STATISTICAL SOLUTION OF INVERSE PROBLEMS

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INVERSE PROBLEM

MAXIMUM LIKELIHOOD OBJECTIVE FUNCTION

$$S_{ML}(\mathbf{P}) = [\mathbf{Y} - \mathbf{T}(\mathbf{P})]^T \mathbf{W} [\mathbf{Y} - \mathbf{T}(\mathbf{P})]$$

where **P** = vector of unknown parameters
Y = vector of measured temperatures
T(**P**) = vector of estimated temperatures
W = Inverse of the covariance matrix of the measurements

INVERSE PROBLEM

Hypotheses:

- The errors are additive, with zero mean and normally distributed.
- The statistical parameters describing the errors are known.
- There are no errors in the independent variables.
- There is no prior information about **P**.

INVERSE PROBLEM

THE LEVENBERG-MARQUARDT METHOD

$$\mathbf{P}^{k+1} = \mathbf{P}^{k} + [\mathbf{J}^{T}\mathbf{W}\mathbf{J} + \lambda^{k}\mathbf{\Omega}^{k}]^{-1}\mathbf{J}^{T}\mathbf{W}[\mathbf{Y} - \mathbf{T}(\mathbf{P}^{k})]$$

where λ^k is the *damping parameter* and $\mathbf{\Omega}^k$ is a *diagonal matrix.*

- The Levenberg-Marquardt Method is related to ***Tikhonov's regularization*** approach.
- Compromise between steepest-descent method and Gauss' method.
- Simple, powerful and straightforward iterative procedure.
- Capable of treating complex physical situations.
- Easy to program.
- Stable and converges fast.

INVERSE PROBLEM

Remark: With the statistical hypotheses described above, the minimization of the least-squares norm yields *maximum likelihood* estimates, that is, the values estimated for the unknown parameters **P** are those most likely to produce the measured data **Y**.

Remark: Although very popular and useful in many situations, the minimization of the least-squares norm is a non-Bayesian estimator. A Bayesian estimator is basically concerned with the analysis of the *posterior probability density*, which is the conditional probability of the parameters **P** given the measurements **Y.**

INVERSE PROBLEM

BAYES' FORMULA

$$\pi_{posterior}(\mathbf{P}) = \pi(\mathbf{P}|\mathbf{Y}) = \frac{\pi_{prior}(\mathbf{P})\pi(\mathbf{Y}|\mathbf{P})}{\pi(\mathbf{Y})}$$

Where: $\pi_{posterior}(\mathbf{P})$ = posterior probability density (conditional probability of the parameters **P** given the measurements **Y**)

$\pi_{prior}(\mathbf{P})$ = prior density (information about the parameters prior to the measurements)

$\pi(\mathbf{Y}|\mathbf{P})$ = likelihood function (expresses the likelihood of different measurement outcomes **Y** with **P** given)

$\pi(\mathbf{Y})$ = probability density of the measurements (normalizing constant)

$$posterior \propto prior \times likelihood$$

<u>INVERSE PROBLEM</u>

The **<u>statistical inversion approach</u>** is based on the following principles:

1. All variables included in the model are modeled as random variables.
2. The randomness describes our degree of information concerning their realizations.
3. The degree of information concerning these values is coded in the probability distributions.
4. The solution of the inverse problem is the posterior probability distribution.

• Jari P. Kaipio and Erkki Somersalo, *Computational and Statistical Methods for Inverse Problems*, Springer, 2004.

• S. Tan, C. Fox, G. Nicholls, *Inverse Problems*, Course Notes for Physics 707, University of Auckland

EXAMPLE

- Heat Flux: $q(t)$
- Thermal Conductivity: $k(T) = B_1 + B_2 e^{-T/B_3}$
- Volumetric Heat Capacity: $C(T) = A_1 + A_2 e^{-T/A_3}$

$$\mathbf{P} = [q_1, q_2, \ldots, q_I, A_1, A_2, A_3, B_1, B_2, B_3]$$

INVERSE PROBLEM

Hypotheses:

- The errors are additive, with zero mean and normally distributed.
- The statistical parameters describing the errors are known.
- There are no errors in the independent variables.
- **P** is a random vector with known mean μ and known covariance matrix **V**.
- **P** is distributed normally and is independent of **Y**.

MAXIMUM A POSTERIORI

Likelihood

$$\pi(\mathbf{Y}|\mathbf{P}) = (2\pi)^{-I/2}\left|\mathbf{W}^{-1}\right|^{-1/2}\exp\left[-\frac{1}{2}(\mathbf{Y}-\mathbf{T})^T\mathbf{W}(\mathbf{Y}-\mathbf{T})\right]$$

where I = number of observations
$\mathbf{W}$ = inverse of the covariance matrix of the measurements

For uncorrelated measurements:

$$\mathbf{W} = \begin{bmatrix} 1/\sigma_1^2 & & & 0 \\ & 1/\sigma_2^2 & & \\ & & \ddots & \\ 0 & & & 1/\sigma_I^2 \end{bmatrix}$$

MAXIMUM A POSTERIORI

Normal Prior

$$\pi(\mathbf{P}) = (2\pi)^{-N/2} \left|\mathbf{V}\right|^{-1/2} \exp\left[-\frac{1}{2} (\mathbf{P} - \boldsymbol{\mu})^T \mathbf{V}^{-1} (\mathbf{P} - \boldsymbol{\mu}) \right]$$

where N = number of parameters
$\boldsymbol{\mu}$ = known mean for **P**
V = known covariance matrix for **P**

Bayes' Formula:

$$\pi_{posterior}(\mathbf{P}) = \pi(\mathbf{P}|\mathbf{Y}) \propto \pi_{prior}(\mathbf{P})\pi(\mathbf{Y}|\mathbf{P})$$

MAXIMUM A POSTERIORI

$$\ln\left[\pi(\mathbf{P}\,|\,\mathbf{Y})\right] = -\frac{1}{2}\left[(I+N)\ln 2\pi + \ln|\mathbf{W}^{-1}| + \ln|\mathbf{V}| + S_{MAP}\right]$$

Maximum a Posteriori Objective Function

$$S_{MAP}(\mathbf{P}) = \left[\mathbf{Y}-\mathbf{T}(\mathbf{P})\right]^T \mathbf{W}\left[\mathbf{Y}-\mathbf{T}(\mathbf{P})\right] + (\mu-\mathbf{P})^T\,\mathbf{V}^{-1}(\mu-\mathbf{P})$$

MAXIMUM A POSTERIORI

For the minimization of $S_{MAP}(\mathbf{P})$:

$$\frac{\partial S_{MAP}(\mathbf{P})}{\partial P_1} = \frac{\partial S_{MAP}(\mathbf{P})}{\partial P_2} = \cdots = \frac{\partial S_{MAP}(\mathbf{P})}{\partial P_N} = 0$$

$$\boxed{-2\,\mathbf{J}^T\,\mathbf{W}[\mathbf{Y}-\mathbf{T}(\mathbf{P})] - 2\mathbf{V}^{-1}[\mu - \mathbf{P}] = 0}$$

where **J** is the *Sensitivity Matrix*.

MAXIMUM A POSTERIORI

$$-2\,\mathbf{J}^T\mathbf{W}[\mathbf{Y}-\mathbf{T}(\mathbf{P})]-2\mathbf{V}^{-1}[\mu-\mathbf{P}]=0$$

Linear Problems: $\mathbf{J}$ does not depend on $\mathbf{P}$ ⇨ $\mathbf{T}(\mathbf{P})=\mathbf{J}\,\mathbf{P}$

$$\mathbf{P}=[\mathbf{J}^T\mathbf{W}\,\mathbf{J}+\mathbf{V}^{-1}]^{-1}[\mathbf{J}^T\mathbf{W}\,\mathbf{Y}+\mathbf{V}^{-1}\mu]$$

Nonlinear Problems: $\mathbf{J}\equiv\mathbf{J}(\mathbf{P})$ ⇨ $\mathbf{T}(\mathbf{P})=\mathbf{T}(\mathbf{P}^k)+\mathbf{J}^k(\mathbf{P}-\mathbf{P}^k)$

$$\mathbf{P}^{k+1}=\mathbf{P}^k+[\mathbf{J}^T\mathbf{W}\mathbf{J}+\mathbf{V}^{-1}]^{-1}\{\mathbf{J}^T\mathbf{W}[\mathbf{Y}-\mathbf{T}(\mathbf{P}^k)]+\mathbf{V}^{-1}(\mu-\mathbf{P}^k)\}$$

SEQUENTIAL PARAMETER ESTIMATION TECHNIQUE

- Utilizes the measurements in a sequential manner in order to estimate the parameters.
- Avoids matrix inversions.
- Permits the identification of improper mathematical models.
- Possible to identify if a sufficient number of transient measurements and if a sufficiently long experimental time have been used in the experiment.

COMPUTATIONAL ALGORITHM FOR THE NONLINEAR CASE

Step 1. Initialize the iterative procedure by setting the iteration index k to 0 and making $\mathbf{P}^0 = \mu$.

Step 2. Compute the estimate for the vector of unknown parameters sequentially, for i=0,…,(I-1), by using

$$\mathbf{A} = \mathbf{V}_i \mathbf{J}_{i+1}^T$$

$$\Delta = \mathbf{J}_{i+1} \mathbf{A} + W_{i+1}^{-1}$$

$$\mathbf{K} = \mathbf{A}\Delta^{-1}$$

$$E_{i+1} = Y_{i+1} - T_{i+1}(\mathbf{P}^k)$$

$$\mathbf{P}_{i+1}^{k+1} = \mathbf{P}_i^{k+1} + \mathbf{K}[E_{i+1} - \mathbf{J}_{i+1}(\mathbf{P}_i^{k+1} - \mathbf{P}^k)]$$

$$\mathbf{V}_{i+1} = \mathbf{V}_i - \mathbf{K}\mathbf{J}_{i+1}\mathbf{V}_i$$

COMPUTATIONAL ALGORITHM FOR THE NONLINEAR CASE

Step 3. Check convergence of the values estimated sequentially with all I measurements

$$\left\| \mathbf{P}_I^{k+1} - \mathbf{P}_I^k \right\| < \varepsilon$$

If the convergence criterion is not satisfied, increment k, make

$$\mathbf{P}^k = \mathbf{P}_I^k$$

and return to step 2.

SAMPLED SOLUTIONS TO INVERSE PROBLEMS

- In many cases, the Posterior Probability Distribution is analytically intractable, p. ex., if the prior probability distribution involves information which is difficult to express in analytic terms.
- Draw samples from the set $\boldsymbol{\Omega}$ of all possible **P**'s, each sample with probability $\pi(\mathbf{P}|\mathbf{Y})$.
- Get a set $\Theta = \{\mathbf{P}_1, \mathbf{P}_2, \ldots, \mathbf{P}_M\}$ of samples distributed like the posterior distribution.
- Inference on $\pi(\mathbf{P}|\mathbf{Y})$ becomes inference on $\Theta = \{\mathbf{P}_1, \mathbf{P}_2, \ldots, \mathbf{P}_M\}$, for example the mean of the samples in Θ give us an estimation of the average values of $\pi(\mathbf{P}|\mathbf{Y})$.
- We generally need the constant that normalizes the probability distribution to sample: **MARKOV CHAIN MONTE-CARLO METHODS**

4. MARKOV CHAIN MONTE CARLO METHODS

METROPOLIS-HASTINGS ALGORITHM

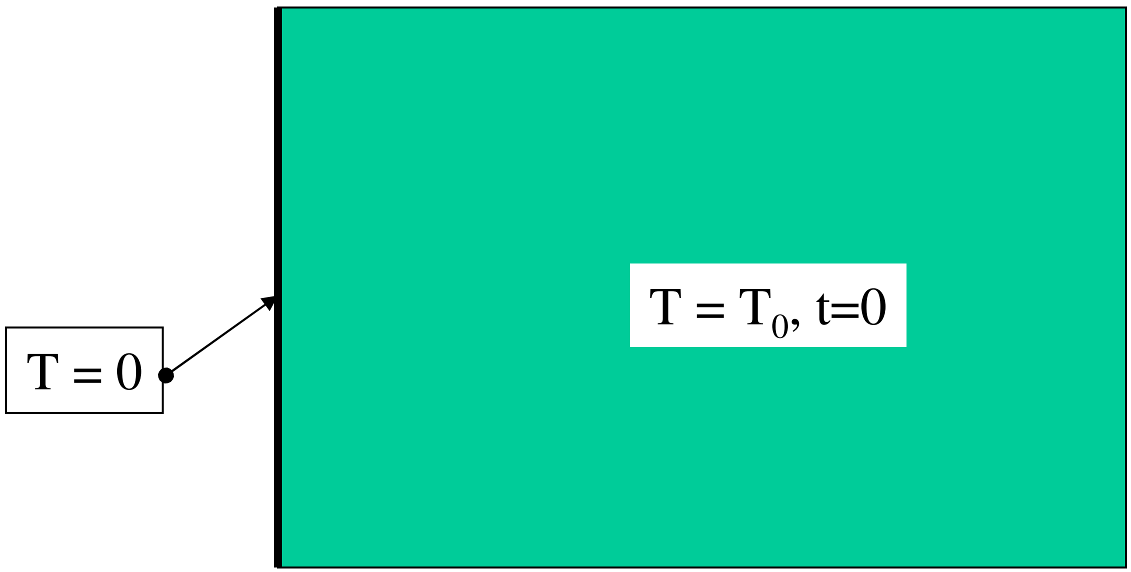
1. Sample a *Candidate Point* $\mathbf{P}^*$ from a jumping distribution $q(\mathbf{P}^*,\mathbf{P}^{(t-1)})$.
2. Calculate:

$$\alpha = \min\left[1, \frac{\pi(\mathbf{P}^* \mid \mathbf{Y})\, q(\mathbf{P}^{(t-1)}, \mathbf{P}^*)}{\pi(\mathbf{P}^{(t-1)} \mid \mathbf{Y})\, q(\mathbf{P}^*, \mathbf{P}^{(t-1)})}\right]$$

3. Generate a random value U which is uniformly distributed on (0,1).
4. If $U \leq \alpha$, define $\mathbf{P}^{(t)} = \mathbf{P}^*$; otherwise, define $\mathbf{P}^{(t)} = \mathbf{P}^{(t-1)}$.
5. Return to step 1 in order to generate the sequence $\{\mathbf{P}^{(1)}, \mathbf{P}^{(2)}, \ldots, \mathbf{P}^{(n)}\}$.

Remark: Ignore $\mathbf{P}^{(i)}$ until the chain has reached equilibrium.

EXAMPLE



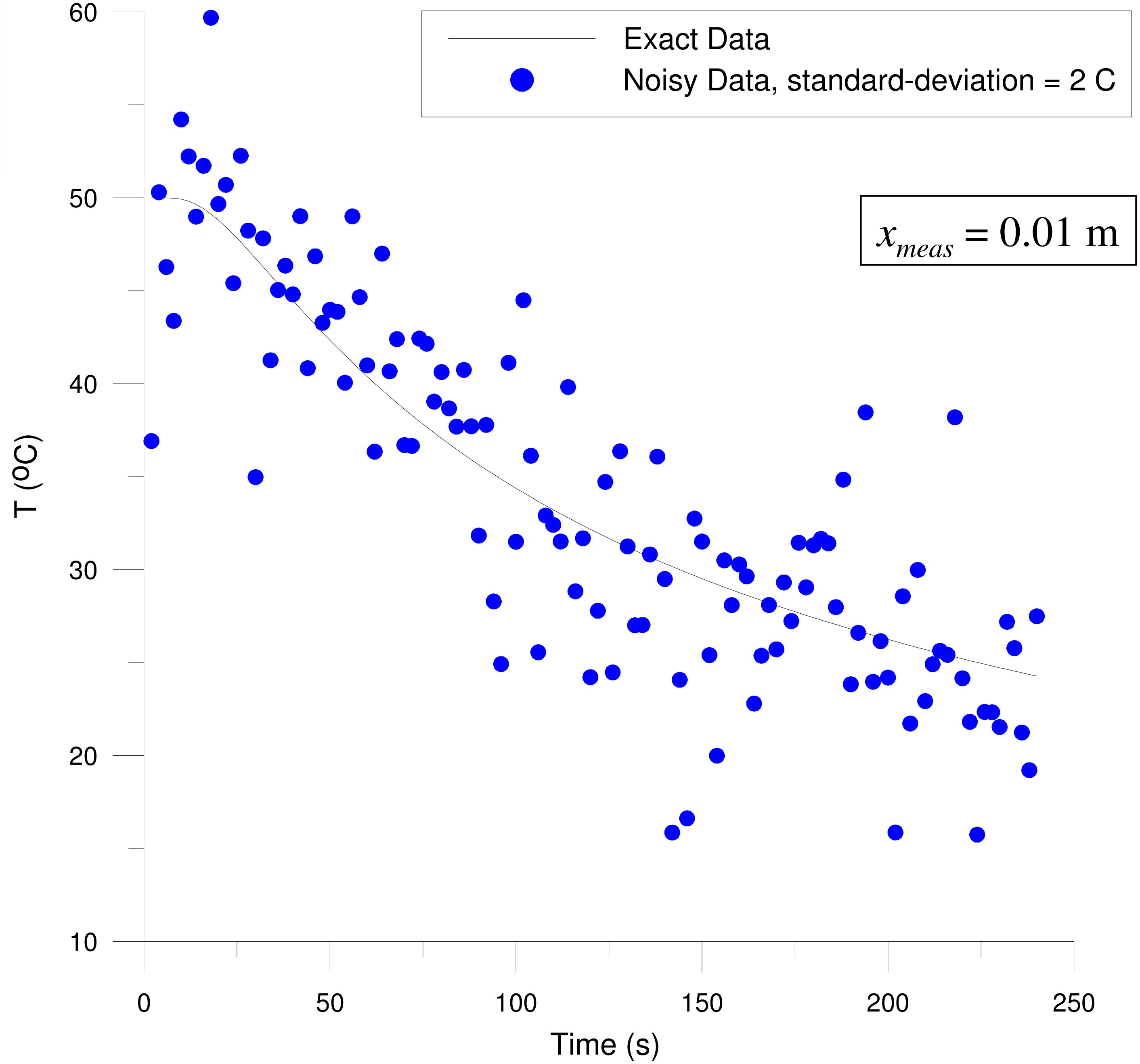
$$T(x,t) = T_0 \, erf\left(\frac{x}{\sqrt{4\alpha t}}\right)$$

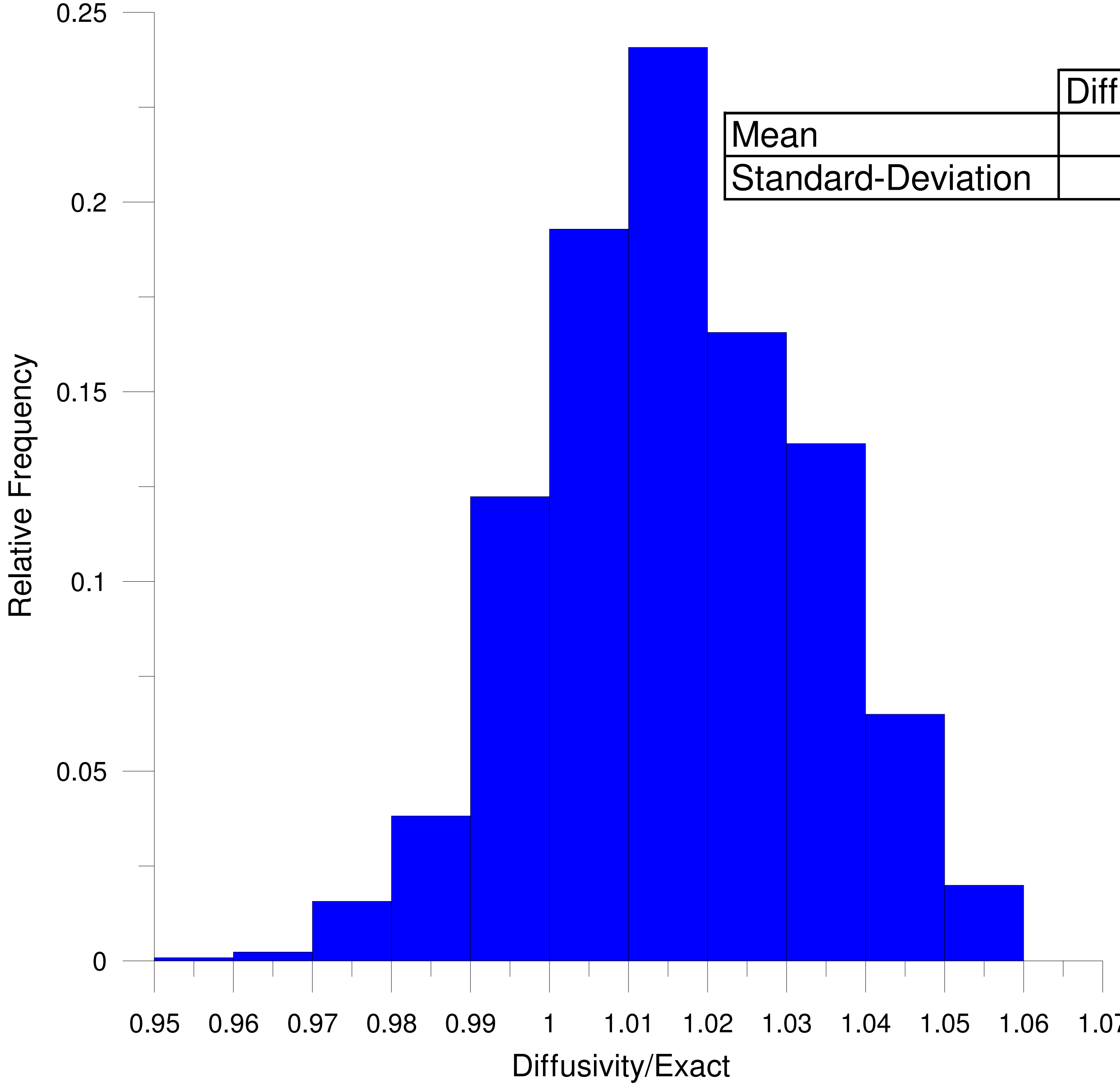
$T_0 = 50\ ^oC$

Concrete: $\alpha = 4.9 \times 10^{-7}\ m^2/s$

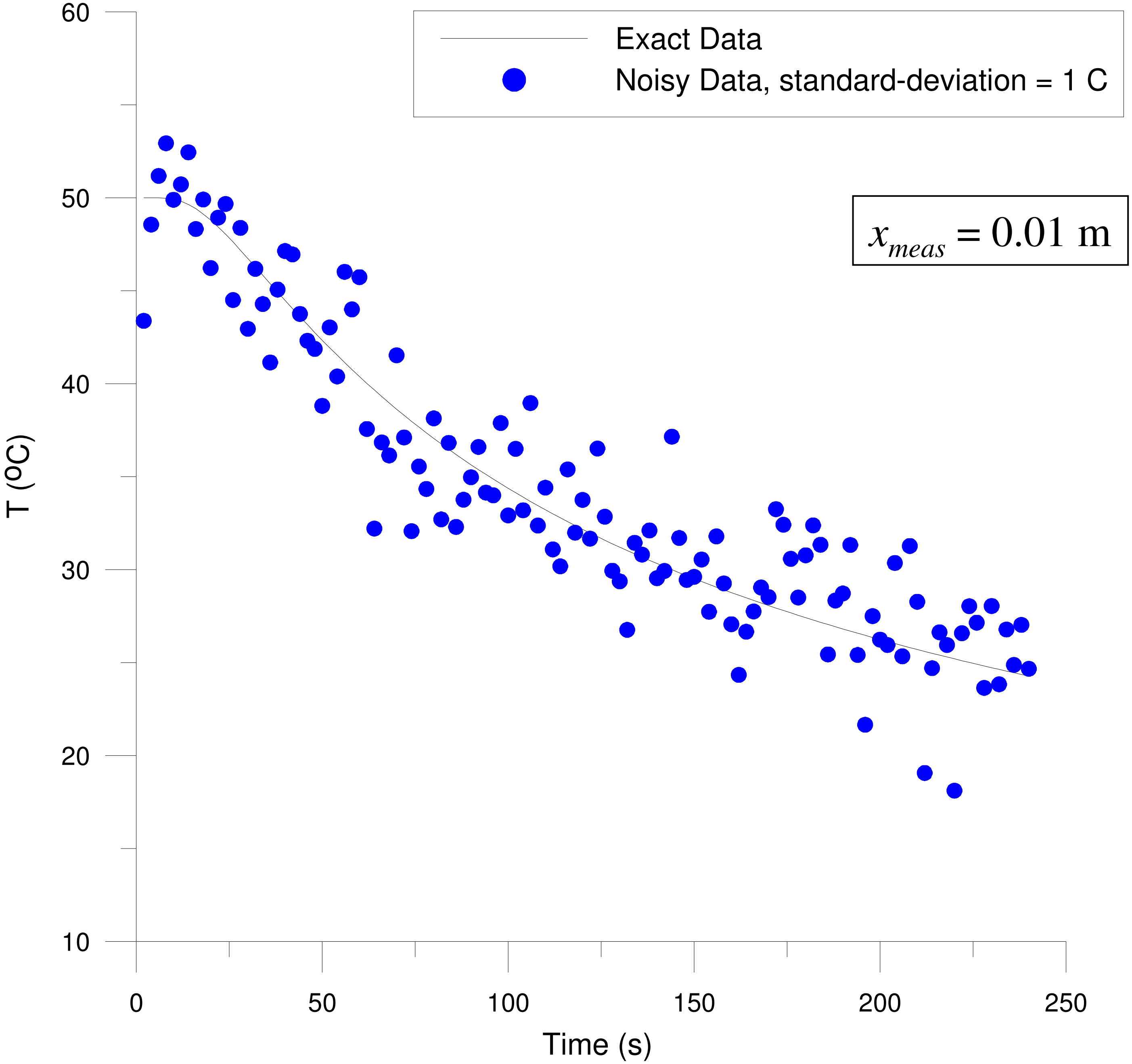
EXAMPLE

- Estimation of α.
- Prior for α: Uniform distribution $(10^{-7},10^{-5})$ m^2/s.
- Start the chain in the middle of the interval.

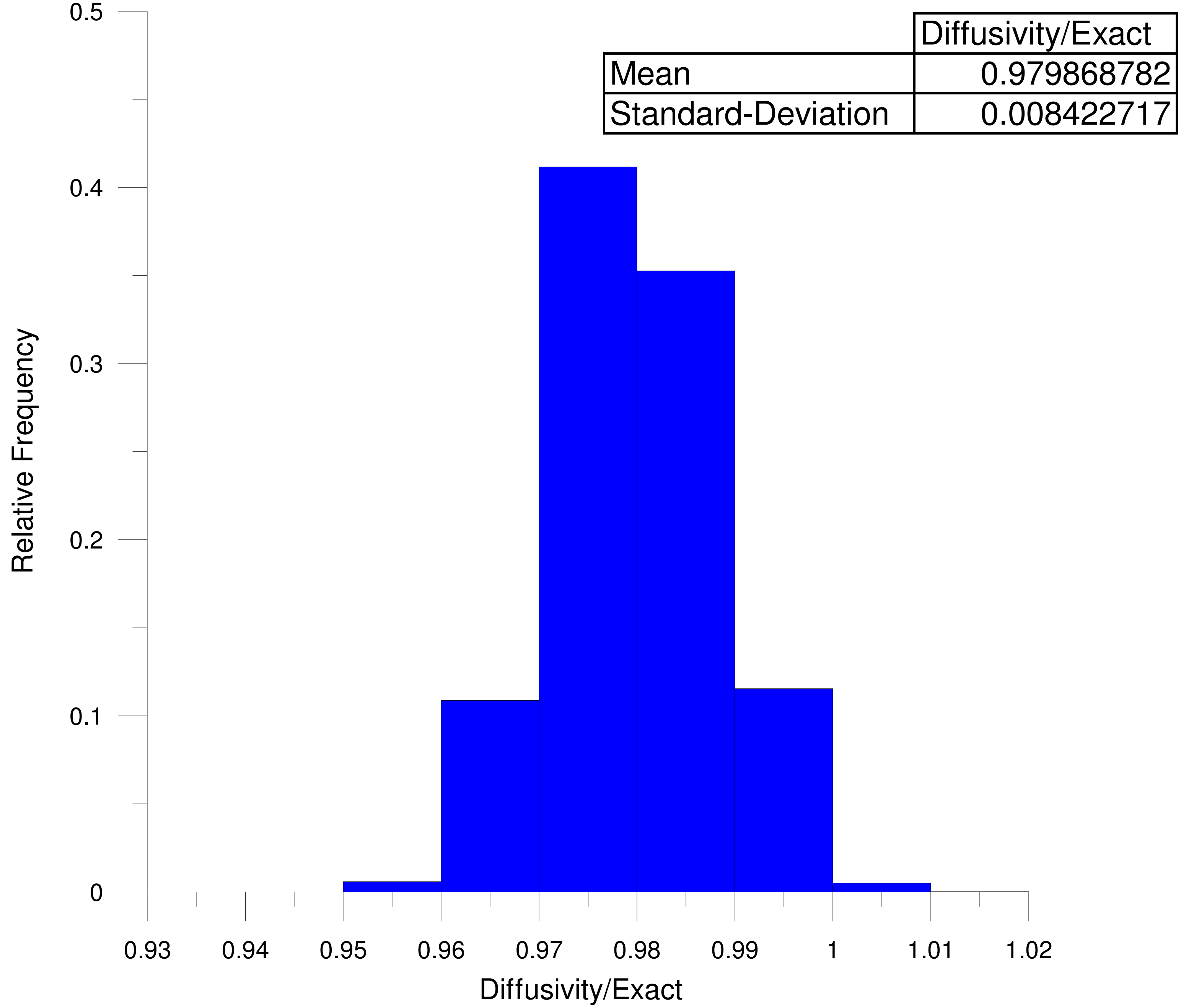

Exact Data
Noisy Data, standard-deviation = 2 C
$x_{meas} = 0.01$ m
T (ºC)
Time (s)
10
20
30
40
50
60
0
50
100
150
200
250



	Diffusivity/Exact
Mean	1.016224796
Standard-Deviation	0.017660818



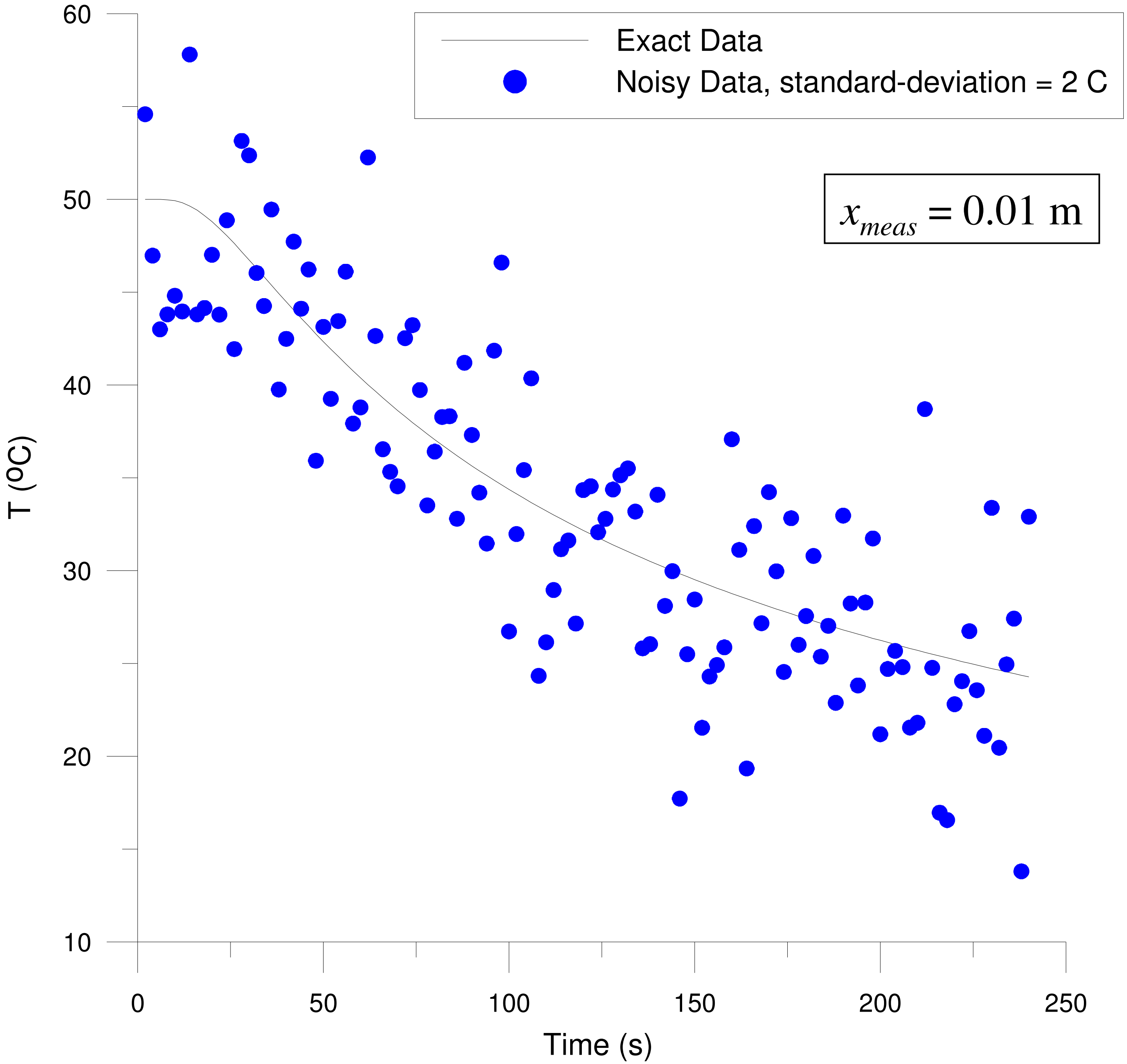
Exact Data
Noisy Data, standard-deviation = 1 C
$x_{meas} = 0.01$ m
T (ºC)
Time (s)
60
50
40
30
20
10
0
50
100
150
200
250

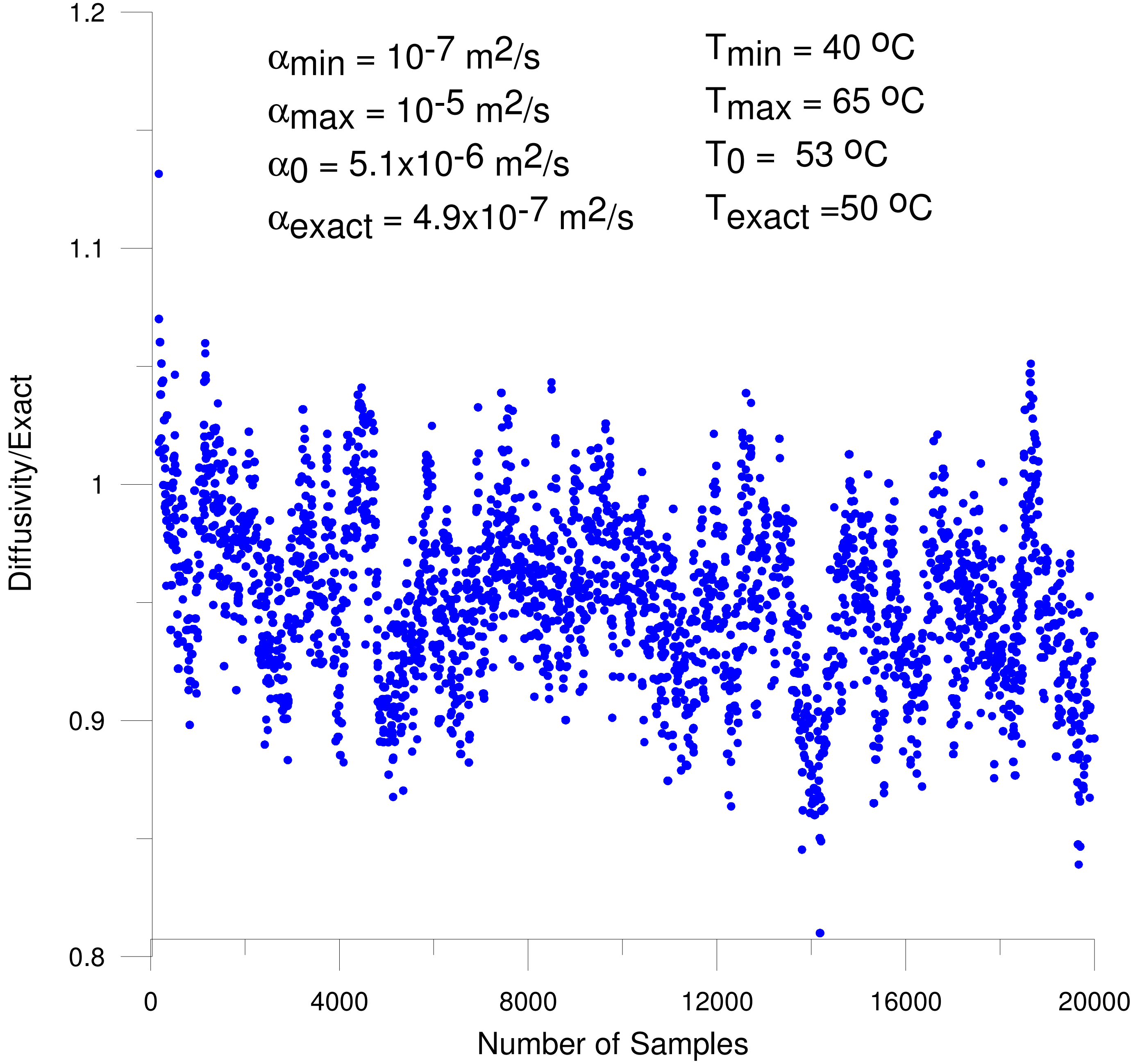


Diffusivity/Exact
Mean
0.979868782
Standard-Deviation
0.008422717
Relative Frequency
0.5
0.4
0.3
0.2
0.1
0
0.93
0.94
0.95
0.96
0.97
0.98
0.99
1
1.01
1.02
Diffusivity/Exact

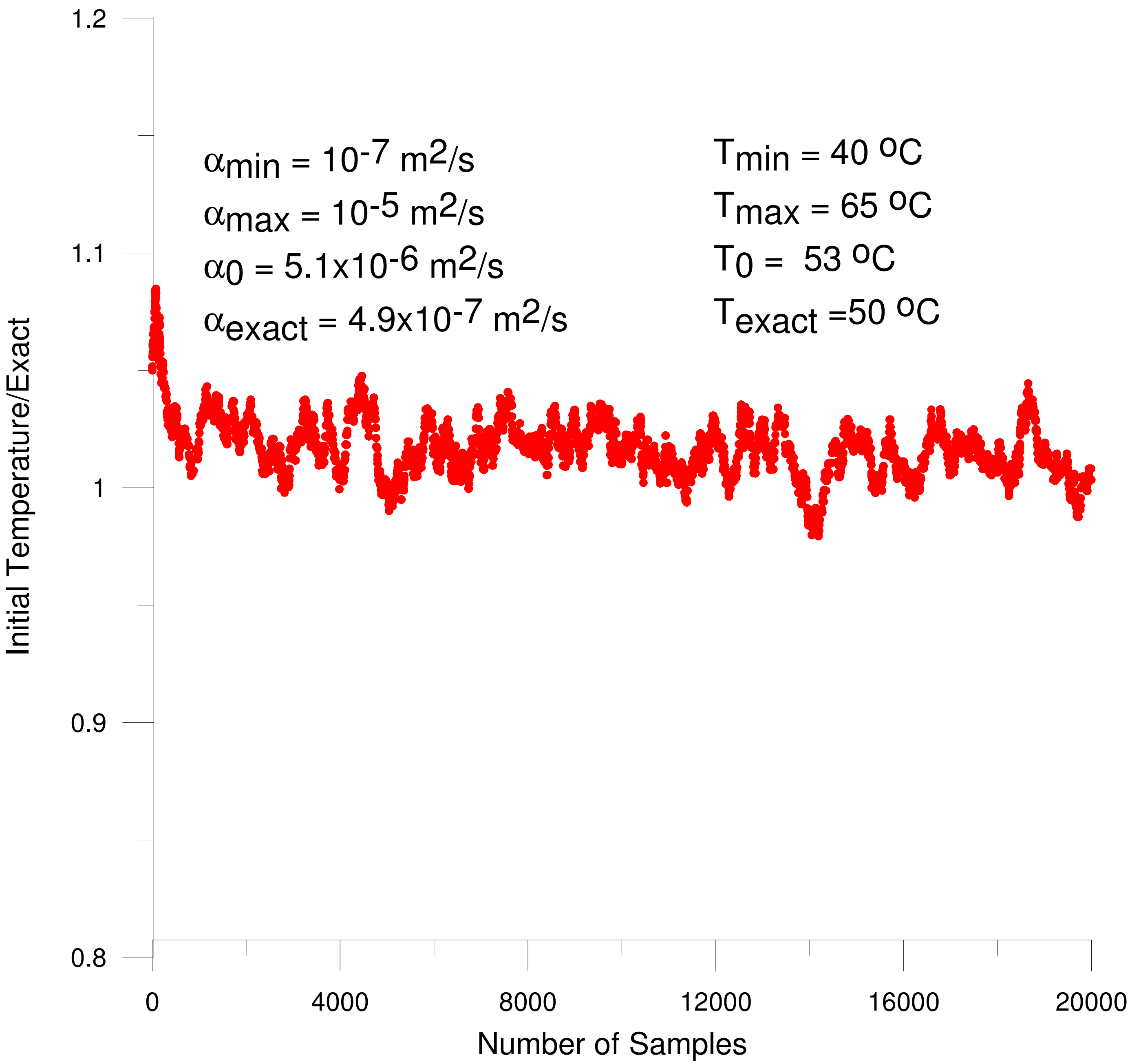
EXAMPLE

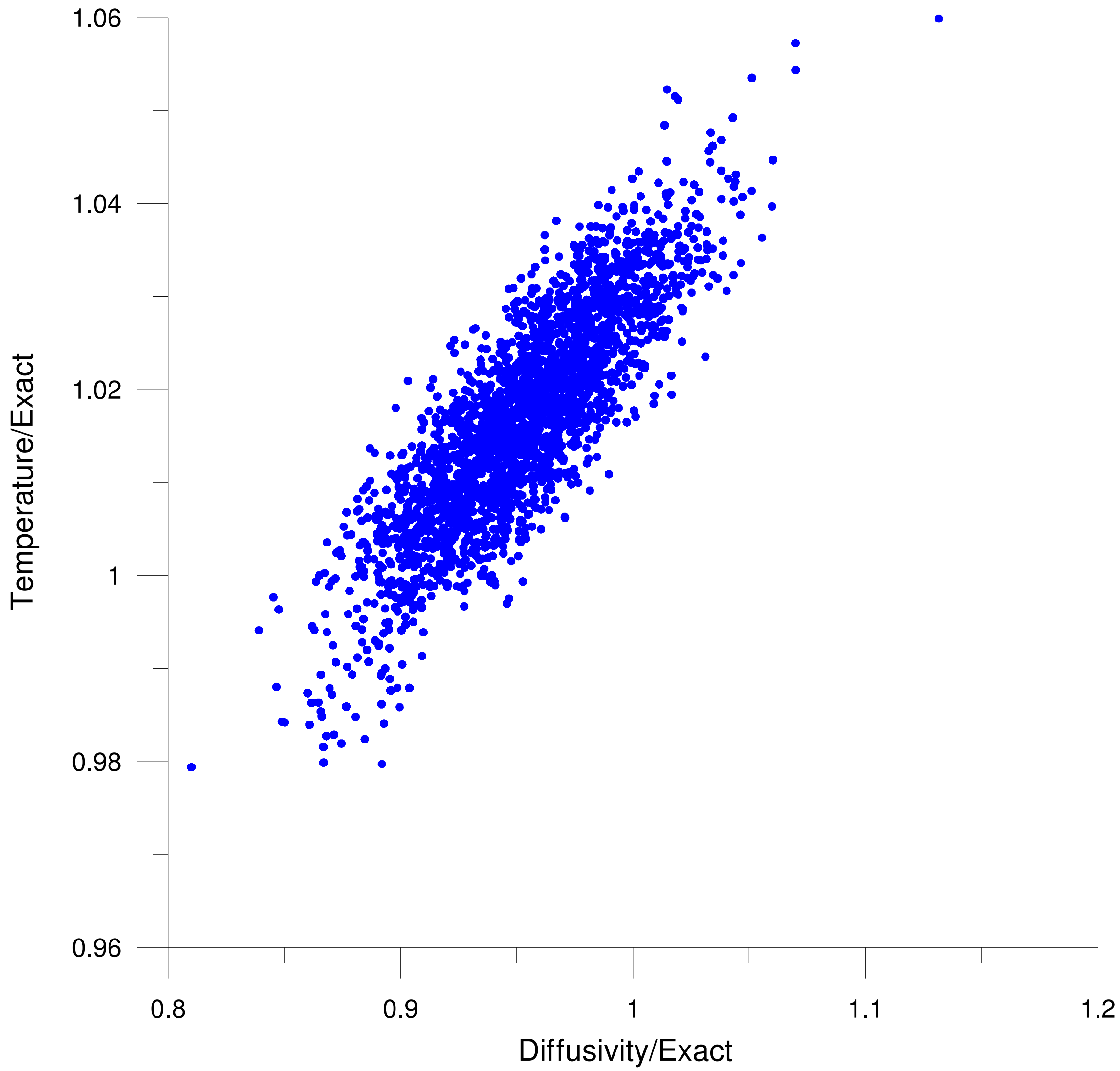
- Simultaneous estimation of T_0 and α.
- Prior for T_0 : Uniform distribution (40, 65) ^oC
- Prior for α: Uniform distribution $(10^{-7},10^{-5})$ m^2/s
- Start the chain in the middle of the intervals


Exact Data
Noisy Data, standard-deviation = 2 C
$x_{meas} = 0.01$ m
T (°C)
Time (s)
60
50
40
30
20
10
0
50
100
150
200
250

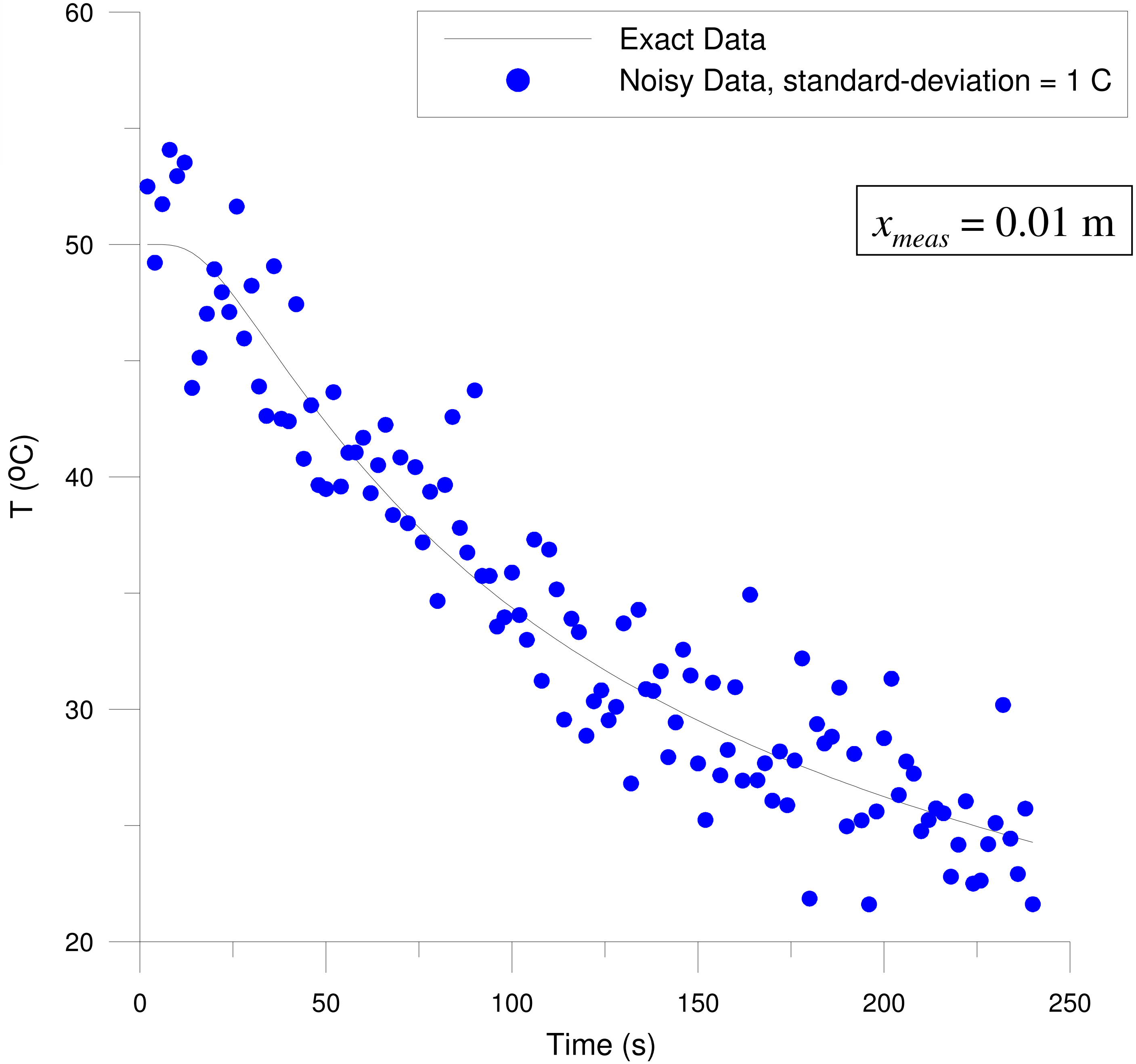


$\alpha_{min} = 10^{-7}$ m^2/s
$\alpha_{max} = 10^{-5}$ m^2/s
$\alpha_0 = 5.1 \times 10^{-6}$ m^2/s
$\alpha_{exact} = 4.9 \times 10^{-7}$ m^2/s
$T_{min} = 40\ ^oC$
$T_{max} = 65\ ^oC$
$T_0 = 53\ ^oC$
$T_{exact} = 50\ ^oC$
Diffusivity/Exact
1.2
1.1
1
0.9
0.8
0
4000
8000
12000
16000
20000
Number of Samples

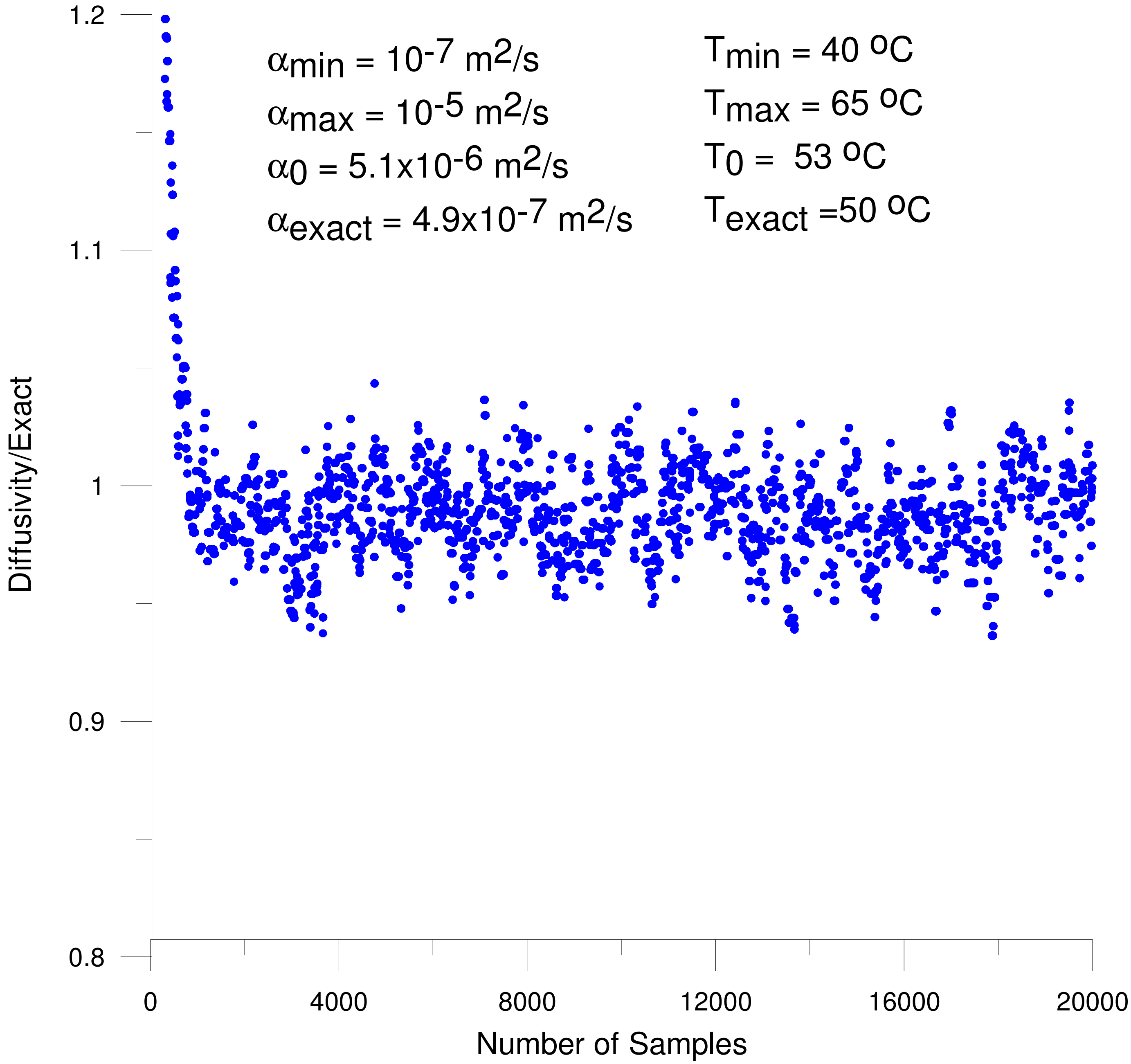

$\alpha_{min} = 10^{-7}\ m^2/s$
$\alpha_{max} = 10^{-5}\ m^2/s$
$\alpha_0 = 5.1x10^{-6}\ m^2/s$
$\alpha_{exact} = 4.9x10^{-7}\ m^2/s$
$T_{min} = 40\ ^oC$
$T_{max} = 65\ ^oC$
$T_0 = 53\ ^oC$
$T_{exact} = 50\ ^oC$
Initial Temperature/Exact
Number of Samples
1.2
1.1
1
0.9
0.8
0
4000
8000
12000
16000
20000



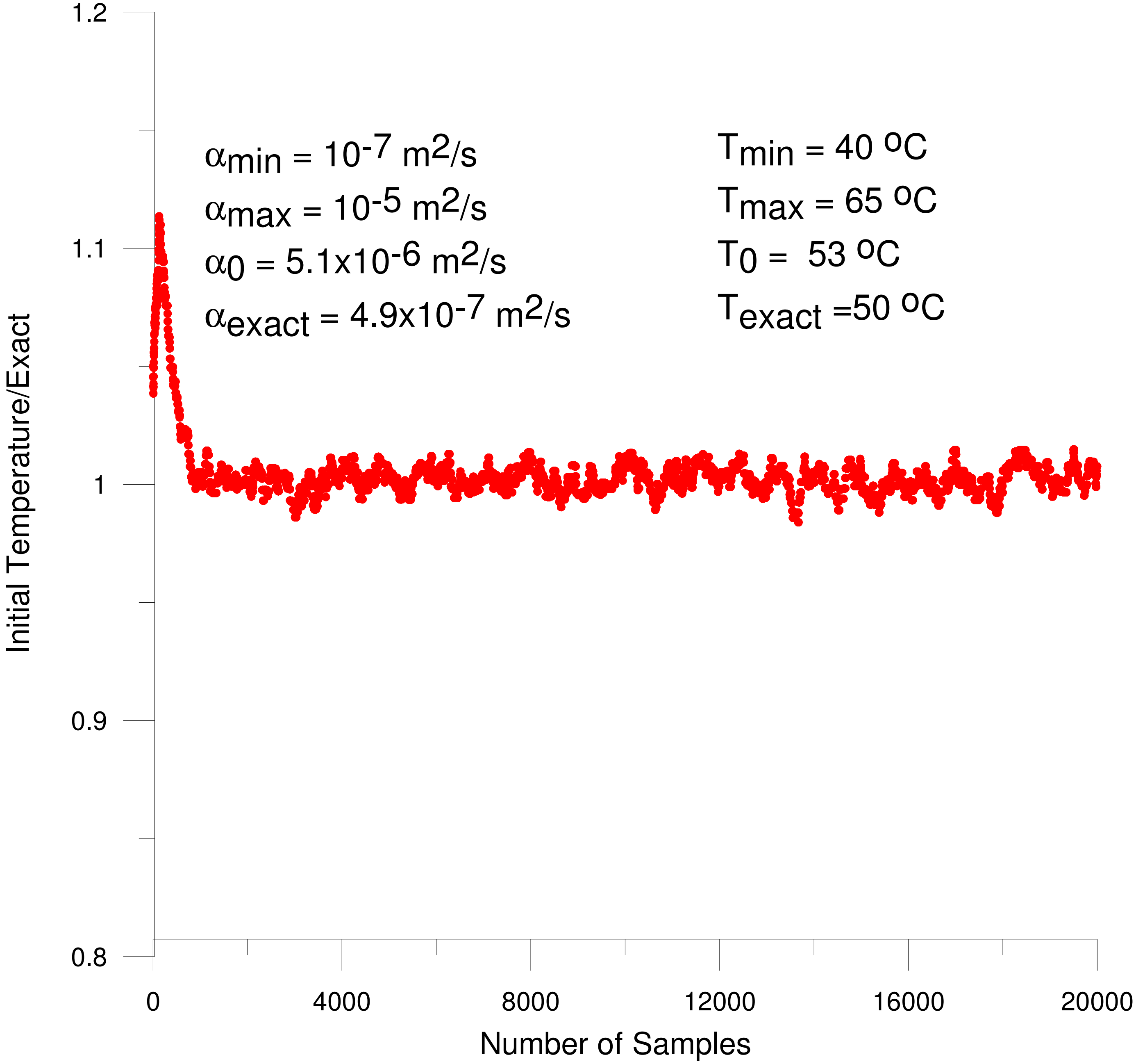
	Diffusivity/Exact	Temperature/Exact
Mean	0.950617158	1.016337295
Standard-Deviation	0.034386526	0.011192818



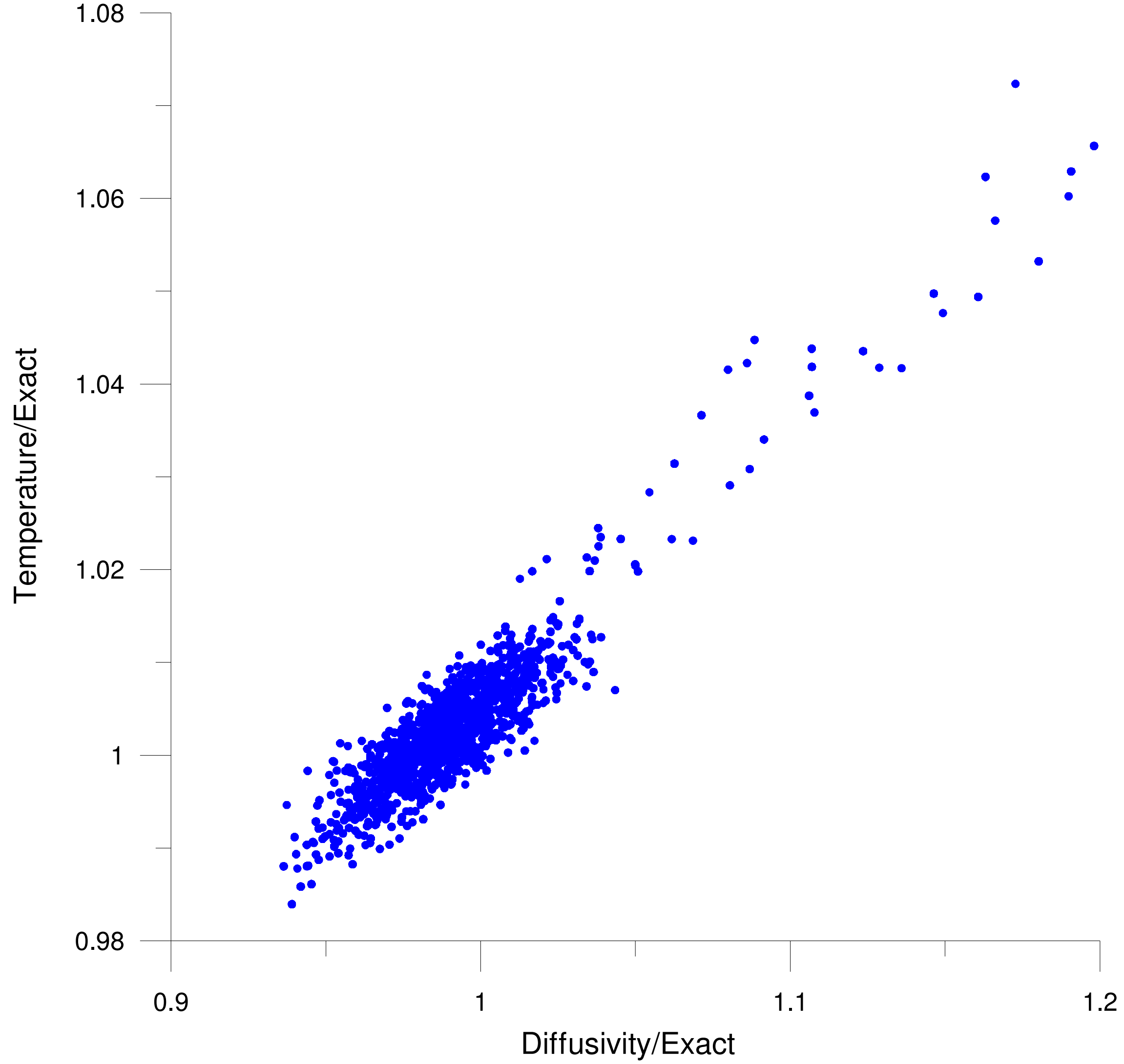
Exact Data
Noisy Data, standard-deviation = 1 C
$x_{meas} = 0.01$ m
T (°C)
Time (s)
60
50
40
30
20
0
50
100
150
200
250



αmin = 10-7 m2/s
αmax = 10-5 m2/s
α0 = 5.1x10-6 m2/s
αexact = 4.9x10-7 m2/s
Tmin = 40 oC
Tmax = 65 oC
T0 = 53 oC
Texact =50 oC
Diffusivity/Exact
Number of Samples
1.2
1.1
1
0.9
0.8
0
4000
8000
12000
16000
20000

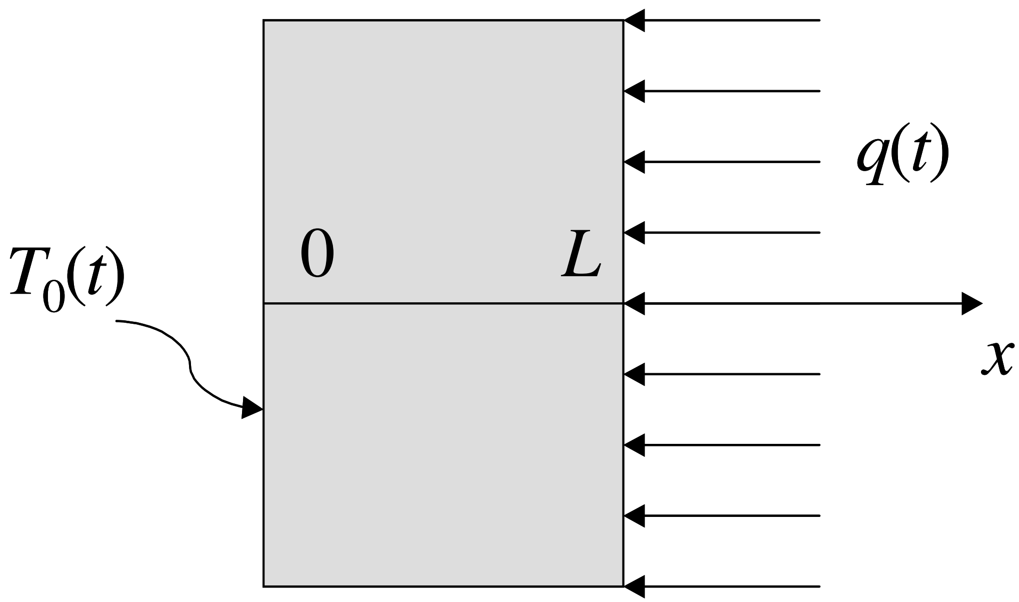


$\alpha_{min} = 10^{-7}$ m^2/s
$\alpha_{max} = 10^{-5}$ m^2/s
$\alpha_0 = 5.1\text{x}10^{-6}$ m^2/s
$\alpha_{exact} = 4.9\text{x}10^{-7}$ m^2/s
$T_{min} = 40$ ^oC
$T_{max} = 65$ ^oC
$T_0 = 53$ ^oC
$T_{exact} = 50$ ^oC
Initial Temperature/Exact
Number of Samples
1.2
1.1
1
0.9
0.8
0
4000
8000
12000
16000
20000



	Diffusivity/Exact	Temperature/Exact
Mean	0.991879086	1.003147487
Standard-Deviation	0.030681073	0.009687663

EXAMPLE



EXAMPLE

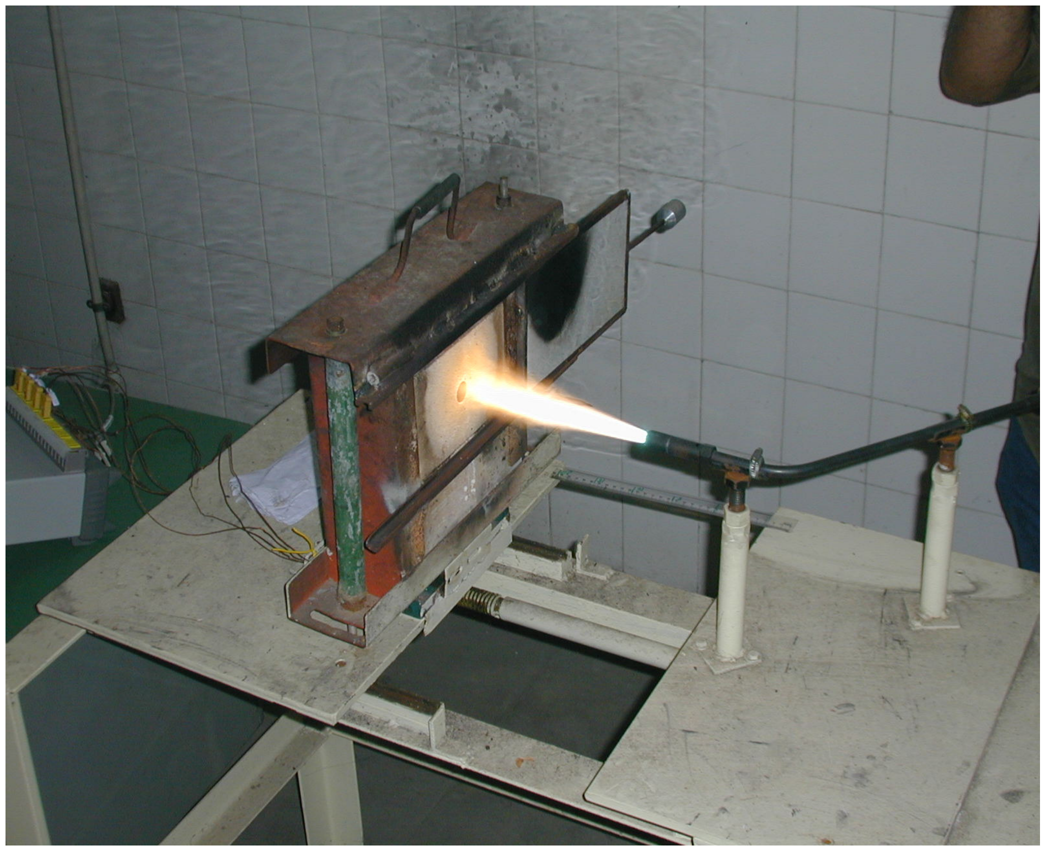
$$C(T)\frac{\partial T(x,t)}{\partial t} = \frac{\partial}{\partial x}\left[k(T)\frac{\partial T}{\partial x}\right] \quad \text{in} \quad 0 < x < L,\ t > 0$$

$$T = T_0(t) \quad \text{at} \quad x = 0, \quad t > 0$$

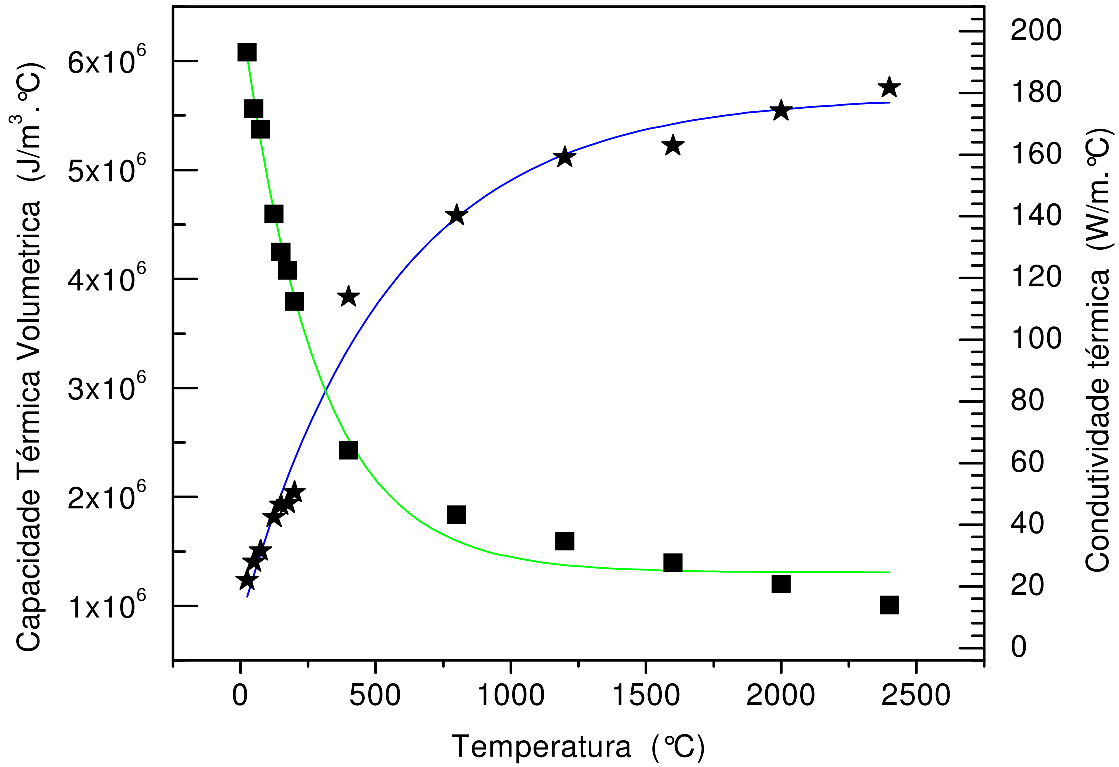
$$k(T)\frac{\partial T}{\partial x} = q(t) \quad \text{at} \quad x = L, \quad t > 0$$

$$T = T_{ini} \quad \text{for } t = 0, \text{ in} \quad 0 < x < L$$

EXAMPLE



EXAMPLE



Capacidade Térmica Volumetrica (J/m^3. °C)
6x10^6
5x10^6
4x10^6
3x10^6
2x10^6
1x10^6
0
500
1000
1500
2000
2500
Temperatura (°C)
200
180
160
140
120
100
80
60
40
20
0
Condutividade térmica (W/m. °C)

PROPRIEDADES TERMOFÍSICA DO MATERIAL

Equações e parâmetros das curvas ajustadas para as propriedades termofísicas.

$$C(T) = A_1 + A_2 e^{-T/A_3}$$

$$k(T) = B_1 + B_2 e^{-T/B_3}$$

Propriedade	Parâmetros	Desvio Padrão
Capacidade térmica volumétrica	A1= 5.681.006 J/m^3.ºC	163.262 J/m^3.ºC
	A2= -4.813.057 J/m^3.ºC	171.948 J/m^3.ºC
	A3= 547,00 ºC	71,42 ºC
Condutividade Térmica	B1= 24,52 W/mºC	2,79 W/mºC
	B2= 183,05 W/mºC	5,22 W/mºC
	B3= 277,00 ºC	20,24 ºC

Estes dados serão utilizados como informação a *priori* das propriedades termofísicas.

PROBLEMA INVERSO

MÉTODO MCMC-MH

Formulação Matemática

Para se determinar a função conjugada de probabilidades a ***priori*** $p(\mathbf{P})$ devemos primeiro defini-la para cada parâmetro a ser estimado. Assim, para o problema em questão, temos:

Para o fluxo de calor:

$$\pi(\mathbf{q}) \propto \alpha^{I/2} \exp\left\{-\frac{1}{2}\alpha\sqrt{\mathbf{q}^T\mathbf{Z}\mathbf{q}}\right\}$$

Onde I é dimensão de q e α é um parâmetro escalar de regularização.

Para as propriedades termofísicas:

$$\pi(\mathbf{A}) \propto \exp\left[-(\mathbf{A}-\boldsymbol{\mu}_A)^T\,\mathbf{W}_A(\mathbf{A}-\boldsymbol{\mu}_A)\right]$$

$$\pi(\mathbf{B}) \propto \exp\left[-(\mathbf{B}-\boldsymbol{\mu}_B)^T\,\mathbf{W}_B(\mathbf{B}-\boldsymbol{\mu}_B)\right]$$

PROBLEMA INVERSO

MÉTODO MCMC-MH

$$\boxed{\mathbf{Z} = \mathbf{D}^T \mathbf{D}}$$

$$\mathbf{D} = \begin{bmatrix} -1 & 1 & 0 & \cdots & 0 \\ 0 & -1 & 1 & \cdots & 0 \\ & & \ddots & & \vdots \\ 0 & \cdots & 0 & -1 & 1 \end{bmatrix}$$

$$\mathbf{A} = \left[A_1, A_2, A_3 \right] \qquad \mathbf{B} = \left[B_1, B_2, B_3 \right]$$

$$\boldsymbol{\mu}_A = \left[\mu_{A_1}, \mu_{A_2}, \mu_{A_3} \right] \qquad \boldsymbol{\mu}_B = \left[\mu_{B_1}, \mu_{B_2}, \mu_{B_3} \right]$$

$$\mathbf{W}_A = \begin{pmatrix} 1/\sigma_{A_1}^2 & 0 & 0 \\ 0 & 1/\sigma_{A_2}^2 & 0 \\ 0 & 0 & 1/\sigma_{A_3}^2 \end{pmatrix} \qquad \mathbf{W}_B = \begin{pmatrix} 1/\sigma_{B_1}^2 & 0 & 0 \\ 0 & 1/\sigma_{B_2}^2 & 0 \\ 0 & 0 & 1/\sigma_{B_3}^2 \end{pmatrix}$$

PROBLEMA INVERSO

MÉTODO MCMC-MH

Assim, temos a seguinte função densidade de probabilidade a ***posteriori*** (PPDF):

$$\pi(\mathbf{P} \mid \mathbf{Y}) \propto \pi(\mathbf{Y} \mid \mathbf{P})\pi(\mathbf{P})$$

$$\pi(\mathbf{q}, \mathbf{A}, \mathbf{B} \mid \mathbf{Y}) \propto \exp\left\{-\frac{\left[(\mathbf{Y} - \mathbf{T}(\mathbf{q}, \mathbf{A}, \mathbf{B})\right]^T \left[(\mathbf{Y} - \mathbf{T}(\mathbf{q}, \mathbf{A}, \mathbf{B})\right]}{2\sigma^2}\right\} \mathrm{x}$$

$$\exp\left[-\frac{1}{2}\alpha\ \sqrt{\mathbf{q}^T Z \mathbf{q}}\right] \exp\left[-(\mathbf{A} - \boldsymbol{\mu}_A)^T \mathbf{W}_A (\mathbf{A} - \boldsymbol{\mu}_A)\right] \exp\left[-(\mathbf{B} - \boldsymbol{\mu}_B)^T \mathbf{W}_B (\mathbf{B} - \boldsymbol{\mu}_B)\right]$$

RESULTADOS E DISCUSSÕES

EXPERIMENTO SIMULADO

Teste de desempenho dos métodos de Gauss-MAP e MCMC (Markov Chain Monte Carlo)

Problema Direto

- **Impôs-se uma função fluxo de calor de forma e magnitude previamente conhecida no contorno quente da amostra.**
- **No contorno frio impôs-se uma temperatura fixa igual à condição inicial.** $T_L = T_0 = 25°C$
- **Obtenção dos dados experimentais de temperatura simulados.**

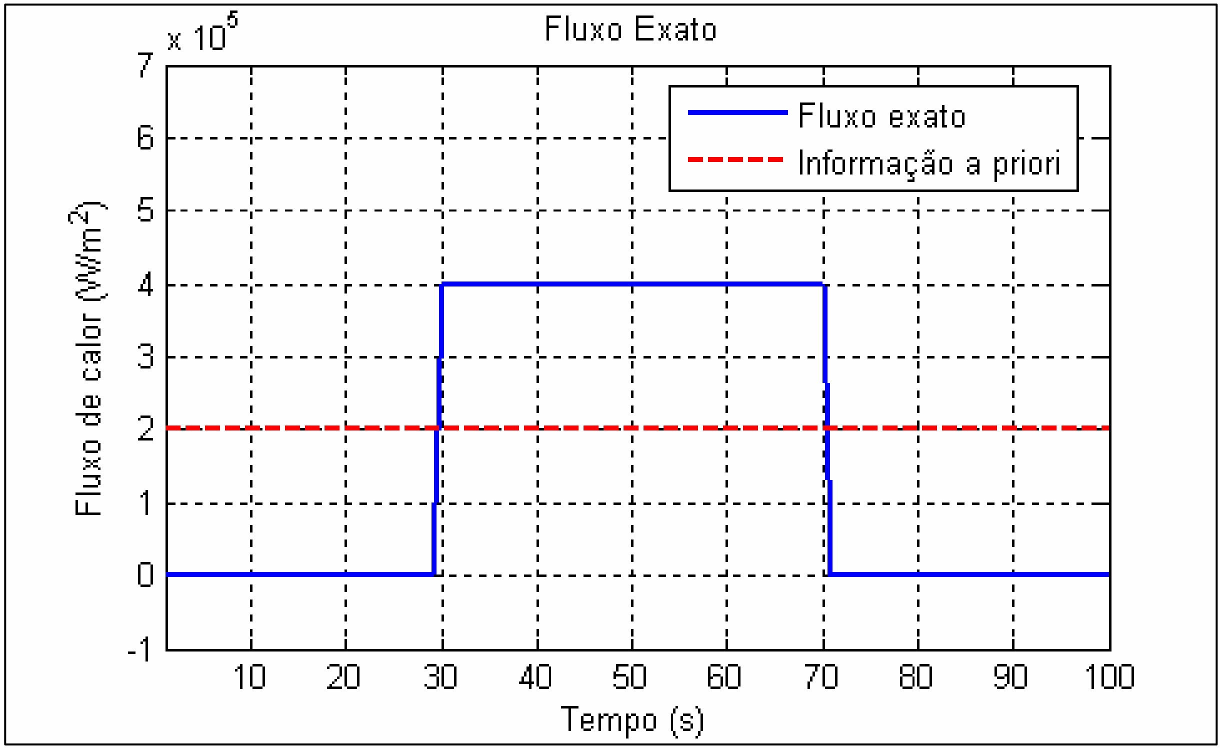
Problema Inverso

- **Partindo dos dados experimentais simulados, estimar a função fluxo de calor original.**
- **No contorno frio impôs-se uma temperatura fixa igual à condição inicial.** $T_L = T_0 = 25°C$
- **Estimativa inicial do fluxo imposto pobre ou pouco informativa.**

RESULTADOS E DISCUSSÕES

EXPERIMENTO SIMULADO

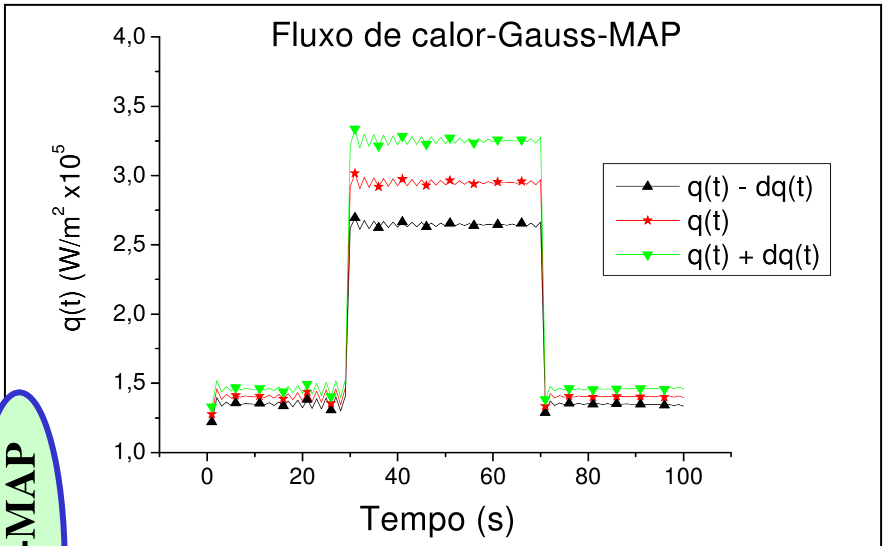
Função fluxo de calor exato e informação a priori do fluxo de calor

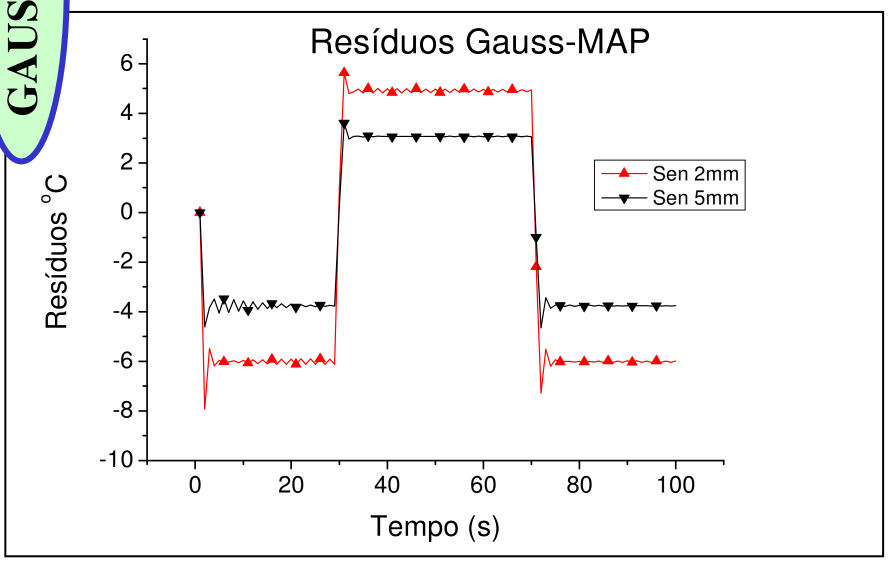


RESULTADOS E DISCUSSÕES

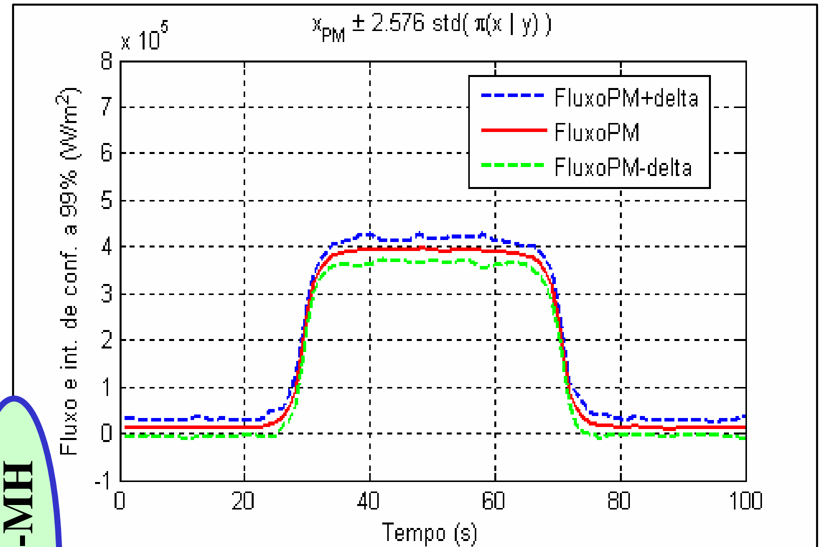
EXPERIMENTO SIMULADO

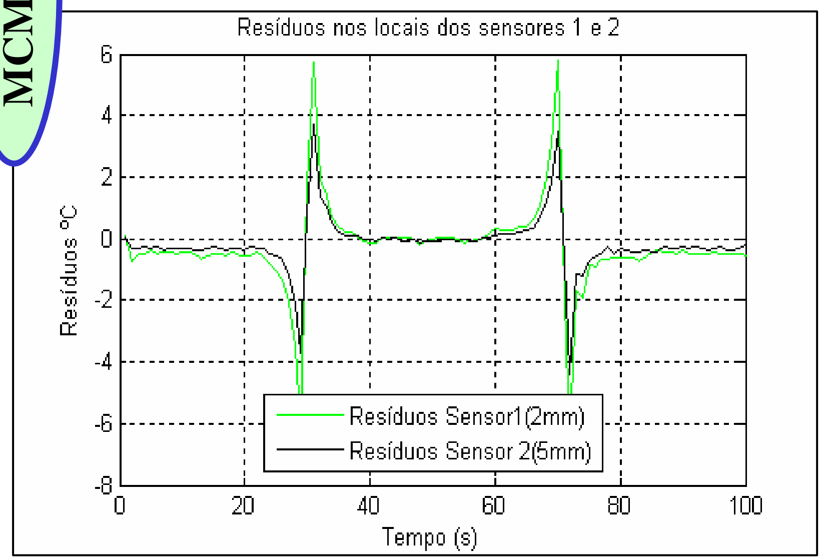
GAUSS-MAP





MCMC-MH





PROBLEMA INVERSO

MÉTODO MCMC-MH

A função de auto-covariância (ACF)

$$C_{ff} \equiv \mathrm{cov}(f(\mathbf{P}_n), f(\mathbf{P}_{(n+s)}))$$

$$\rho_{ff}(s) = C_{ff}(s) / C_{ff}(0) = C_{ff}(s) / \mathrm{var}(f)$$

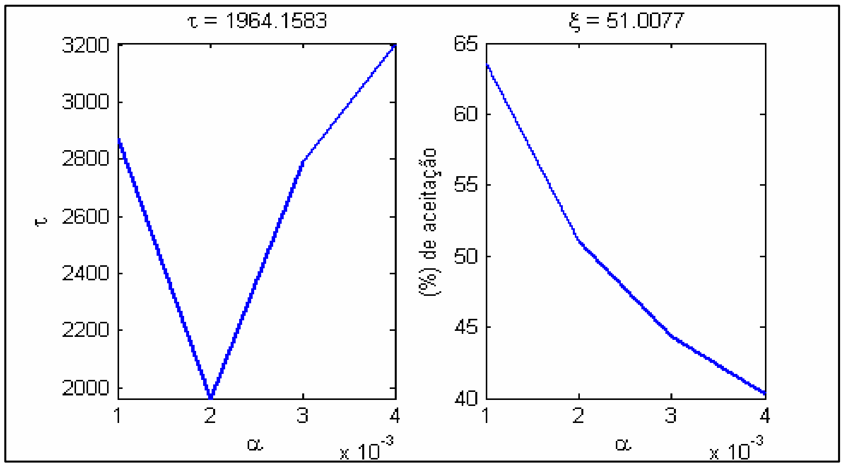
Tempo de Auto-covariância

$$\tau_f = 1 + 2\sum_{s=1}^{M} \rho_{ff}(s)$$

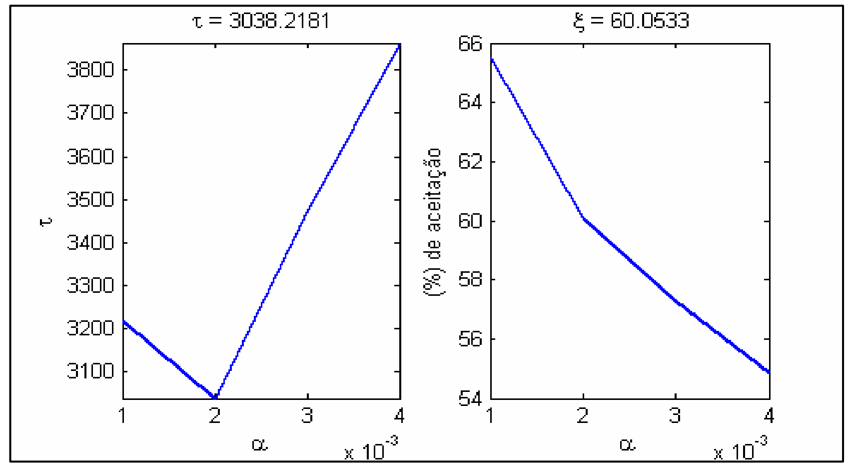
RESULTADOS E DISCUSSÕES

Resultados com o método MCMC-MH

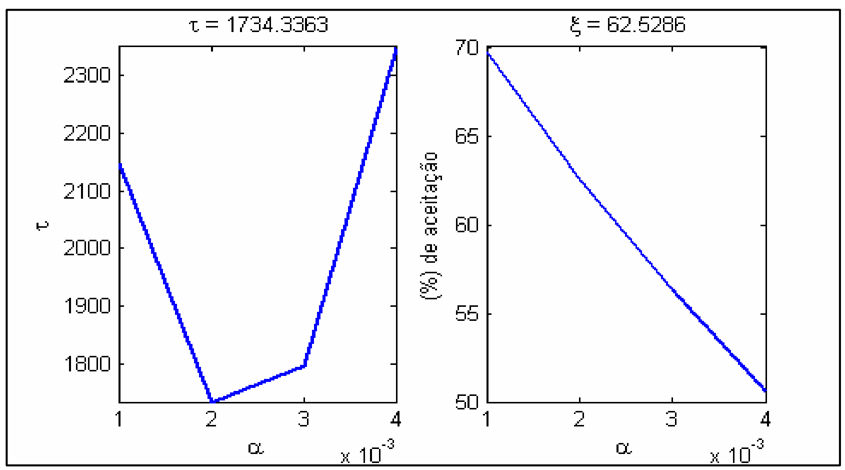
Estudo do IACT e da taxa de aceitação em função de α.



Experimento 1



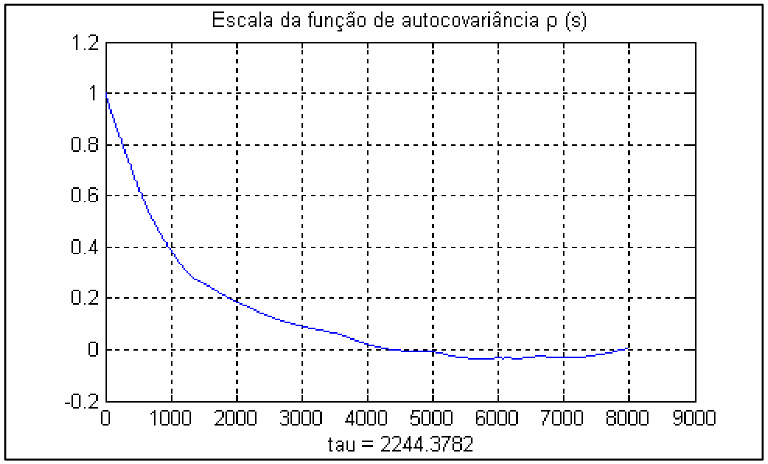
Experimento 2



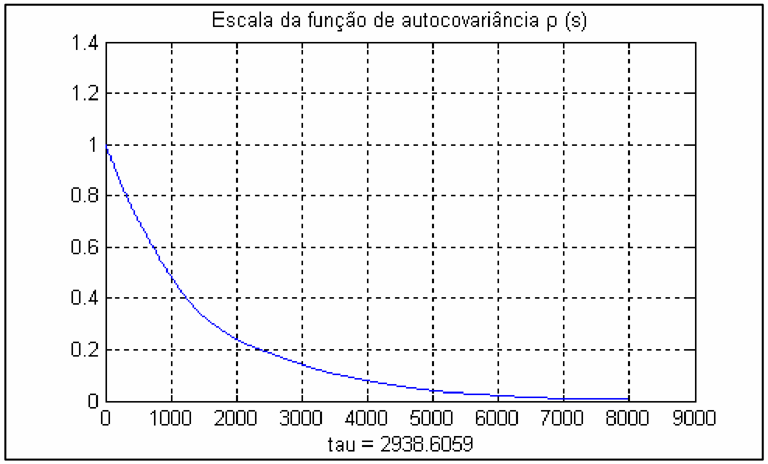
Experimento 3

Resultados com o método MCMC-MH

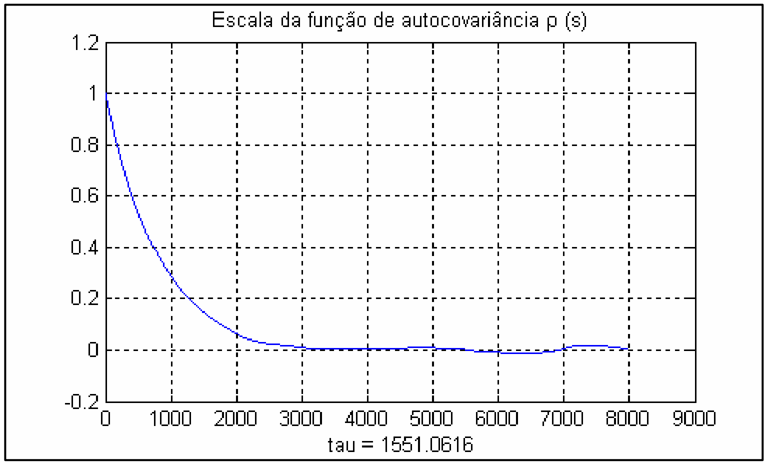
Funções de covariância normalizada para o valor ótimo de α .



Experimento 1



Experimento 2



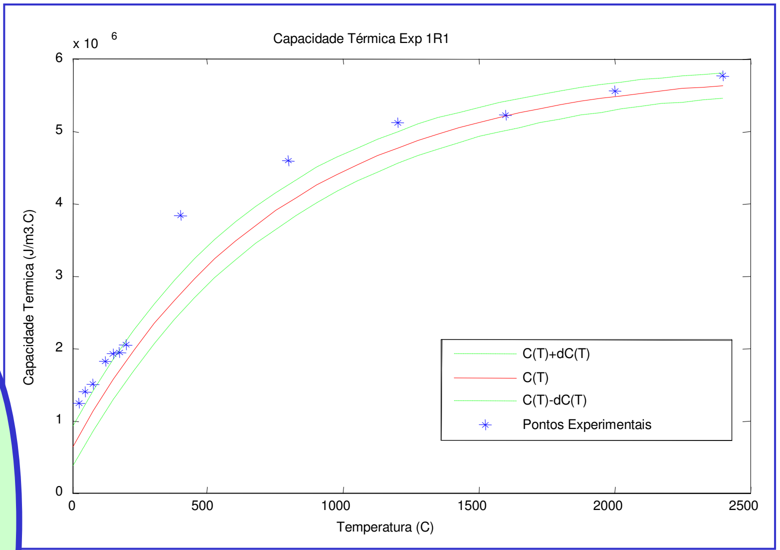
Experimento 3

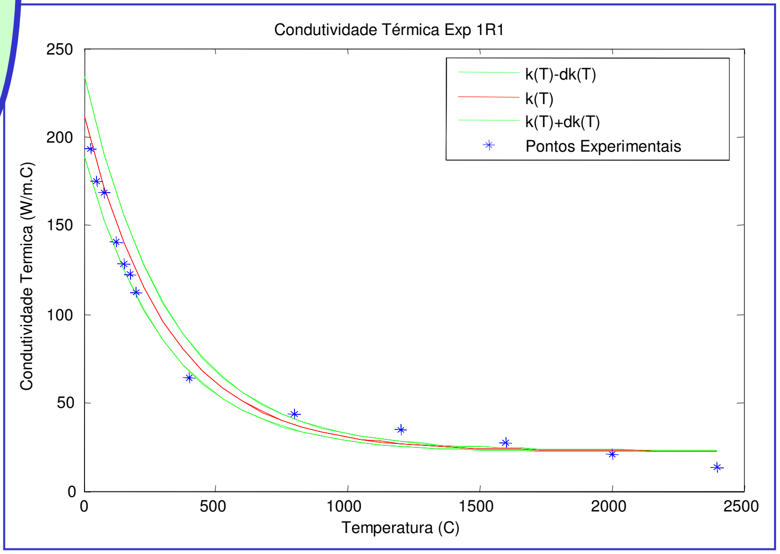
RESULTADOS E DISCUSSÕES

Análise comparativa dos resultados

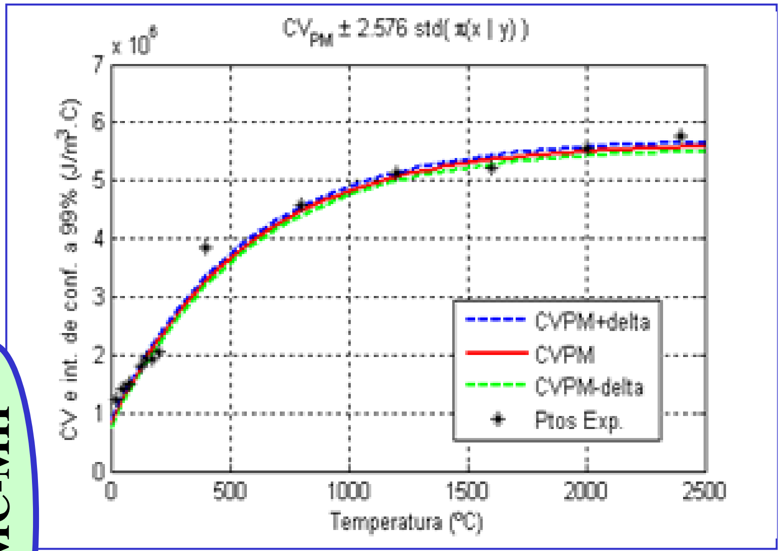
Resultados do experimento 1R1 – Propriedades

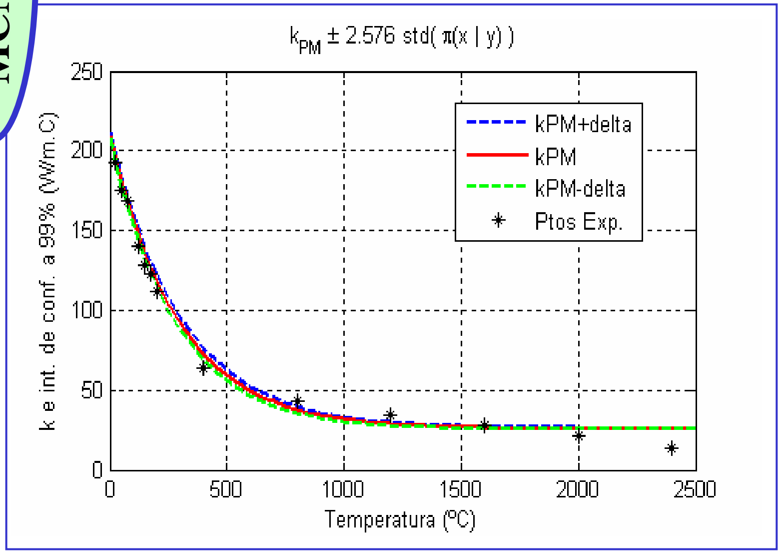
GAUSS-MAP





MCMC-MH

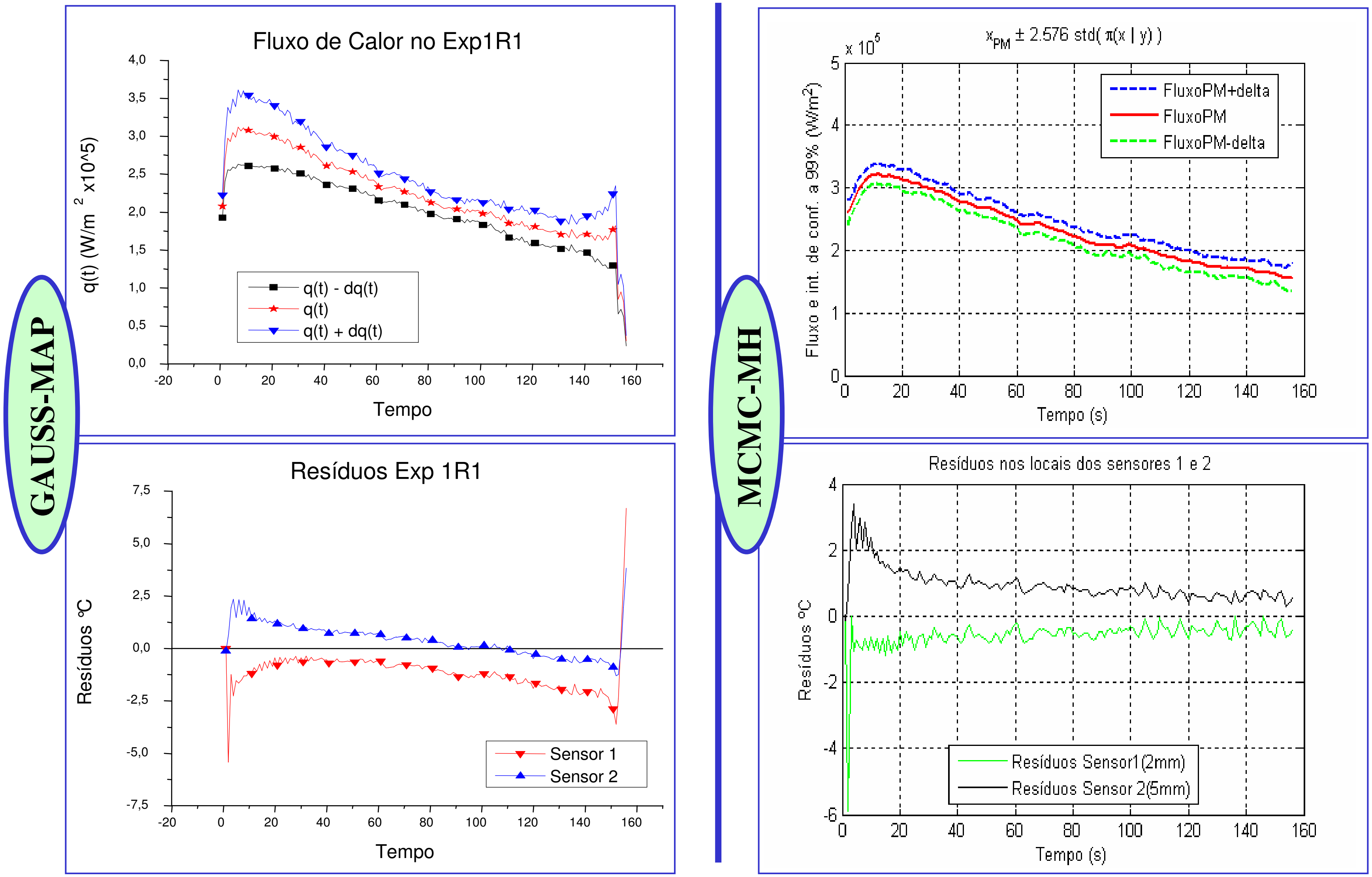




RESULTADOS E DISCUSSÕES

Análise comparativa dos resultados

Resultados do experimento 1R1 –Fluxo e Resíduos

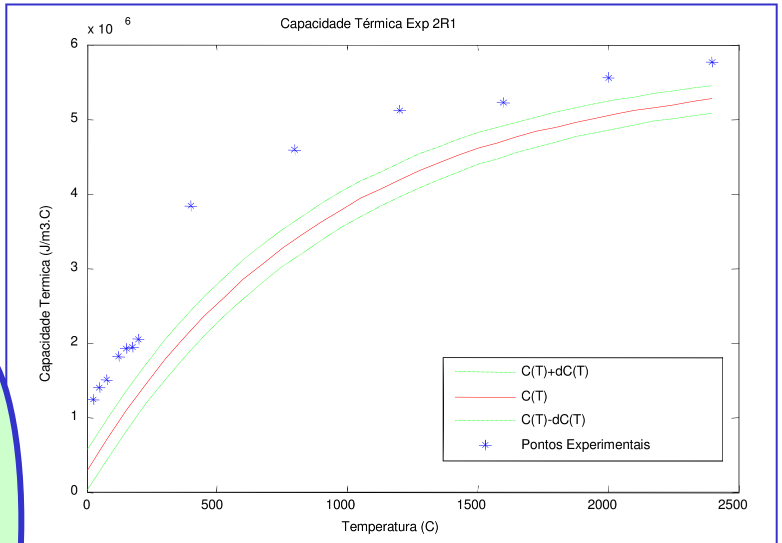


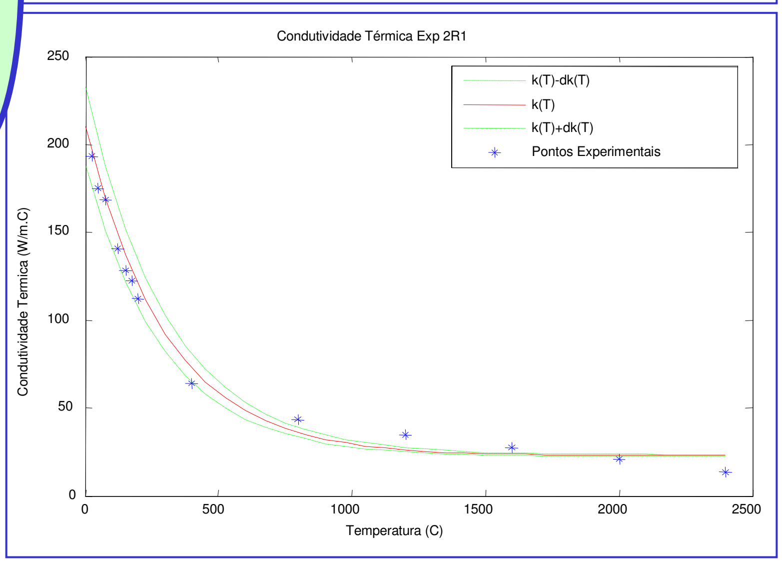
RESULTADOS E DISCUSSÕES

Análise comparativa dos resultados

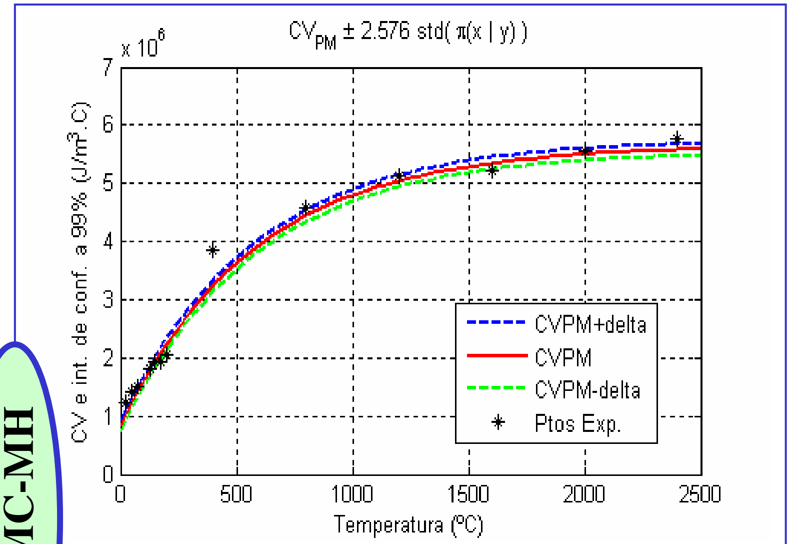
Resultados do experimento 2R1 – Propriedades

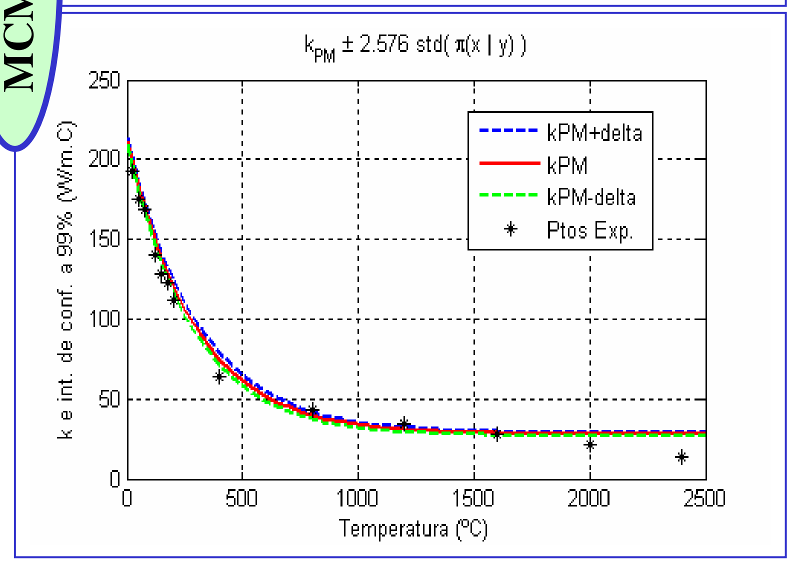
GAUSS-MAP





MCMC-MH



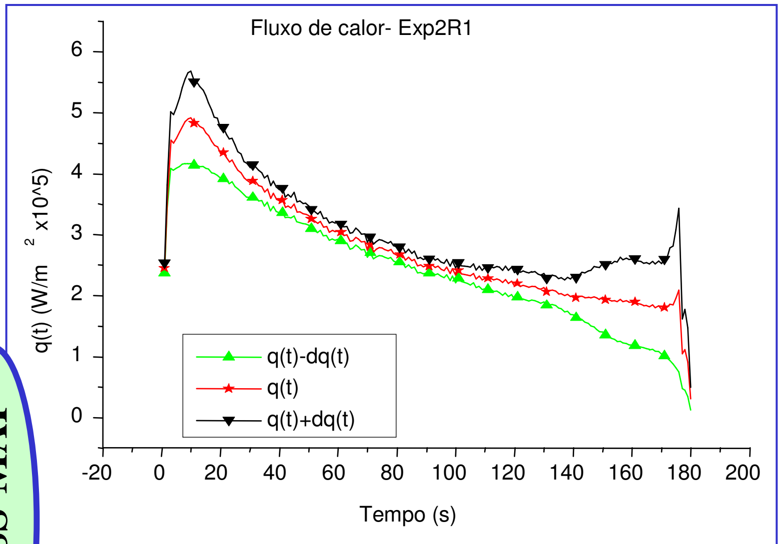


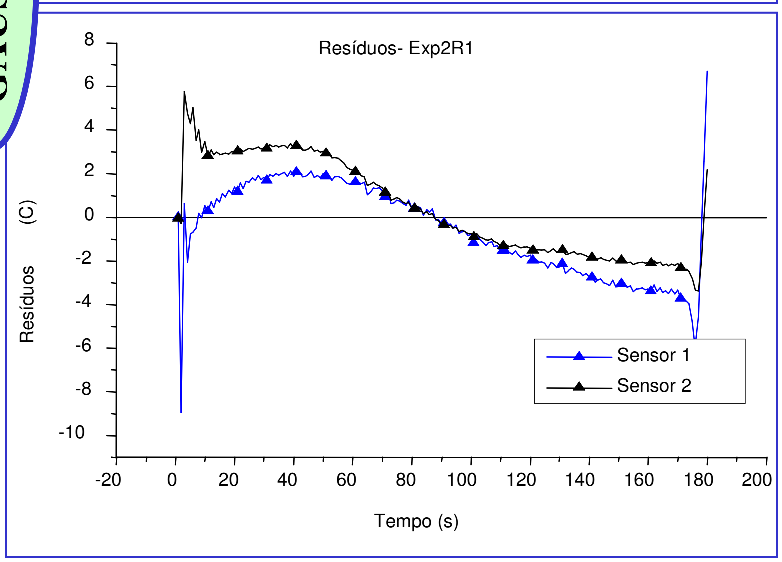
RESULTADOS E DISCUSSÕES

Análise comparativa dos resultados

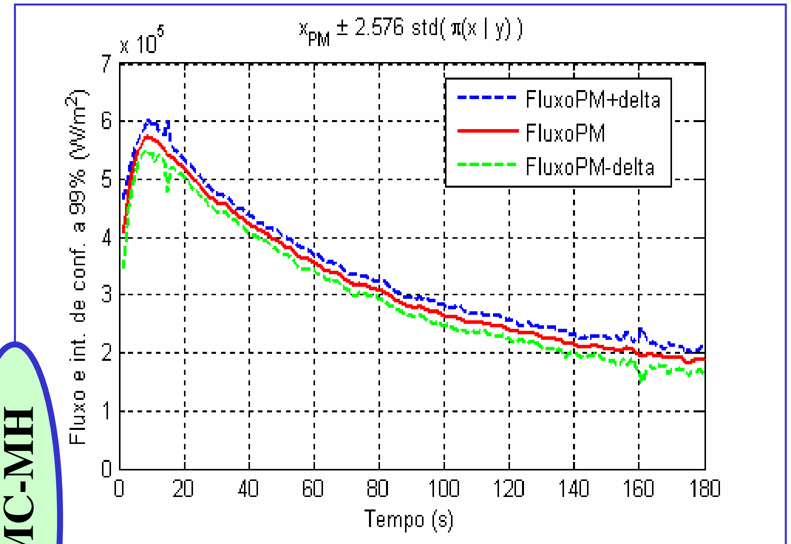
Resultados do experimento 2R1 –Fluxo e Resíduos

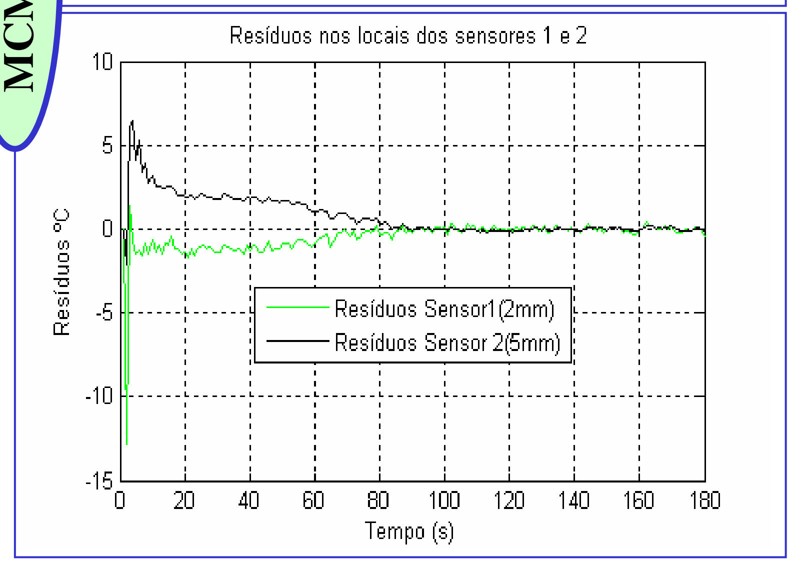
GAUSS-MAP





MCMC-MH



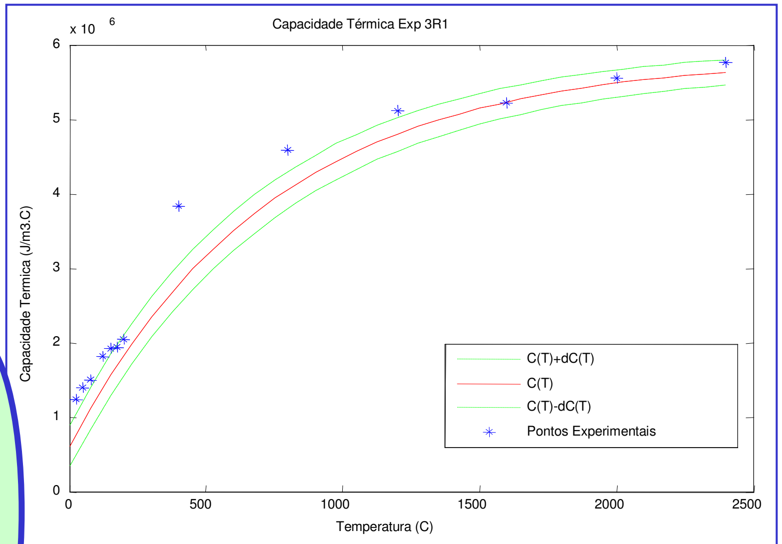


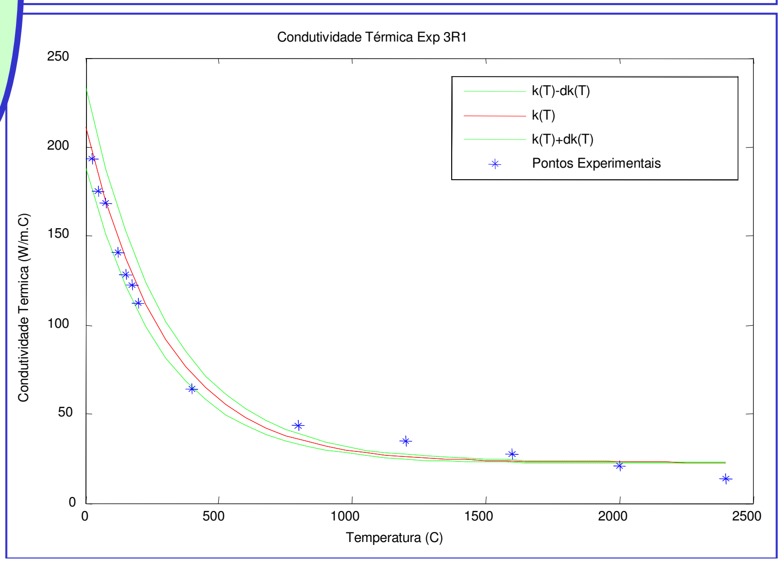
RESULTADOS E DISCUSSÕES

Análise comparativa dos resultados

Resultados do experimento 3R1 – Propriedades

GAUSS-MAP





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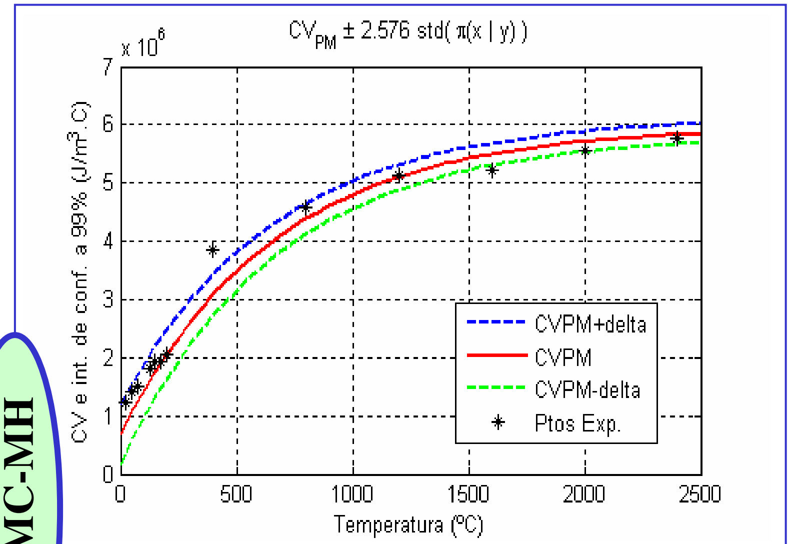
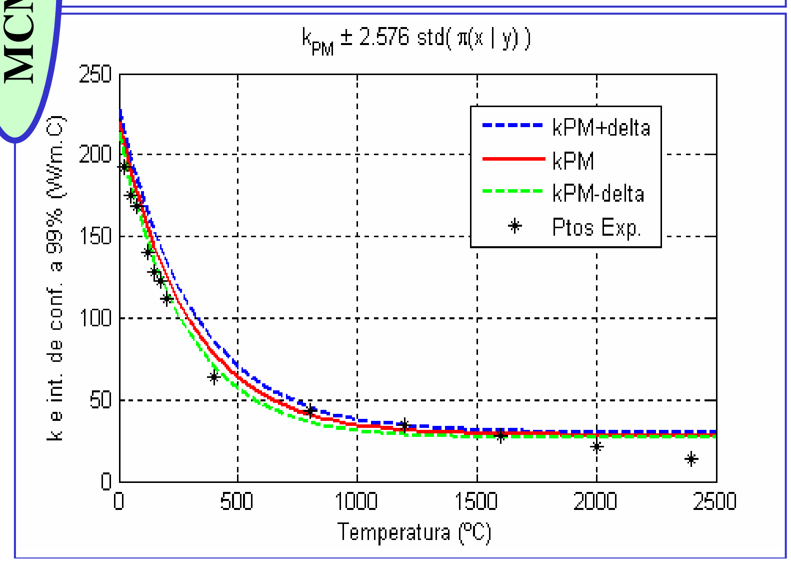


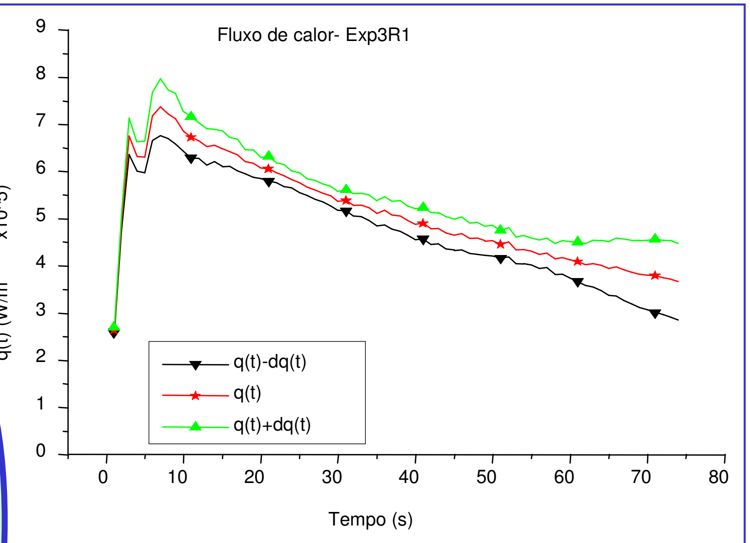


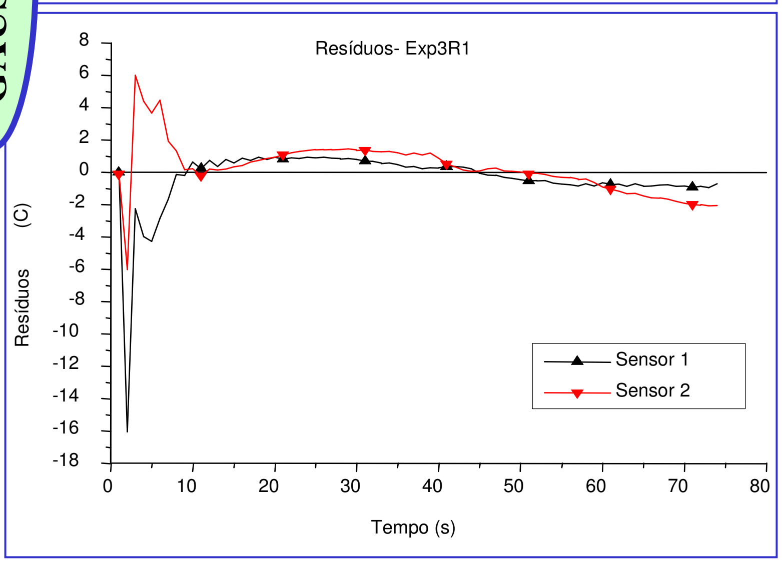
RESULTADOS E DISCUSSÕES

Análise comparativa dos resultados

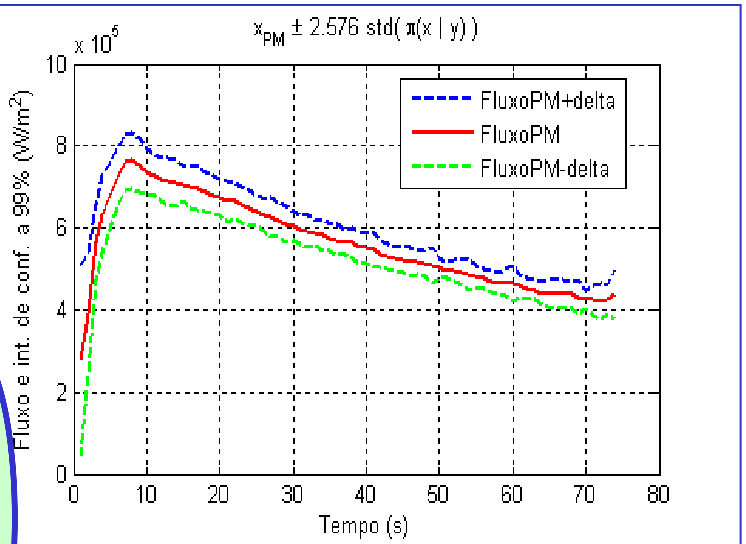
Resultados do experimento 3R1 – Fluxo e Resíduos

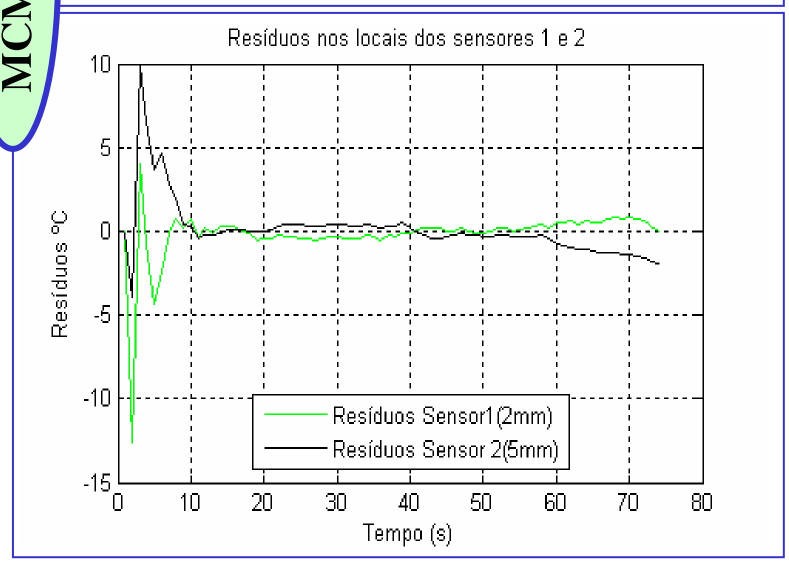
GAUSS-MAP





MCMC-MH





5. INTERPOLATION OF THE LIKELIHOOD FUNCTION

$$f\left(\mathbf{x}\right)=\sum_{j=1}^{N}\alpha_j\phi\left(\left|\mathbf{x}-\mathbf{x}_j\right|\right)+\sum_{k=1}^{M}\sum_{i=1}^{L}\beta_{i,k}\,p_k\left(x_i\right)+\beta_0$$

$p_k(x_i)$ is one of the M terms of a given basis of polynomials

5. INTERPOLATION OF THE LIKELIHOOD FUNCTION

RADIAL BASIS FUNCTIONS

Multiquadrics: $\phi\left(\left|\mathbf{x}_i - \mathbf{x}_j\right|\right) = \sqrt{\left(\mathbf{x}_i - \mathbf{x}_j\right)^2 + c_j^2}$

Squared multiquadrics: $\phi\left(\left|\mathbf{x}_i - \mathbf{x}_j\right|\right) = \left(\mathbf{x}_i - \mathbf{x}_j\right)^2 + c_j^2$

Gaussian: $\phi\left(\left|\mathbf{x}_i - \mathbf{x}_j\right|\right) = \exp\left[-c_j^2\left(\mathbf{x}_i - \mathbf{x}_j\right)^2\right]$

Cubical multiquadrics: $\phi\left(\left|\mathbf{x}_i - \mathbf{x}_j\right|\right) = \left[\sqrt{\left(\mathbf{x}_i - \mathbf{x}_j\right)^2 + c_j^2}\right]^3$

- Automatic selection of the best interpolating function
- Cross-validation procedure
- Polynomials up to degree 6 without crossed terms

6. RESULTS FOR A TEST-CASE

6. RESULTS FOR A TEST-CASE

$$R\frac{\partial c(z,t)}{\partial t} = D\frac{\partial^2 c(z,t)}{\partial z^2} - V\frac{\partial c(z,t)}{\partial z}$$ for $0 < z < L$ and $t > 0$

$$c(z,0) = C_0$$ for $t = 0$ in $0 < z < L$

$$c(0,t) = C_0$$ at $z = 0$ for $t > 0$

$$D\frac{\partial c(L,t)}{\partial z} + h_m\, c(L,t) = h_m C_b$$ at $z = L$ for $t > 0$

$$\mathbf{P}^{\mathbf{T}} = [\, D\, ,\, R\, ,\, h_m\, ,\, V\,]$$

6. RESULTS FOR A TEST-CASE

- Errors in the measured variables are additive, uncorrelated, normally distributed, with zero mean and known constant standard-deviation
- Simulated experimental data: constant standard-deviation of 0.05
- Column with length $L = 5.4$ cm
- $R = 14.4$
- $D = 11.08$ cm^2/min
- $h_m = 0.39$ cm/min
- $V = 0.59$ cm/min
- 90 measurements of the outflow concentration
- Number of samples: 20000
- Prior information: uniform distribution

$$9 \leq R \leq 20$$

$$9 \text{ cm}^2/\text{min} \leq D \leq 20 \text{ cm}^2/\text{min}$$

$$0.3 \text{ cm/min} \leq h_m \leq 0.6 \text{ cm/min}$$

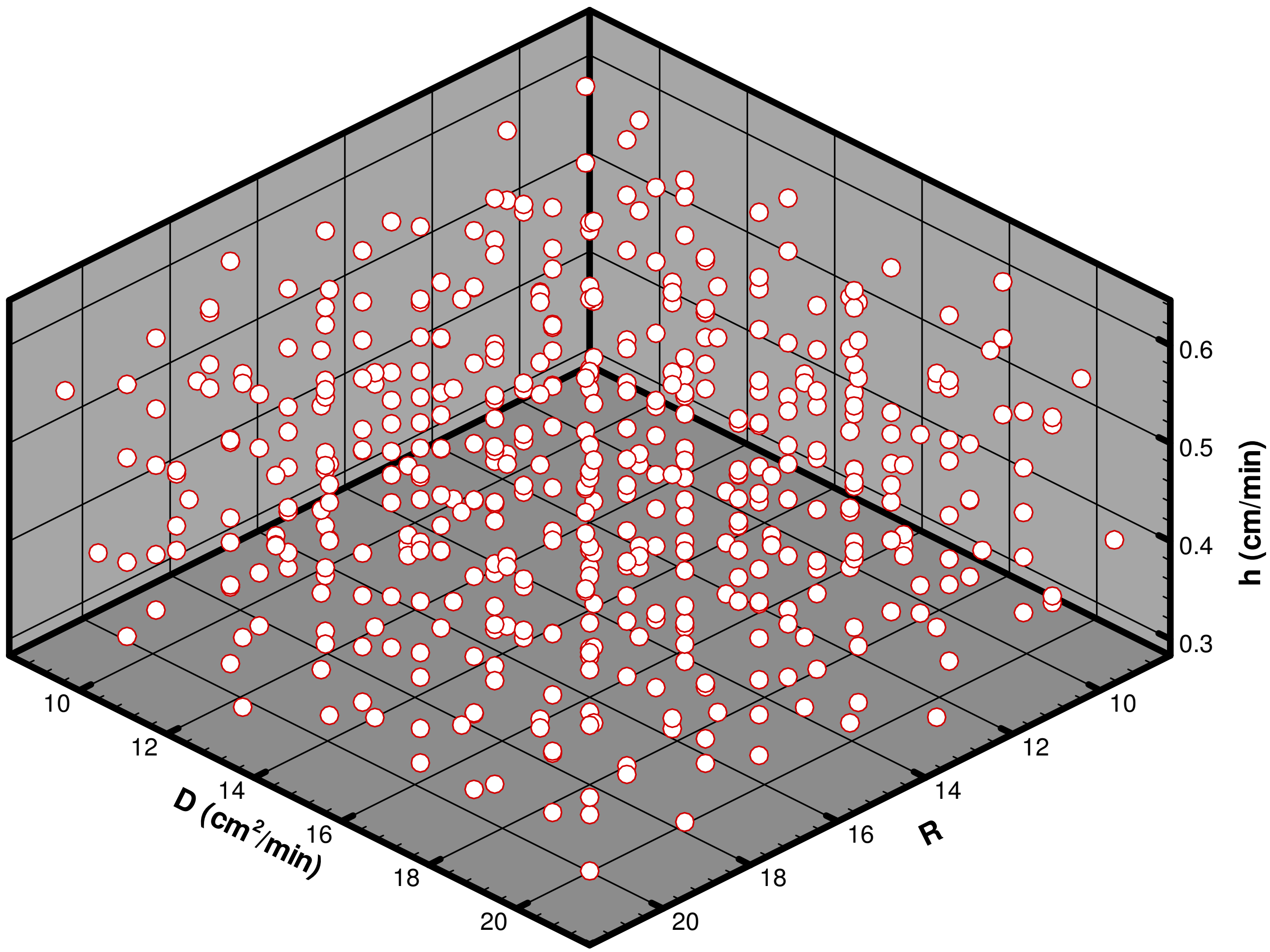
$$0.58 \text{ cm/min} \leq V \leq 0.60 \text{ cm/min}$$

$9 \le R \le 20$

$9\ \text{cm}^2/\text{min} \le D \le 20\ \text{cm}^2/\text{min}$

$0.3\ \text{cm/min} \le\ h_m \le 0.6\ \text{cm/min}$

$0.58\ \text{cm/min} \le\ V \le 0.60\ \text{cm/min}$

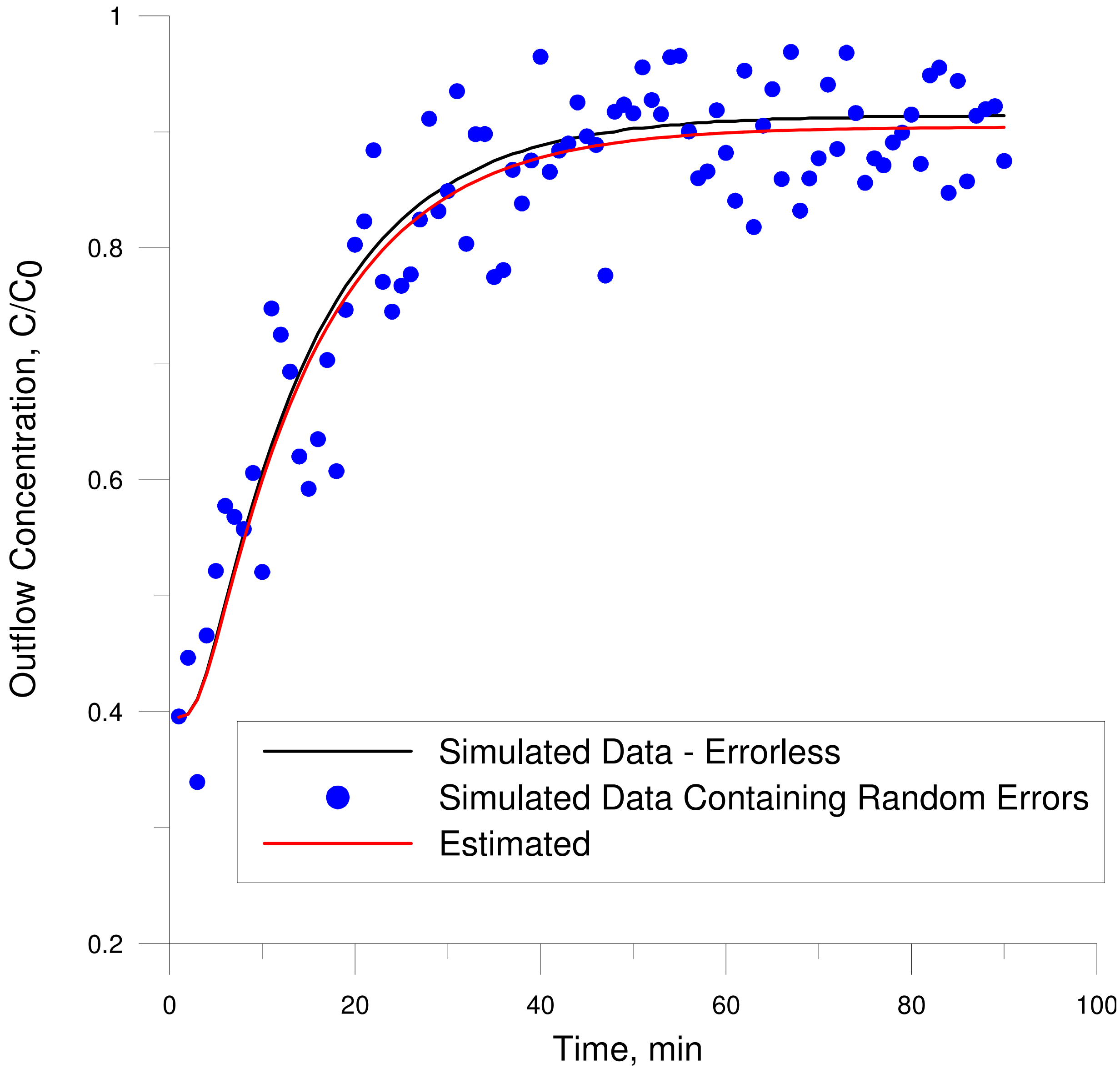


6. RESULTS FOR A TEST-CASE

Technique 1: Without interpolation

Parameter	Mean	Standard-Deviation
R	16.7	1.9
D (cm^2/min).	12.7	1.5
h_m (cm/min)	0.50	0.06
V (cm/min)	0.59	0.01

- $R = 14.4$
- $D = 11.08$ cm^2/min
- $h_m = 0.39$ cm/min
- $V = 0.59$ cm/min



Outflow Concentration, C/C0
Time, min
Simulated Data - Errorless
Simulated Data Containing Random Errors
Estimated
1
0.8
0.6
0.4
0.2
0
20
40
60
80
100

6. RESULTS FOR A TEST-CASE

Technique 2: Interpolation with Multiquadrics RBFs

Parameter	Mean	Standard-Deviation	Number of Interpolating Points
R	18.3	2.2	300
D (cm^2/min).	14.7	1.6	
h_m (cm/min)	0.57	0.03	
V (cm/min)	0.58	0.01	
R	18.9	0.7	500
D (cm^2/min).	15.2	0.7	
h_m (cm/min)	0.57	0.03	
V (cm/min)	0.59	0.01	

- R = 14.4
- D = 11.08 cm^2/min
- h_m = 0.39 cm/min
- V = 0.59 cm/min

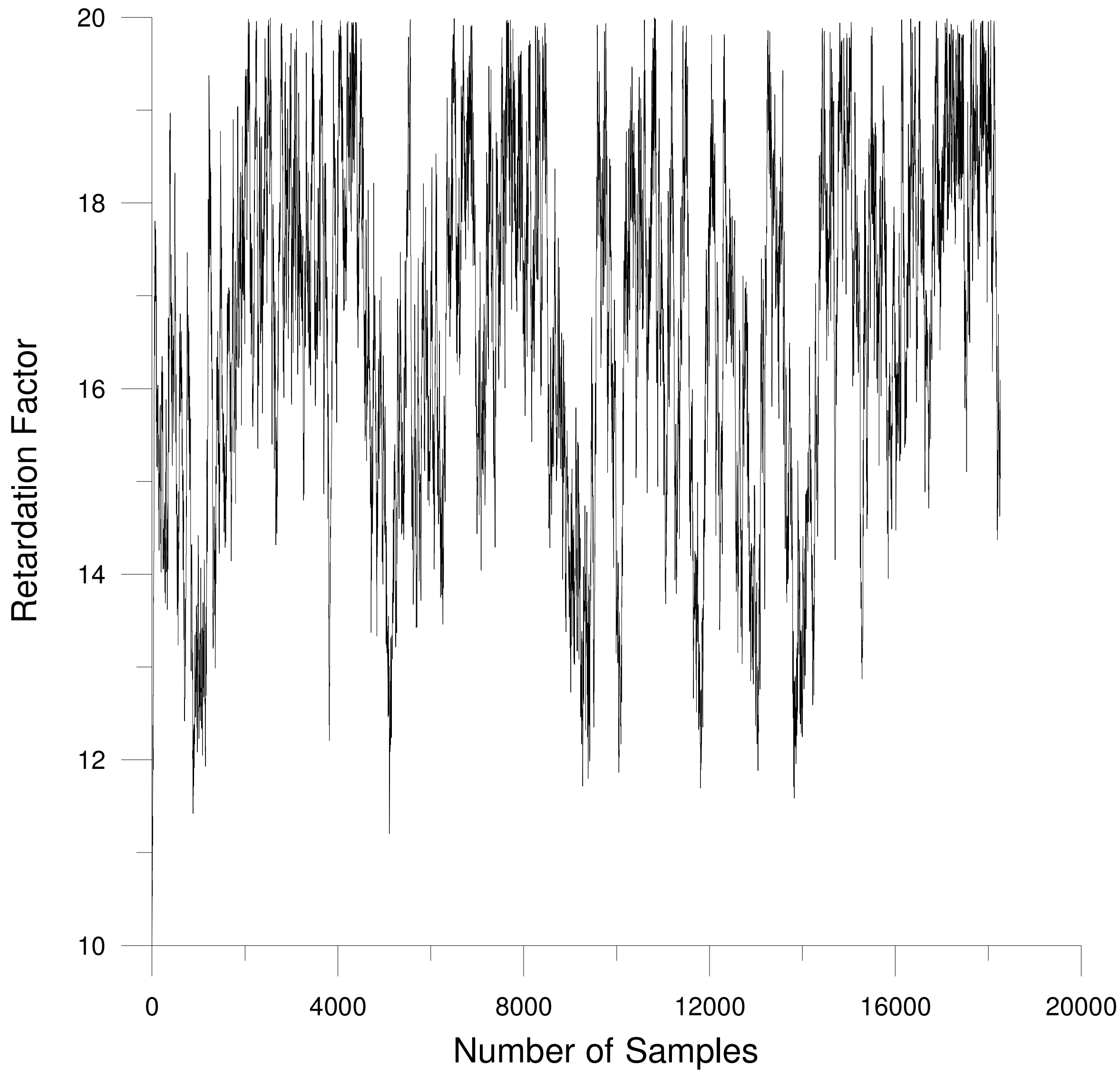
6. RESULTS FOR A TEST-CASE

Technique 3: Iterpolation with RBFs using the cross-validation procedure

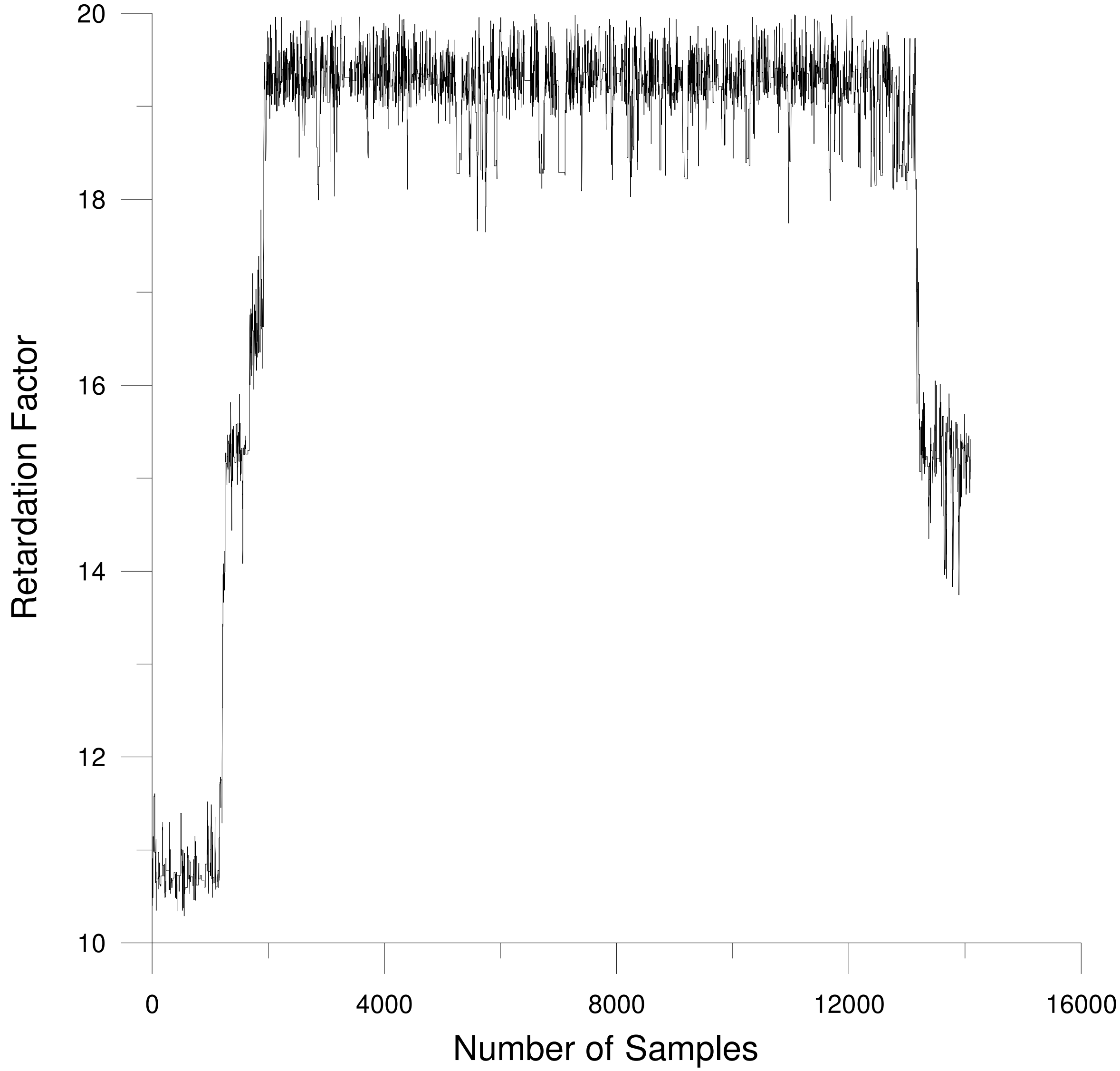
Parameter	Mean	Standard-Deviation	Number of Interpolating Points
R	16.4	1.9	300
D (cm^2/min).	12.6	1.7	
h_m (cm/min)	0.41	0.06	
V (cm/min)	0.58	0.01	
R	17.4	2.0	500
D (cm^2/min).	13.4	1.7	
h_m (cm/min)	0.47	0.07	
V (cm/min)	0.59	0.01	

- R = 14.4
- D = 11.08 cm^2/min
- h_m = 0.39 cm/min
- V = 0.59 cm/min

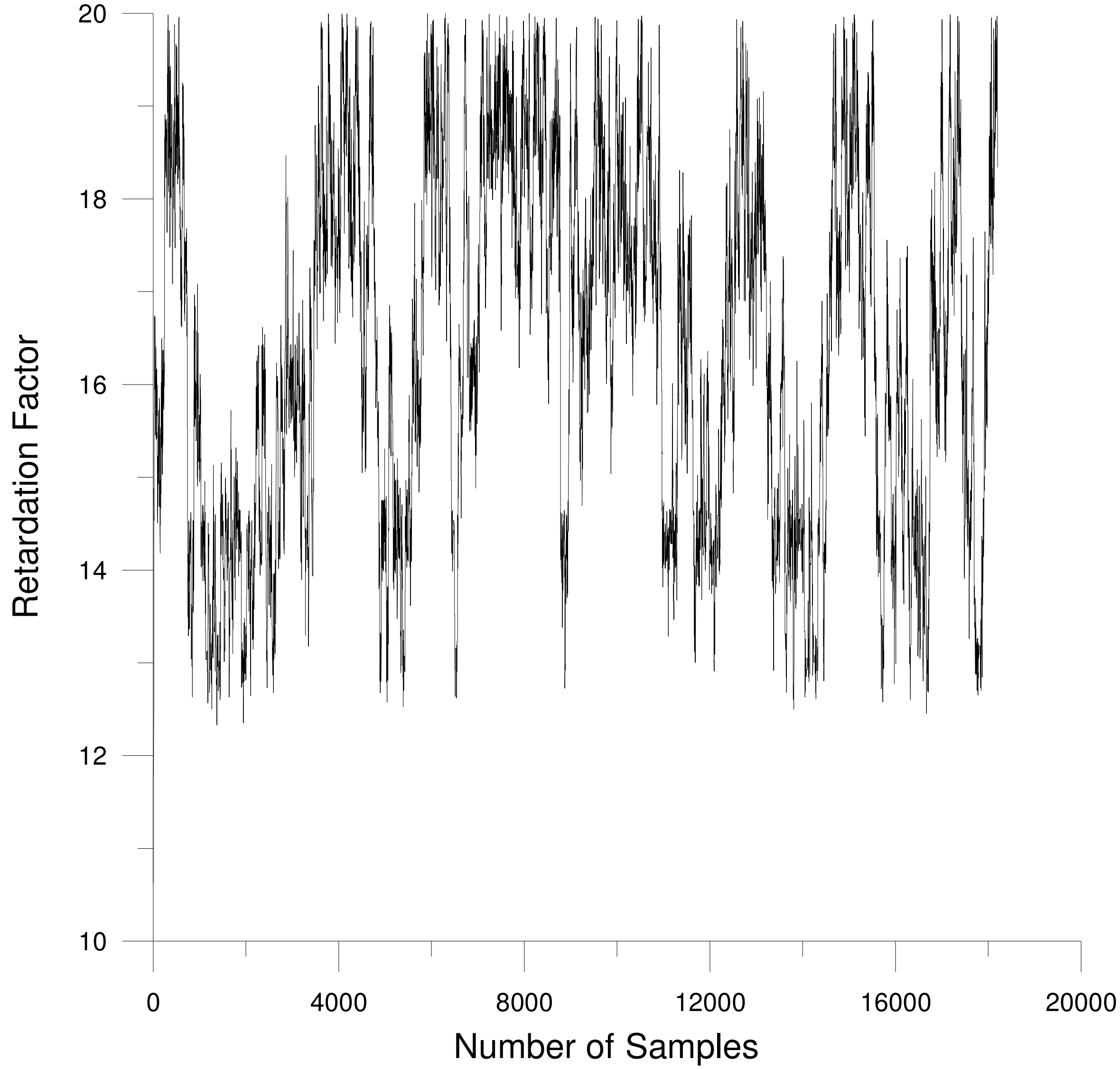
Technique 1: Without interpolation



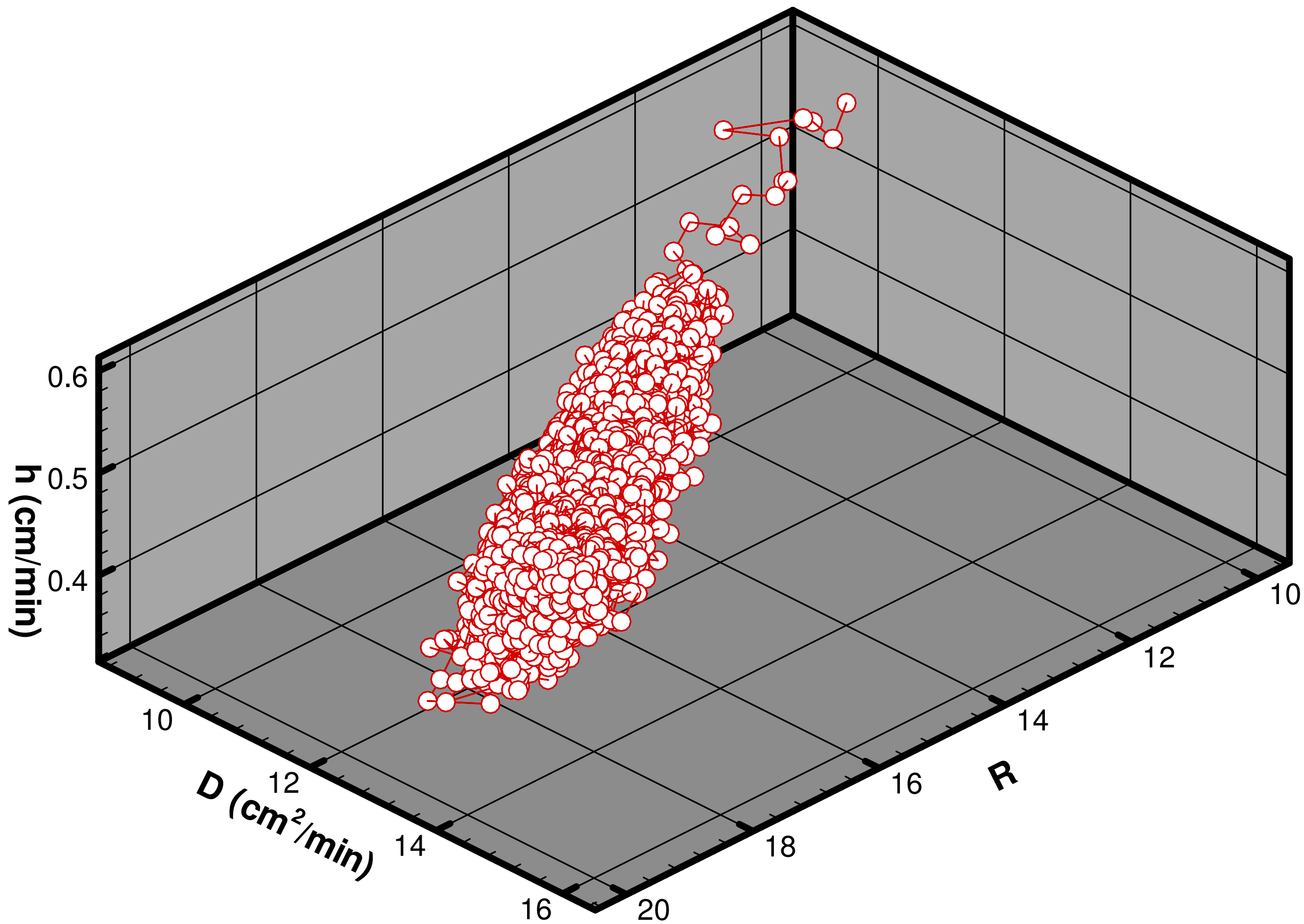
Technique 2: Interpolation with Multiquadrics RBFs



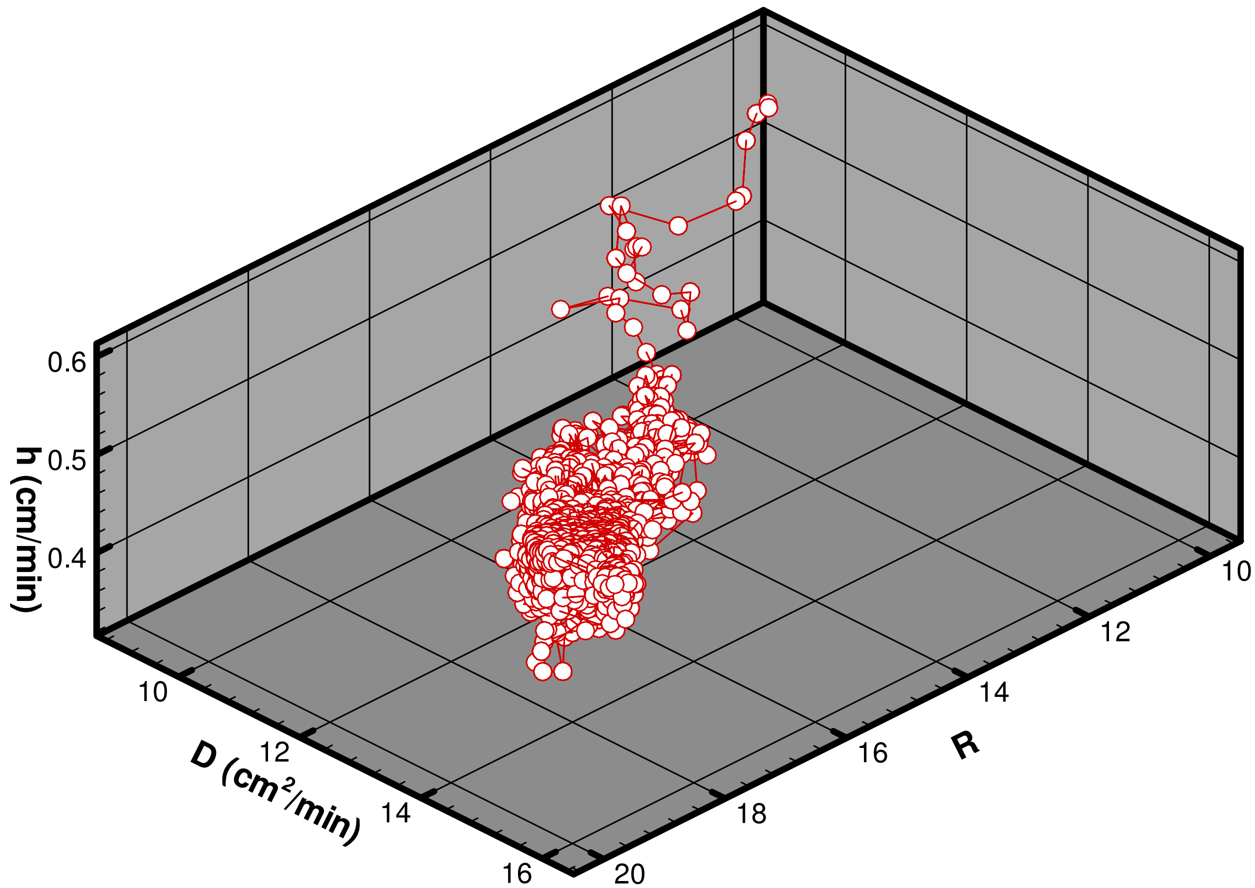
Technique 3: Iterpolation with RBFs using the cross-validation procedure



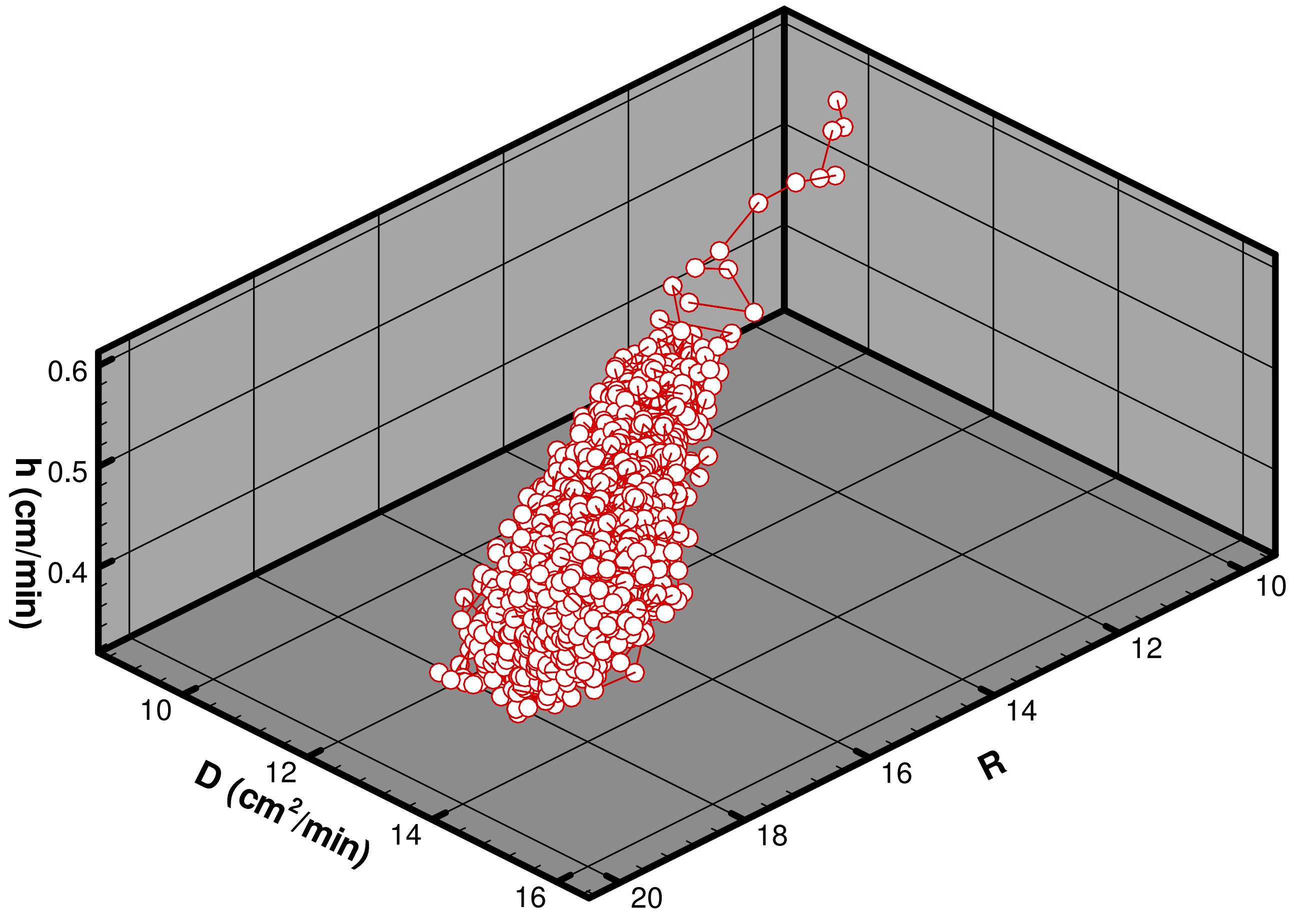
Technique 1: Without interpolation



Technique 2: Interpolation with Multiquadrics RBFs



Technique 3: Iterpolation with RBFs using the cross-validation procedure



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- Prof. Gloria Frontini and the hospitality of UNMDP
- Carlos Alberto de Alencar Mota
- M. D. Mikhailov, R. M. Cotta and M. Colaço
- CNPq-PROSUL, CAPES and FAPERJ

Para non hablar que non me gusta el futebol de Argentina…