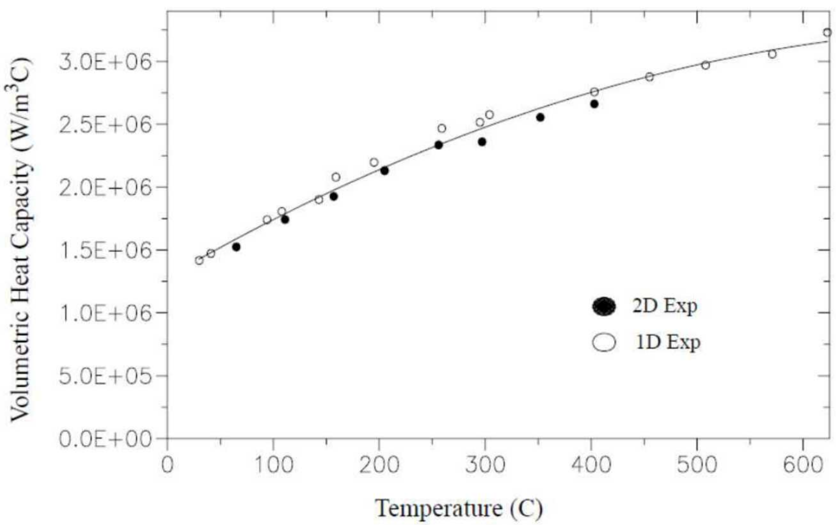
Quartic heating IHCP examples

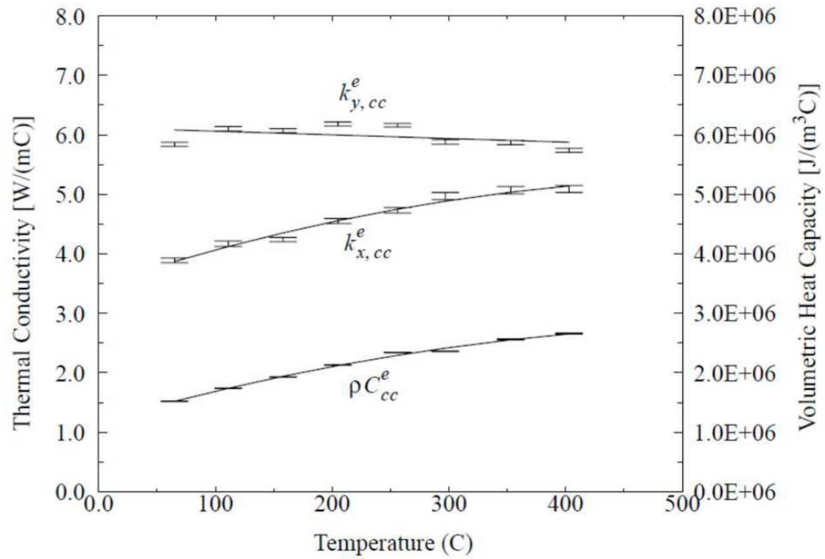
- Keith Woodbury, University of Alabama

Discussion/Questions

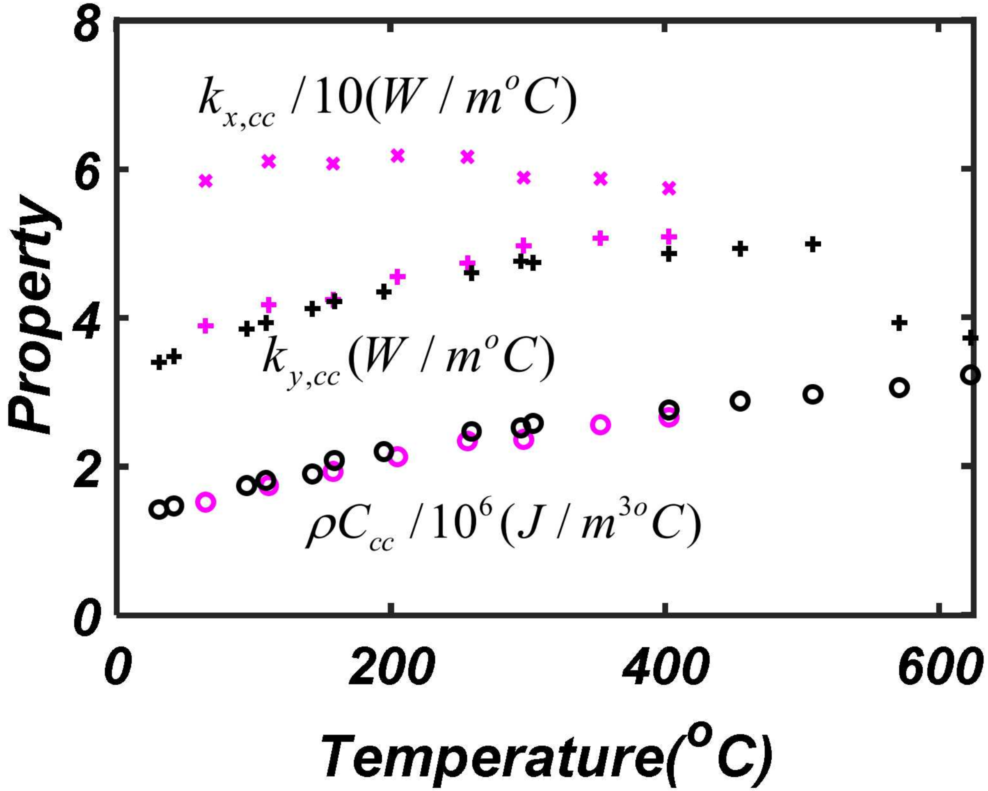
Back-ups


Thermal Conductivity (W/mC)
Temperature (C)
2D Exp
1D Exp
0.0
2.0
4.0
6.0
8.0
0
100
200
300
400
500


Volumetric Heat Capacity (W/m3C)
Temperature (C)
2D Exp
1D Exp
0.0E+00
5.0E+05
1.0E+06
1.5E+06
2.0E+06
2.5E+06
3.0E+06
0
100
200
300
400
500
600


Thermal Conductivity [W/(mC)]
Volumetric Heat Capacity [J/(m3C)]
Temperature (C)
$k^e_{y,cc}$
$k^e_{x,cc}$
ρC^e_{cc}
0.0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
0.0E+06
1.0E+06
2.0E+06
3.0E+06
4.0E+06
5.0E+06
6.0E+06
7.0E+06
8.0E+06
0.0
100
200
300
400
500

Temperature Dependent Properties



Estimates with 1D Exp

Estimates with 2D Exp

Sensitivity Coefficients for the one-dimensional experiment