IDENTIFICAÇÃO DE PROPRIEDADES FÍSICAS EM PROBLEMAS DE TRANSFERÊNCIA DE MASSA

Renato M. Cotta e Helcio R. B. Orlande
Departamento/Programa de Engenharia Mecânica, POLI/COPPE
Universidade Federal do Rio de Janeiro, UFRJ
cotta@serv.com.ufrj.br e helcio@serv.com.ufrj.br

AGRADECIMENTOS

- **Lucilia B. Dantas**, *Estimativa de Parâmetros na Secagem de Meios Porosos-Capilares*, Tese de Doutorado, PEM/COPPE/UFRJ, 2001
- **Leonardo F. Saker**, *Estimativa Simultânea dos Coeficientes de Transferência de Calor e Massa em Meios Porosos Capilares*, Tese de Mestrado, PEM/COPPE/UFRJ, 2002
- **Udilma da Conceição Nascimento**, *Transporte de Contaminantes em Colunas de Meios Porosos Saturados*, Tese de Doutorado, PEM/COPPE/UFRJ, 2005
- **Paulo H. da Silva Moreira**, *Identificação do Coeficiente Aparente de Difusão em Colunas de Meios Porosos Saturados*, Projeto de Fim de Curso, DEM/POLI/UFRJ, 2004

PROF. ROBERTO DE SOUZA

PROJETO CNEN/COPPE

SUMMARY

1. Luikov’s Equations
2. Diffusion and Dispersion in Saturated Columns

2. LUIKOV'S EQUATIONS

- Luikov, A. V., (1935), **On Thermal Diffusion of Moisture**, *Zh. Prikl. Khim.*, vol.8, pp. 1354.
- Luikov, A. V., (1966), *Heat and Mass Transfer in Capillary-porous Bodies*, Pergamon Press, Oxford.
- Luikov, A. V., (1975), Systems of differential equations of heat and mass transfer in capillary-porous bodies (review), *International Journal of Heat and Mass Transfer,* Volume 18, Issue 1, pp. 1-14.
- Kirscher, O., (1942), *Der Warme-und Stoffaustausch im Trocknunsgut*, VDI-Froschungsheft, 415.
- Philip, I. R. and de Vries, D. A. (1957), *Trans. Am. Geophys. Union*, vol.38, pp. 594.

Mikhailov and Ozisik[1]: "…*Krischer's system was identical to that of Luikov. The system defined by de Vries was also of the Luikov type*…".

[1]Mikhailov, M. D. and Özisik, M. N., (1984), *Unified Analysis and Solutions of Heat and Mass Diffusion*, John Wiley, New York

2. LUIKOV'S EQUATIONS

•**Macroscopic model:** the variables of interest are not representative of heat and mass transfer at the pore scale (microscopic level), but at the scale of a small volume containing a sufficient number of pores. This *representative elementary volume* is the smallest differential volume that results in statistically meaningful local average properties such as porosity, saturation and capillary pressure.

•**Unsaturated capillary porous media.**

•**Experimentally confirmed:** Low initial moisture content, narrow pore size distribution and small moisture content heterogeneities**.**

Remark 1: For a microscopic model, see, p.ex., F. Plourde and M. Prat, (2003), Pore network simulations of drying of capillary porous media. Influence of thermal gradients, *International Journal of Heat and Mass Transfer,* Volume 46, pp. 1293-1307.

Remark 2: A body is said to be capillary-porous, and the pores to be capillaries, if the capillary potential is significantly greater than the gravity potential. In this case, the effects of the gravity force can be neglected.

Remark 3: Large-scale heterogeneities of moisture content during drying have been observed for initially saturated porous media.

2. LUIKOV'S EQUATIONS

HYPOTHESES

- Water, in the liquid and vapor phases (i.e., no ice, $T > 0^{o}$C), and air, fill the pores of the capillary-porous body;
- The mass flow rate in the body is extremely slow, so that the temperatures of the interstitial fluids and of the porous matrix are locally identical, that is, they are in thermodynamic equilibrium;
- Phase transitions occur between liquid and vapor only;
- Chemical reactions do not take place in the medium;
- The mass of air, as well as the mass of vapor, is negligible as compared to the mass of liquid water in the pores;
- Changes in the volume and porosity of the body, resulting from changes in the moisture content, are neglected;
- Radiation heat transfer is negligible;
- The medium is isotropic.

2. LUIKOV'S EQUATIONS

Energy Conservation Equation:

$$\rho_0 c \frac{\partial T}{\partial t} = -\nabla.\mathbf{q} + \sum_{i=1}^{2} h_i I_i$$

Mass Conservation Equation:

$$\rho_0 \frac{\partial u_i}{\partial t} = -\nabla.\mathbf{J}_i + I_i$$

$i = 1$ and 2

Subscript $i = 0$ refers to the dry body, $i = 1$ to the water vapor and $i = 2$ to the liquid water

u_i , h_i, I_i and $\mathbf{J}_i$ are the mass content, enthalpy, mass source/sink and mass flux vector for phase i, respectively, while T is the temperature, $\mathbf{q}$ is the heat flux vector, ρ_0 is the density of the dry body and c is the reduced specific heat.

2. LUIKOV'S EQUATIONS

The **moisture content *u*** is defined as the water relative concentration, that is,

$$u = \frac{\sum_{i=1}^{2} m_i}{m_0} = \sum_{i=1}^{2} u_i$$

where $u_i = m_i/m_0$ and m_i is mass of phase i.

Since the mass of vapor is negligible as compared to the mass of liquid water, we have that $u = u_2$.

2. LUIKOV'S EQUATIONS

The **mass source/sink** results from the water phase change:

$$I_1 = -I_2 = \varepsilon \rho_0 \frac{\partial u}{\partial t}$$

where **ε is the phase-change criterion** ($0 \leq \varepsilon \leq 1$).

- **$\varepsilon = 0$:** no phase-change takes place inside the porous medium; moisture is transported in the medium as liquid and the phase change takes place at the body surface.
- **$\varepsilon = 1$:** all the liquid changes phase in the pores and it is then transported through the body as vapor.

2. LUIKOV'S EQUATIONS

The **source/sink term in the energy equation** refers to the phase change in the medium:

$$h_1 I_1 + h_2 I_2 = (h_1 - h_2) I_1 = \varepsilon \, r \, \rho_0 \frac{\partial u}{\partial t}$$

where r is the latent heat of vaporization.

The **reduced specific heat** is given by:

$$c = c_0 + \sum_{i=1}^{2} c_i u_i$$

where c_i is the specific heat of phase i.

2. LUIKOV'S EQUATIONS

Constitutive Equations:

Conduction heat flux: $\mathbf{q} = -k\,\nabla T$

where k is the body effective thermal conductivity.

For capillary-porous media, Luikov has shown that the **diffusive mass flux** can be written in terms of the moisture content gradient and of the temperature gradient.

Diffusive mass flux: $\mathbf{J} = -\rho_0\, a_m (\nabla u + \delta\,\nabla T)$

where δ is the thermogradient coefficient and a_m is the moisture diffusivity.

2. LUIKOV'S EQUATIONS

LUIKOV'S SYSTEM OF EQUATIONS

$$\rho_0 c \frac{\partial T}{\partial t} = \nabla.(k \nabla T) + r\varepsilon\rho_0 \frac{\partial u}{\partial t}$$

$$\frac{\partial u}{\partial t} = \nabla.(a_m \nabla u) + \nabla.(a_m \delta \nabla T)$$

For constant thermophysical properties:

$$\frac{\partial T}{\partial t} = a\nabla^2 T + \frac{r\varepsilon}{c}\frac{\partial u}{\partial t}$$

$$\frac{\partial u}{\partial t} = a_m \nabla^2 u + a_m \delta \nabla^2 T$$

where $a = k/\rho_0 c$ is the thermal diffusivity.

2. LUIKOV'S EQUATIONS

REMARK: A third equation is needed to model fast and intense drying processes, for which vigorous boiling may happen, in special if the temperatures exceed 100 ^{o}C. This additional equation involves the pressure gradient in the medium and is also required when the flow is imposed by a pressure gradient. Also, the energy and mass conservation equations above need to be changed.

2. LUIKOV'S EQUATIONS

BOUNDARY CONDITION – MASS CONSERVATION

$$-a_m \rho_0 \left(\frac{\partial u}{\partial \mathbf{n}} + \delta \frac{\partial T}{\partial \mathbf{n}} \right) + j_m = 0$$

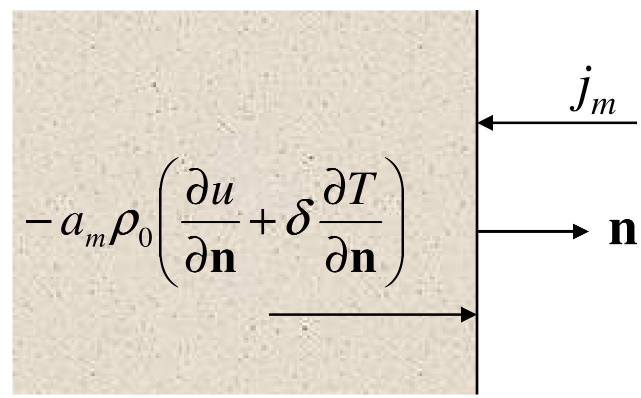
where $\dfrac{\partial}{\partial \mathbf{n}}$ = normal derivative at the boundary surface

δ = thermogradient coefficient

a_m = moisture diffusivity

j_m = imposed mass flux

ρ_0 = density of the dry body



2. LUIKOV'S EQUATIONS

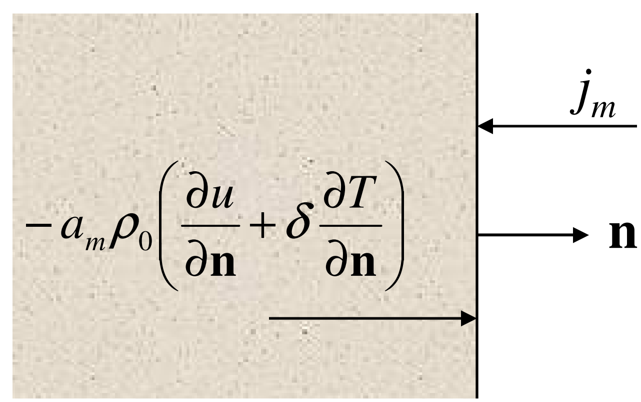
For the body interacting with the surrounding air: $j_m = h_m \, \rho_0 (u^* - u)$

where:

- mass transfer coefficient: h_m [m/s]
- moisture content in equilibrium with the surrounding air: u^*

Therefore:

$$-a_m \left(\frac{\partial u}{\partial \mathbf{n}} + \delta \frac{\partial T}{\partial \mathbf{n}} \right) + h_m (u^* - u) = 0$$



2. LUIKOV'S EQUATIONS

BOUNDARY CONDITION – ENERGY EQUATION

$$-k\frac{\partial T}{\partial \mathbf{n}} + j_q - r\, j_{m2} = 0$$

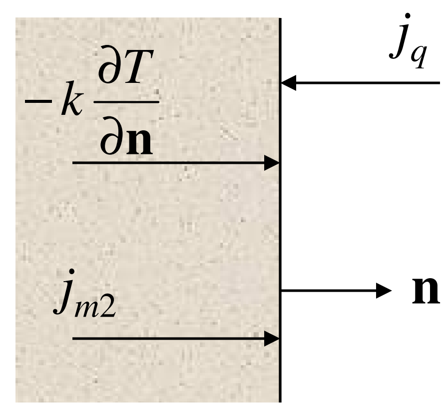
where $\frac{\partial T}{\partial \mathbf{n}}$ = normal derivative of temperature at the boundary surface

k = effective thermal conductivity

j_q = imposed heat flux

j_{m2} = liquid water mass flux

r = latent heat of vaporization



2. LUIKOV'S EQUATIONS

For the body interacting with the surrounding air: $j_q = h(T_s - T)$

where: h = heat transfer coefficient

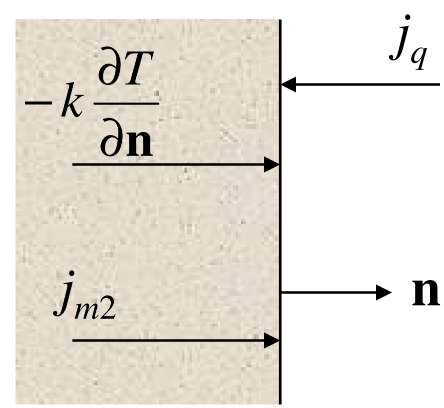
T_s = temperature of the surrounding air

Liquid mass flux: $j_{m2} = -(1-\varepsilon) a_m \rho_0 \left(\frac{\partial u}{\partial \mathbf{n}} + \delta \frac{\partial T}{\partial \mathbf{n}} \right) = -(1-\varepsilon) h_m \rho_0 (u^* - u)$

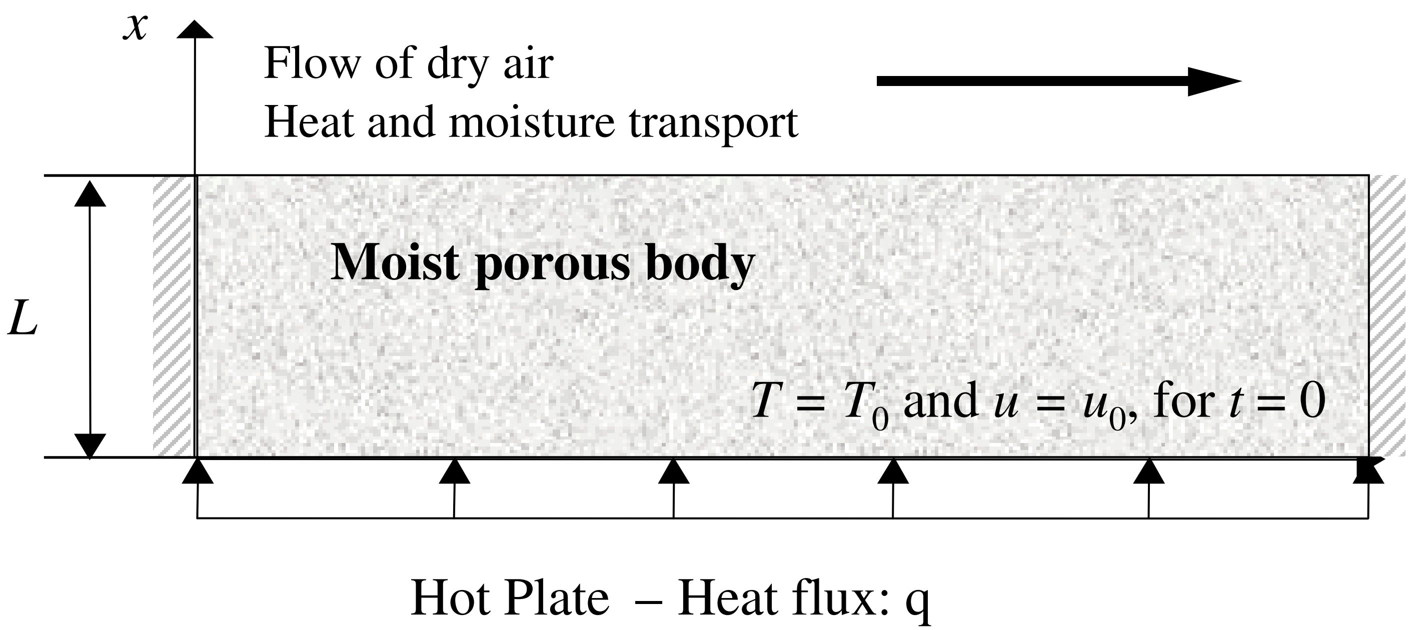
where: ε = phase-change factor

Therefore:

$$-k \frac{\partial T}{\partial \mathbf{n}} + h(T_s - T) + r(1-\varepsilon) h_m \rho_0 (u^* - u) = 0$$



3. PARAMETER ESTIMATION



3. PARAMETER ESTIMATION

$$\theta(X,\tau) = \frac{T(x,t) - T_o}{T_s - T_o},$$

$$\phi(X,\tau) = \frac{u_o - u(x,t)}{u_o - u^*},$$

$$X = \frac{x}{L},$$

$$\tau = \frac{at}{L^2},$$

$$Q = \frac{qL}{k(T_s - T_o)},$$

$$Bi_q = \frac{hL}{k} = \text{Biot number for heat transfer}$$

$$Bi_m = \frac{h_m L}{a_m} = \text{Biot number for mass transfer}$$

3. PARAMETER ESTIMATION

$$Lu = \frac{a_m}{a}$$

$$Pn = \delta \frac{T_s - T_o}{u_o - u^*}$$

$$Ko = \frac{r}{c} \frac{u_o - u^*}{T_s - T_o}$$

- The *Luikov number* is a ratio between the mass and heat diffusivities. Thus, it compares how the mass transfer and the heat transfer processes develop.
- The *Posnov number* indicates the change in moisture content resulting from the temperature gradient relative to the total moisture change.
- The *Kossovitch number* indicates how the heat expended in the evaporation of the liquid compares to that expended for heating the wet body.

3. PARAMETER ESTIMATION

$$\frac{\partial \theta(X,\tau)}{\partial \tau} = \frac{\partial^2 \theta(X,\tau)}{\partial X^2} - \varepsilon Ko \frac{\partial \phi(X,\tau)}{\partial \tau}$$

$$\frac{\partial \phi(X,\tau)}{\partial \tau} = Lu \frac{\partial^2 \phi(X,\tau)}{\partial X^2} - LuPn \frac{\partial^2 \theta(X,\tau)}{\partial X^2}$$

in $0 < X < 1$, for $\tau > 0$

$$\theta(X,0) = 0, \quad \phi(X,0) = 0,$$

for $\tau = 0$ in $0 < X < 1$

$$\frac{\partial \theta(0,\tau)}{\partial X} = -Q, \qquad \frac{\partial \phi(0,\tau)}{\partial X} - Pn \frac{\partial \theta(0,\tau)}{\partial X} = 0,$$

at $X = 0$, for $\tau > 0$

$$\frac{\partial \theta(1,\tau)}{\partial X} - Bi_q [1 - \theta(1,\tau)] + (1-\varepsilon) KoLuBi_m [1 - \phi(1,\tau)] = 0,$$

$$-\frac{\partial \phi(1,\tau)}{\partial X} + Pn \frac{\partial \theta(1,\tau)}{\partial X} + Bi_m [(1 - \phi(1,\tau)] = 0,$$

at $X = 1$, for $\tau > 0$

3. PARAMETER ESTIMATION

DIRECT PROBLEM

Known:

- Boundary and initial conditions
- Lu, Pn, Ko, Bi_q, Bi_m and ε

Determine:

- Temperature distribution $\theta(X, \tau)$
- Moisture content distribution $\phi(X, \tau)$

INVERSE PROBLEM

Known:

- Boundary and initial conditions
- ***Temperature measurements*** $Y_m(\tau_i)$ taken at locations X_m , m=1,…,M and times τ_i, i=1,…,I

Estimate:

- Lu, Pn, Ko, Bi_q, Bi_m and ε

3. PARAMETER ESTIMATION

Minimize: $$S(\mathbf{P}) = [\mathbf{Y} - \boldsymbol{\theta}(\mathbf{P})]^T [\mathbf{Y} - \boldsymbol{\theta}(\mathbf{P})]$$

where:

$$[\mathbf{Y} - \boldsymbol{\theta}(\mathbf{P})]^T \equiv \left[(\vec{Y}_1 - \vec{\theta}_1), (\vec{Y}_2 - \vec{\theta}_2), \ldots, (\vec{Y}_I - \vec{\theta}_I) \right]$$

$$\left(\vec{Y}_i - \vec{\theta}_i \right) = \left[Y_{i1} - \theta_{i1}, Y_{i2} - \theta_{i2}, \ldots, Y_{iM} - \theta_{iM} \right]$$

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**.
- The measurements are uncorrelated.
- The standard-deviation of the measurements is constant.

LEVENBERG-MARQUARDT'S METHOD

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

where μ^k is a positive scalar, $\mathbf{J}^k$ is the sensitivity matrix, $\mathbf{\Omega}^k$ is a diagonal matrix and k is the number of iterations

- 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.

3. PARAMETER ESTIMATION

Test-case: Drying of ceramics

$\rho_0 = 2000$ kg/m^3

$k_q = 0.34$ W/mK , $k_m = 2.4\text{x}10^{-7}$ kg/ms°M

$c_q = 607$ J/kgK , $c_m = 1.8\text{x}10^{-3}$ kg/kg°M

$\delta = 0.56$ °M/K , $r = 2.5\text{x}10^{6}$ J/kg.

$l = 0.05$ m

$T_0 = 24$ °C , $u_0/c_m = 80$ °M

$T_s = 30$ °C , $u^*/c_m = 40$ °M

$h_q = 17$ W/m^{2}K , $h_m = 1.2\text{x}10^{-5}$ kg/m^{2}s°M

⇒

$Bi_q = 2.5$

$Bi_m = 2.5$

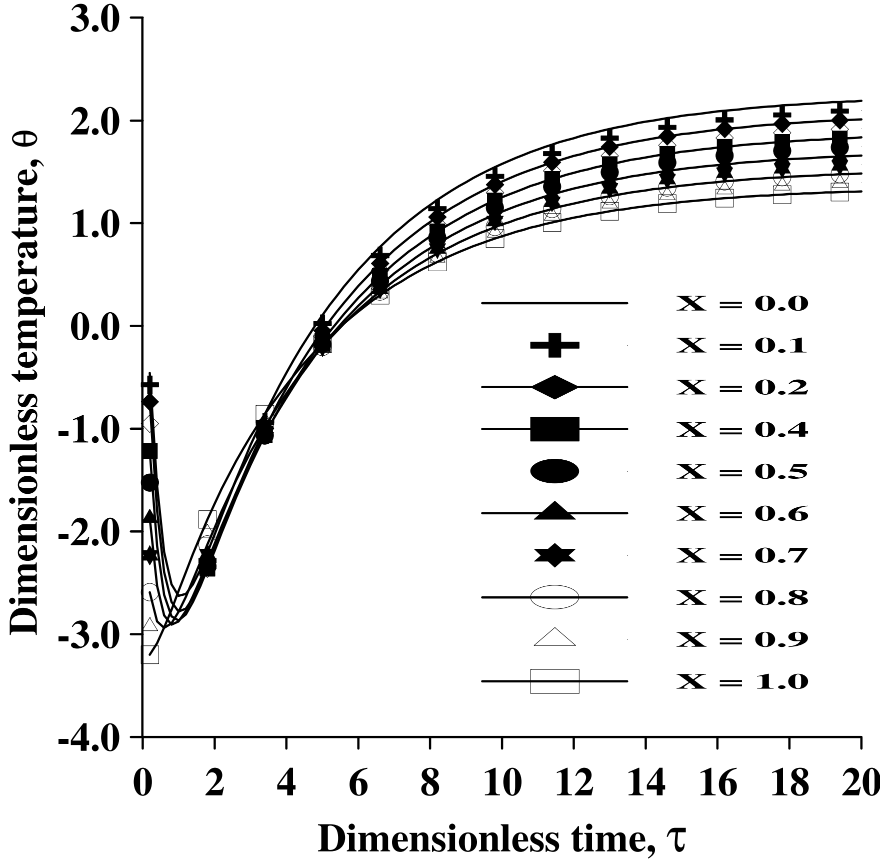
$Lu = 0.2$

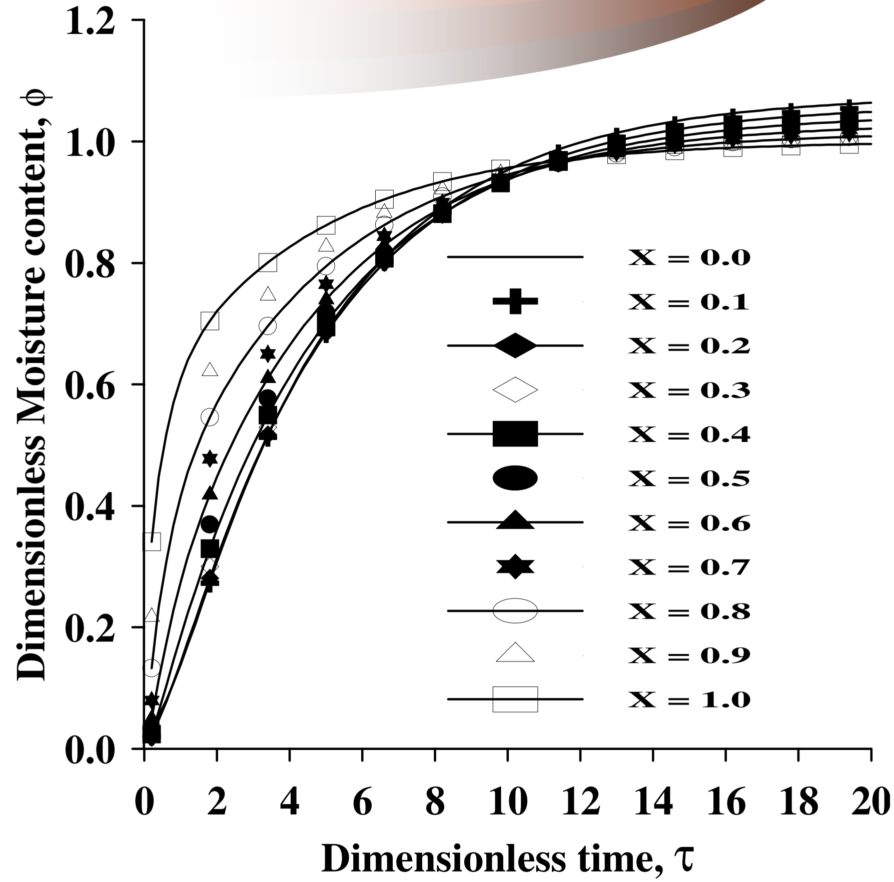
$Pn = 0.084$

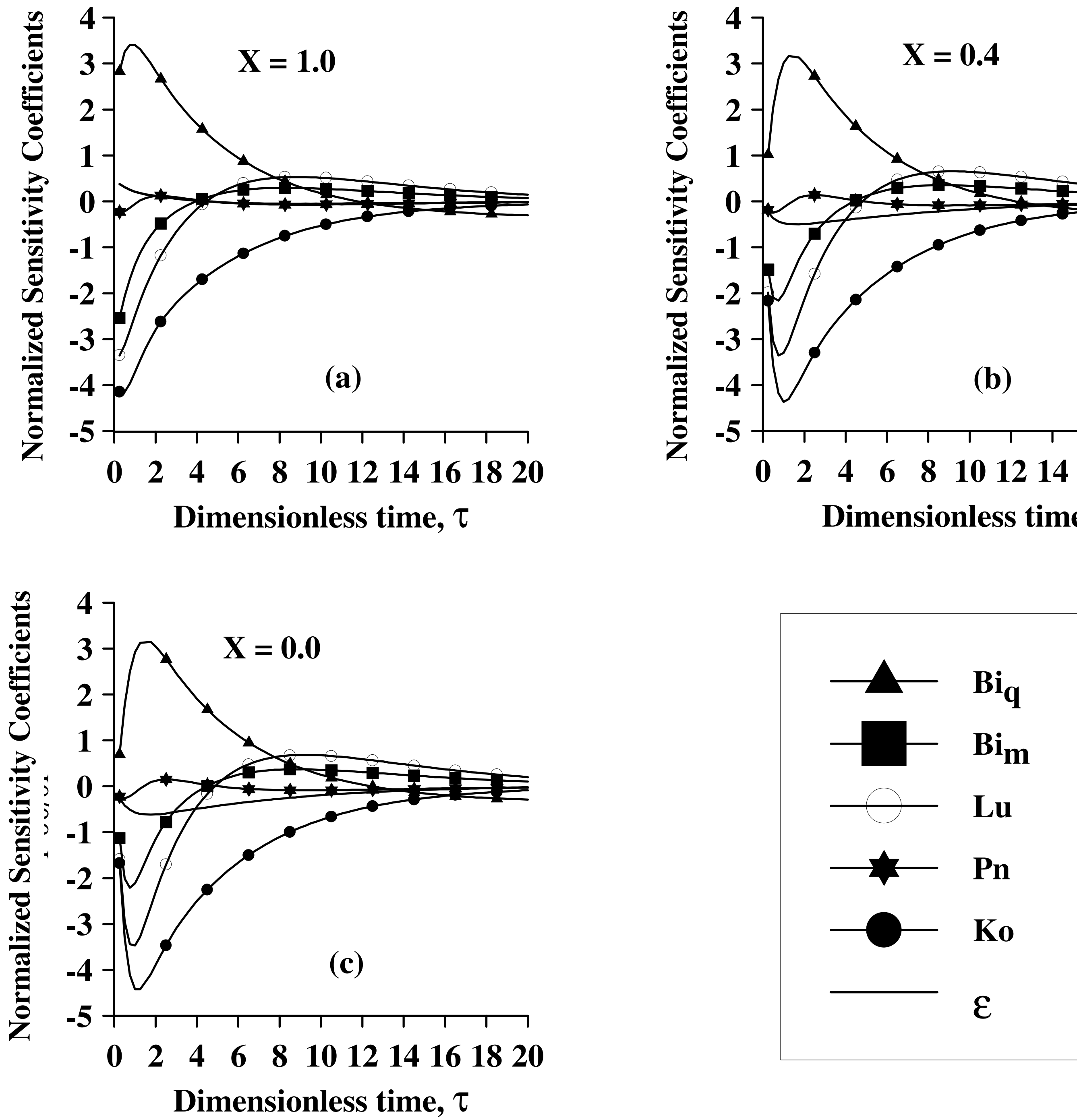
$Ko = 49$

$\varepsilon = 0.2$

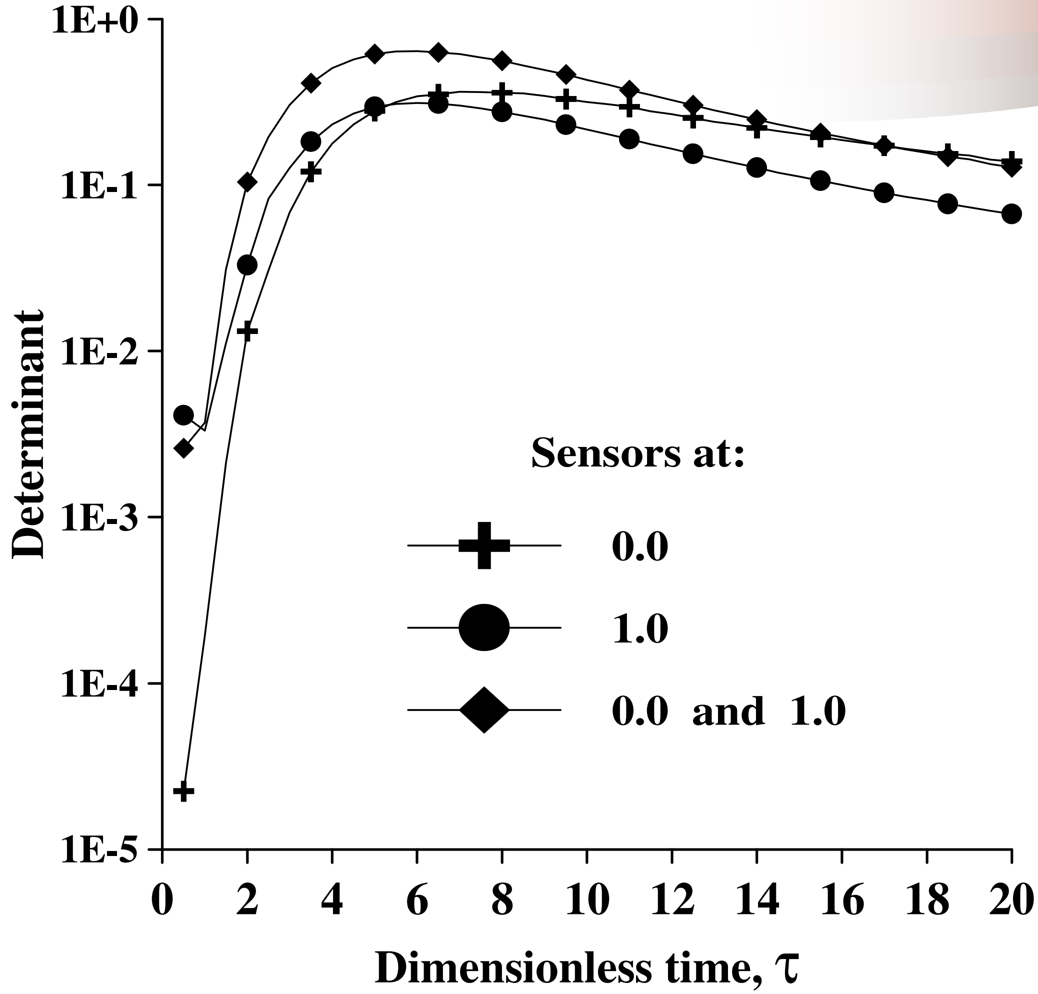
TEMPERATURE AND MOISTURE CONTENT






X = 1.0
(a)
X = 0.4
(b)
X = 0.0
(c)
Normalized Sensitivity Coefficients
Dimensionless time, τ
4
3
2
1
0
-1
-2
-3
-4
-5
0 2 4 6 8 10 12 14 16 18 20
Bi_q
Bi_m
Lu
Pn
Ko
ε

3. PARAMETER ESTIMATION



3. PARAMETER ESTIMATION

Levenberg-Marquardt's Method

Initial-guesses: $Lu^0 = 1.0$, $Bi_q^{\,0} = 5.0$, $Ko^0 = 60.0$

Parameters	Exact	Estimated $\sigma = 0$	Estimated $\sigma = 0.01\ Y_{max}$	Confidence intervals
Bi_q	2.5	2.5	2.500	(2.500,2.502)
Lu	0.2	0.2	0.20	(0.19,0.21)
Ko	49.0	49.0	48.99	(48.92,49.05)

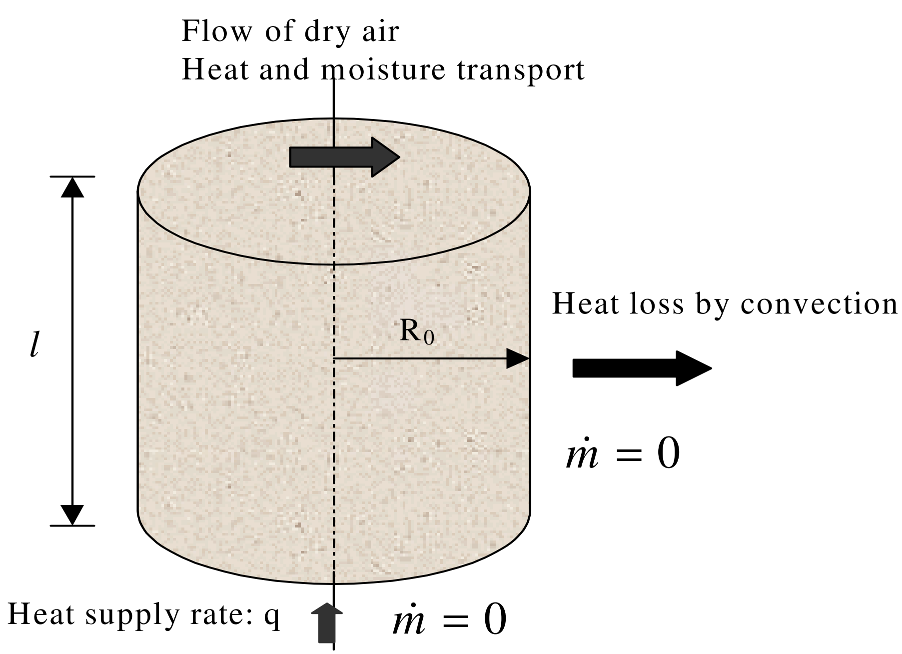
3. PARAMETER ESTIMATION

DIRECT PROBLEM

2D Formulation

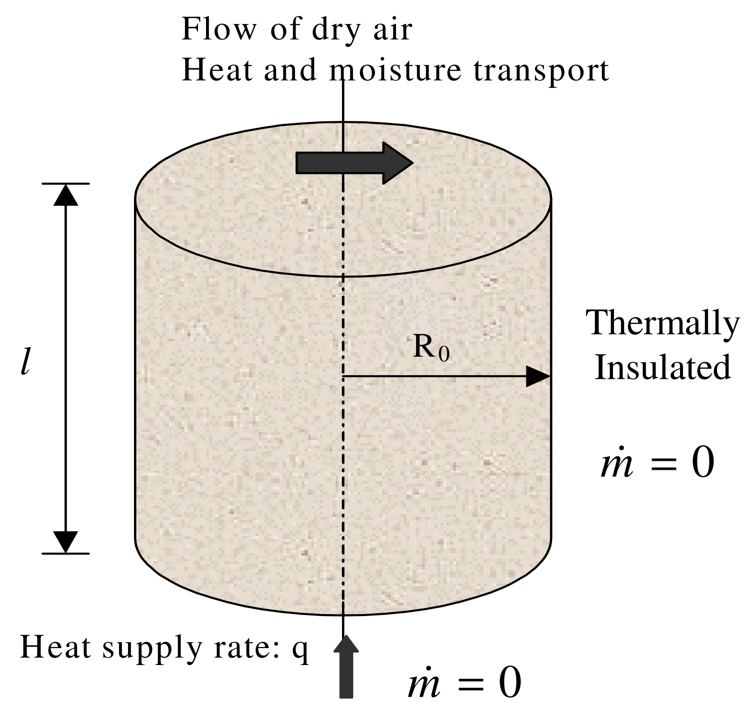
↓

Simulated Measurements



INVERSE PROBLEM

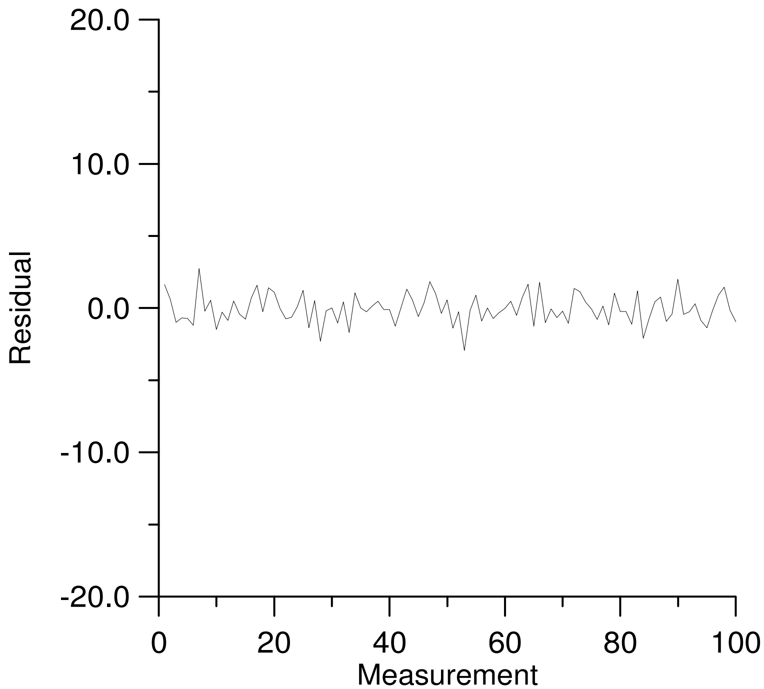
1D Formulation



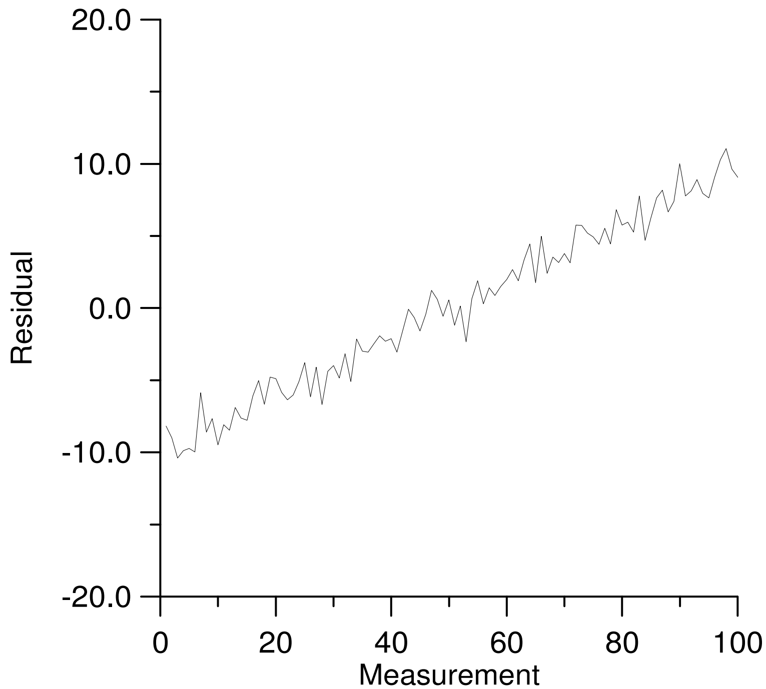
3. PARAMETER ESTIMATION

ANALYSIS OF THE RESIDUALS: $R_{\theta m}(t_i) = Y_{im} - \hat{\theta}_{im}$

Independent

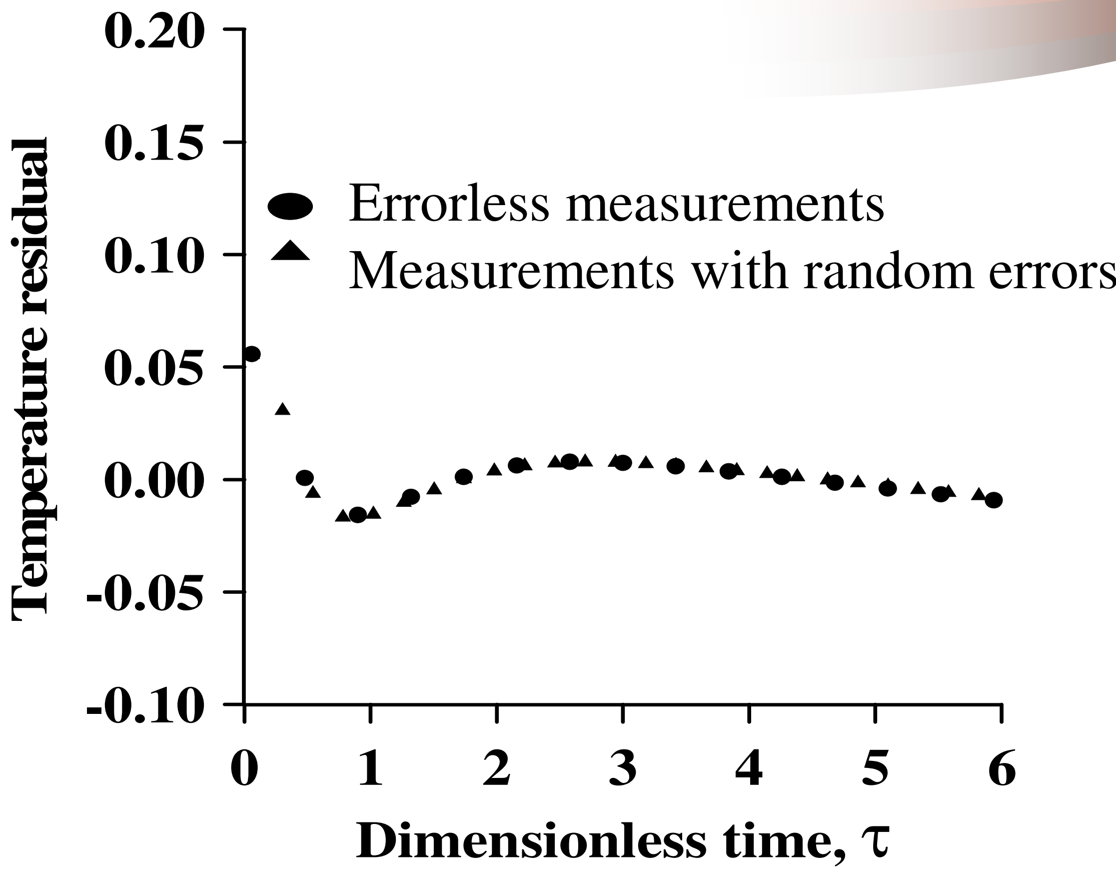


Correlated

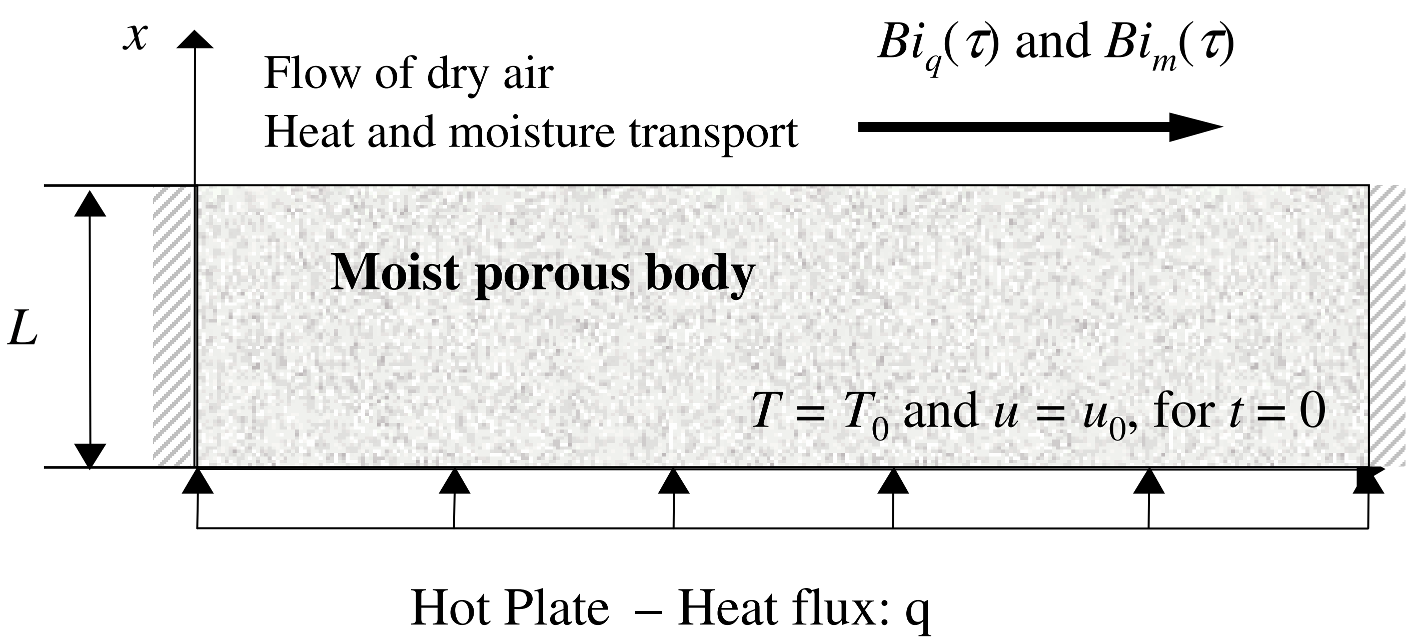


3. PARAMETER ESTIMATION

$r_a=1$
$Bi_{qr}=0.1$



4. FUNCTION ESTIMATION



4. FUNCTION ESTIMATION

$$\left.\begin{aligned}\frac{\partial \theta}{\partial \tau} &= \alpha \frac{\partial^2 \theta}{\partial X^2} - \beta \frac{\partial^2 \phi}{\partial X^2} \\ \frac{\partial \phi}{\partial \tau} &= Lu \frac{\partial^2 \phi}{\partial X^2} - Lu\ Pn \frac{\partial^2 \theta}{\partial X^2}\end{aligned}\right\} \quad \text{in } 0 < X < 1 \text{ and } \tau > 0$$

$$\left.\begin{aligned}\frac{\partial \theta}{\partial X} &= -Q \\ \frac{\partial \phi}{\partial X} &= -Pn\, Q\end{aligned}\right\} \quad \text{at } X = 0 \text{, for } \tau > 0$$

$$\alpha = 1 + \varepsilon\, Ko\, Lu\, Pn$$

$$\beta = \varepsilon\, Ko\, Lu$$

$$\left.\begin{aligned}\frac{\partial \theta}{\partial X} &= Bi_q(\tau)(1-\theta) - (1-\varepsilon) Ko\, Lu\, Bi_m(\tau)(1-\phi) \\ \frac{\partial \phi}{\partial X} &= Pn \frac{\partial \theta}{\partial X} + Bi_m(\tau)(1-\phi)\end{aligned}\right\} \quad \text{at } X = 1 \text{, for } \tau > 0$$

$$\theta(X,0) = \phi(X,0) = 0 \qquad \text{for } \tau = 0 \text{, in } 0 < X < 1$$

4. FUNCTION ESTIMATION

DIRECT PROBLEM

Known:

- Boundary and initial conditions
- Thermophysical properties

↓

Determine:

- Temperature distribution $\theta(X, \tau)$
- Moisture distribution $\phi(X, \tau)$

INVERSE PROBLEM

Known:

- Initial condition
- Boundary condition at X=0
- Thermophysical properties
- *Temperature measurements*
- *Moisture content measurements*
- *Total moisture measurements*

↓

Estimate:

$Bi_m(\tau)$ and $Bi_q(\tau)$

4. FUNCTION ESTIMATION

Minimization of the following functional:

$$S[Bi_m(\tau), Bi_q(\tau)] =$$

$$= \int_{\tau=0}^{\tau_f} \left\{ \sum_{i=1}^{I} [\theta(X_i, \tau; Bi_m, Bi_q) - M_i(\tau)]^2 w_\theta \right\} d\tau +$$

$$+ \int_{\tau=0}^{\tau_f} \left\{ \sum_{n=1}^{N} [\phi(X_n^*, \tau; Bi_m, Bi_q) - C_n(\tau)]^2 w_\phi \right\} d\tau + \int_{\tau=0}^{\tau_f} [\Gamma(\tau; Bi_m, Bi_q) - P(\tau)]^2 w_\Gamma \, d\tau$$

$$w_\theta = \frac{C_\theta}{M_{max}^2} \quad , \quad w_\phi = \frac{C_\phi}{C_{max}^2} \quad , \quad w_\Gamma = \frac{C_\Gamma}{P_{max}^2}$$

$$C_\theta, C_\phi, C_\Gamma = \begin{cases} 0 \\ 1 \end{cases}$$

4. FUNCTION ESTIMATION

Iterative Procedure:

$$Bi_m^{k+1}(\tau) = Bi_m^{k}(\tau) + \beta_1^k d_1^k(\tau)$$
$$Bi_q^{k+1}(\tau) = Bi_q^{k}(\tau) + \beta_2^k d_2^k(\tau)$$

Direction of Descent:

$$d_1^k(\tau) = -\nabla S[Bi_m^k(\tau)] + \gamma^k d_1^{k-1}(\tau) + \psi^k d_1^q(\tau)$$
$$d_2^k(\tau) = -\nabla S[Bi_q^k(\tau)] + \gamma^k d_2^{k-1}(\tau) + \psi^k d_2^q(\tau)$$

Conjugation Coefficients:

Polak-Ribiere's version of the conjugate gradient method

Search steps size: β_1^k *and* β_2^k

and

Gradient Directions: $\begin{cases} \nabla S[Bi_m^k(\tau)] \\ \nabla S[Bi_q^k(\tau)] \end{cases}$

→

Sensitivity Problems
and
Adjoint Problem

4. FUNCTION ESTIMATION

Test-case: Ceramics

$k = 0.34\ W/mK$

$k_m = 2.4\text{x}10^{-7} kg/ms^oM$

$c = 607\ J/kgK$

$r = 2.5\text{x}106 J/kg$

$T_0 = 24^oC$

$u_0 = 80^oM$

$\delta = 0.56^oM/K$

$t_{final} = 1785$ s

$L = 0.05$m

$Lu = 0.2$

$\text{Pn} = 0.084$

$\text{Ko} = 49$

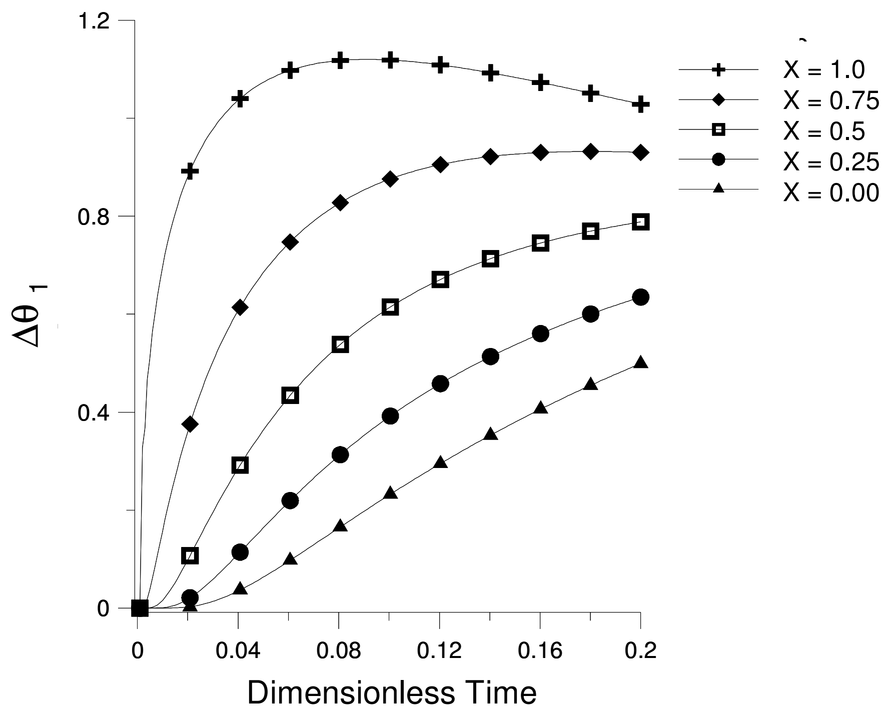
$\varepsilon = 0.2$

$Q = 0.9$

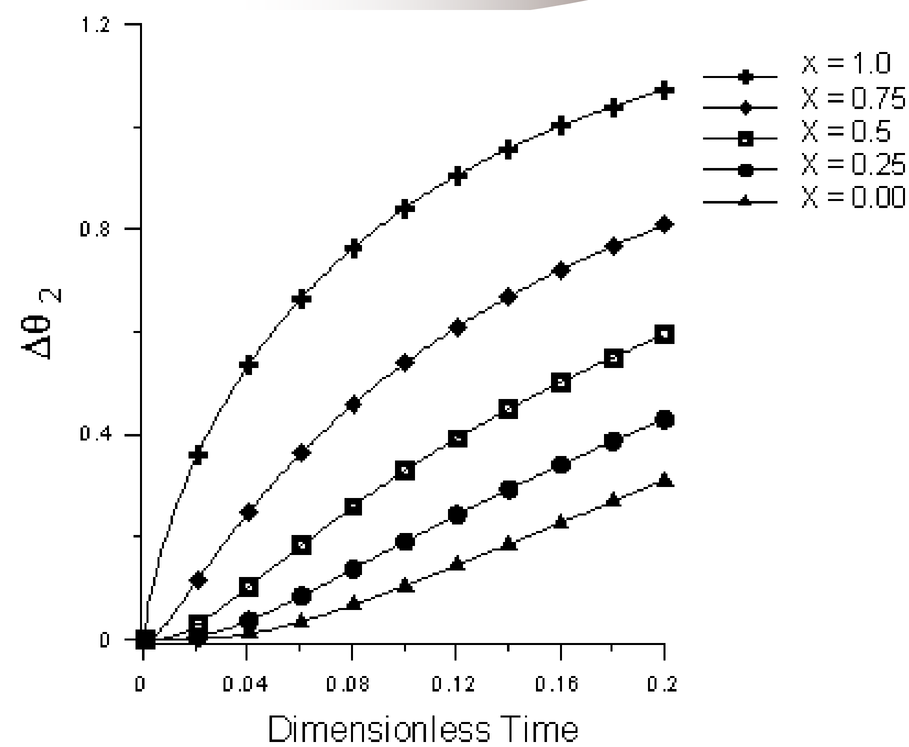
$\tau_f = 0.2$

4. FUNCTION ESTIMATION

$$Bi_m(\tau) = Bi_q(\tau) = 2.5$$



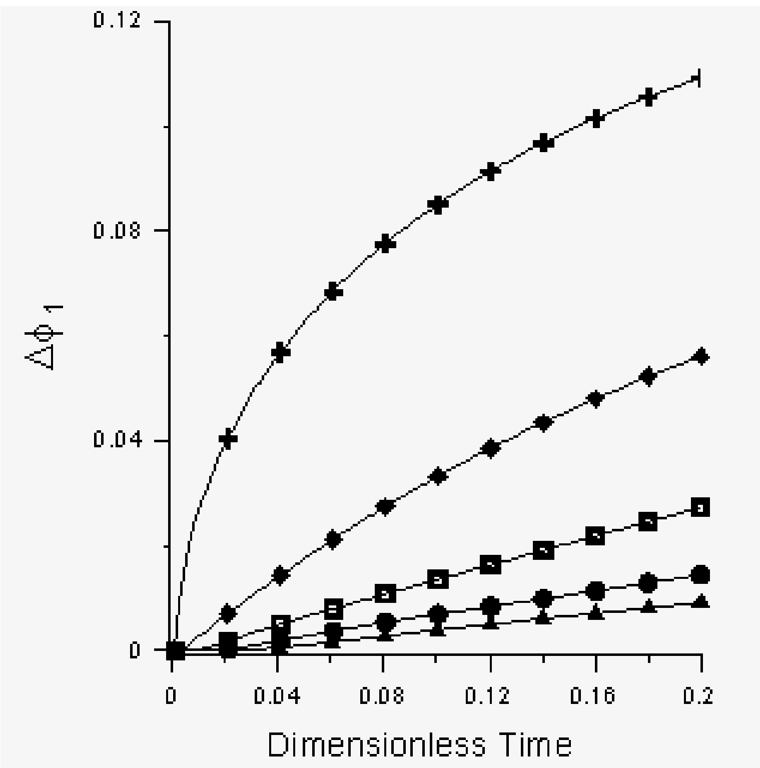
Temperature sensitivity function resulting from variations in $Bi_m(\tau)$



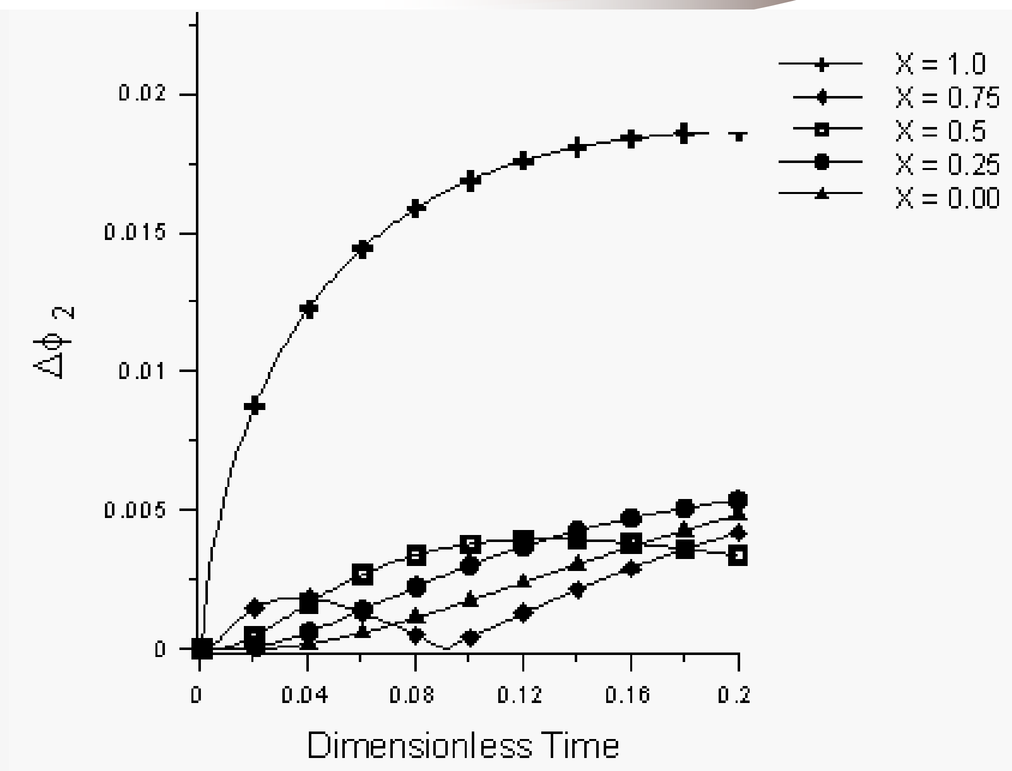
Temperature sensitivity function resulting from variations in $Bi_q(\tau)$

4. FUNCTION ESTIMATION

$$Bi_m(\tau) = Bi_q(\tau) = 2.5$$

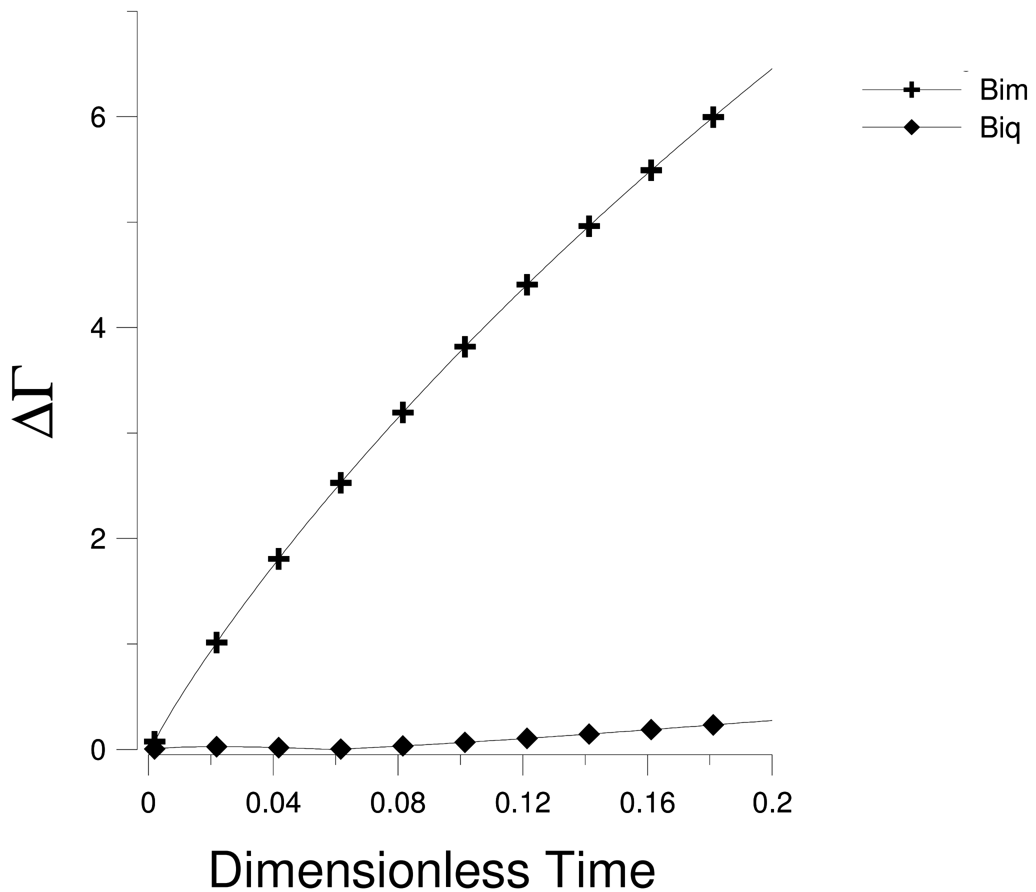


Moisture content sensitivity function resulting from variations in $Bi_m(\tau)$



Moisture content sensitivity function resulting from variations in $Bi_q(\tau)$

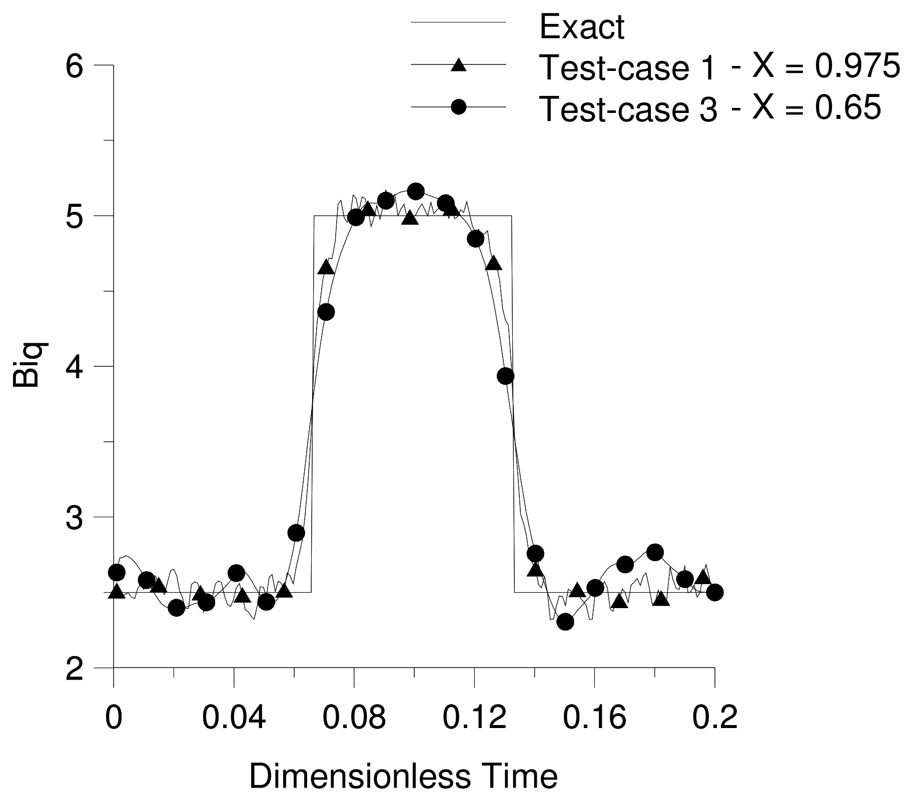
4. FUNCTION ESTIMATION



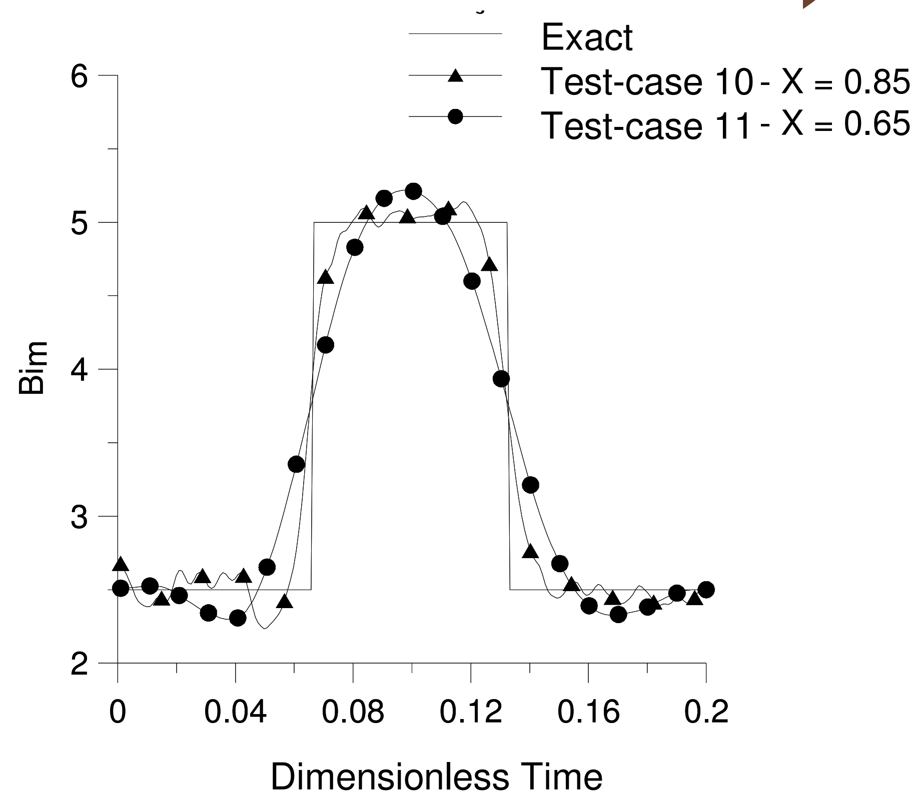
Moisture content total weight sensitivity function

$$Bi_m(\tau) = Bi_q(\tau) = 2.5$$

4. FUNCTION ESTIMATION

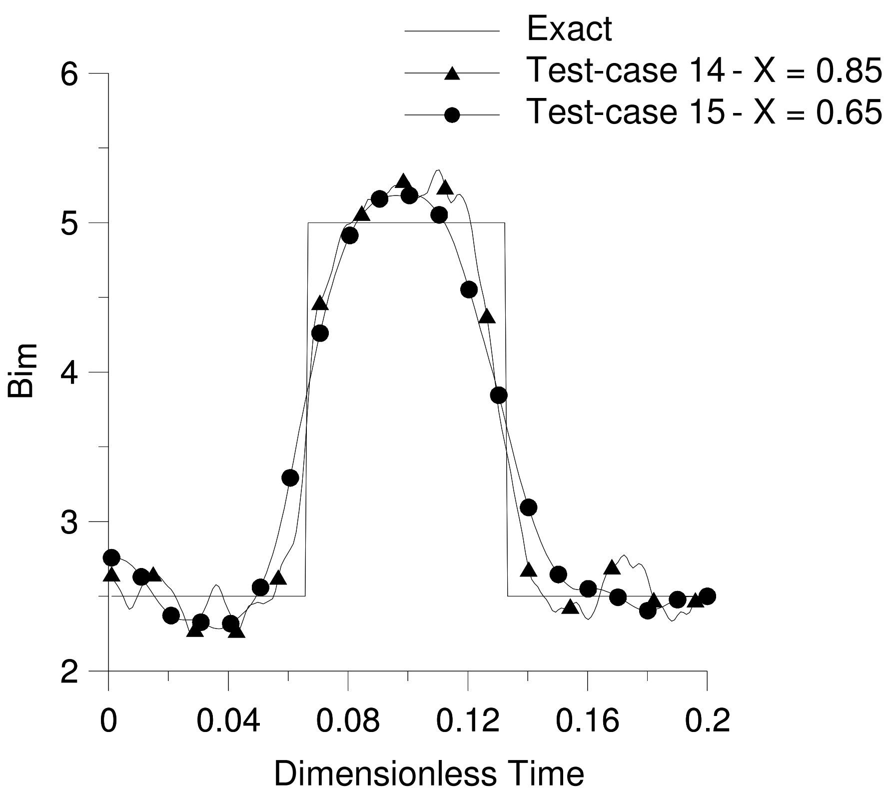


Estimation of $Bi_q(\tau)$ by using only temperature measurements

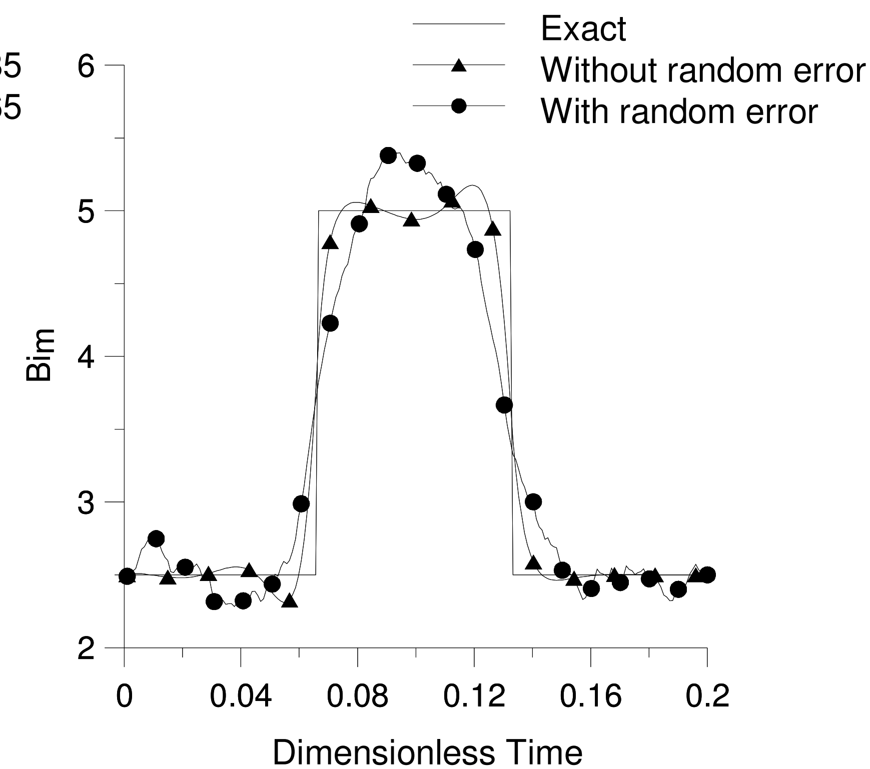


Estimation of $Bi_m(\tau)$ by using only temperature measurements

4. FUNCTION ESTIMATION

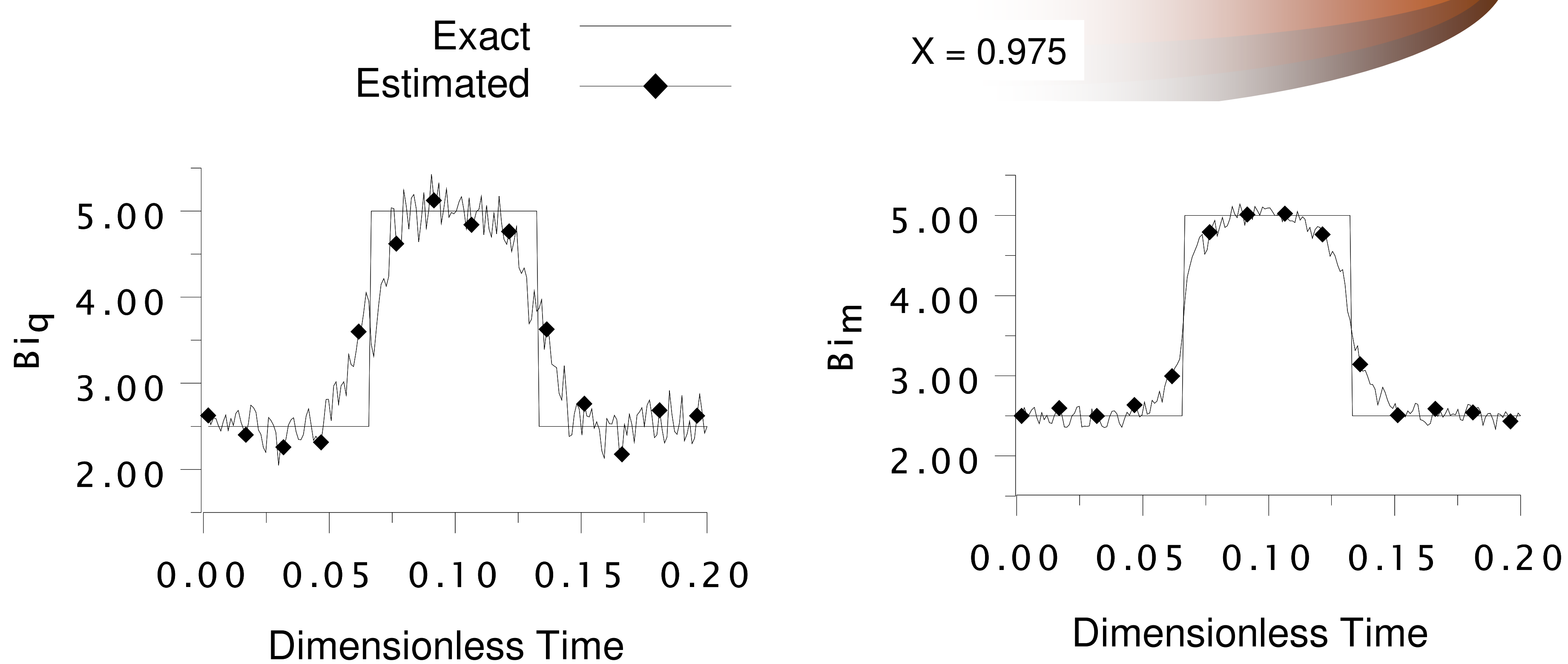


Estimation of $Bi_m(\tau)$ by using only moisture content measurements



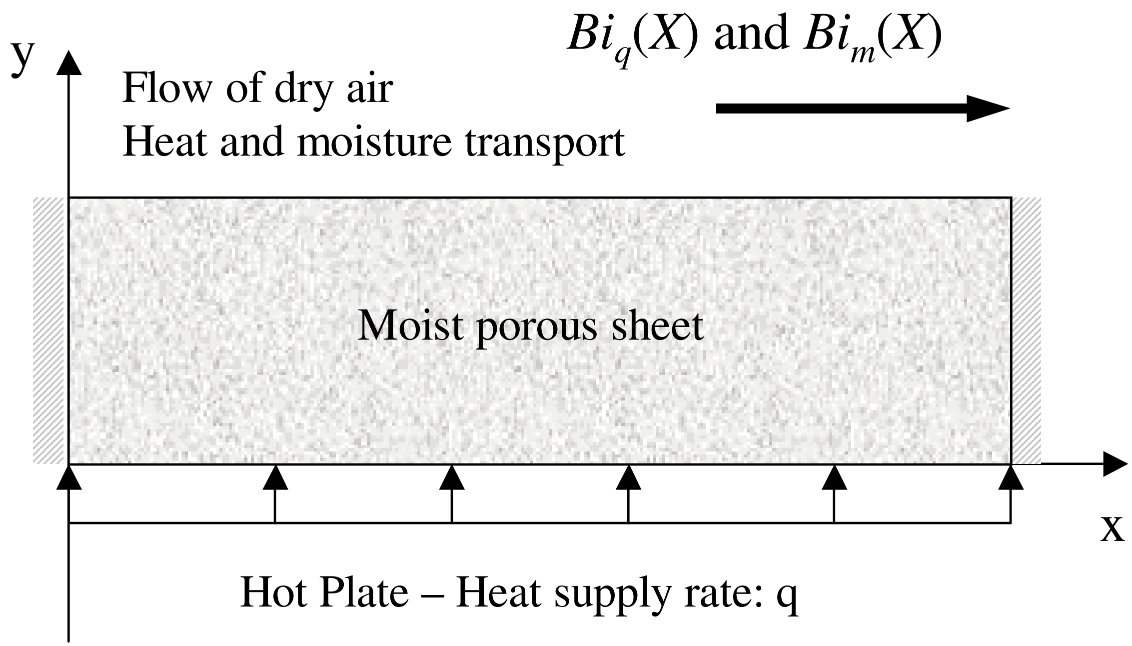
Estimation of $Bi_m(\tau)$ by using only total moisture weight measurements

4. FUNCTION ESTIMATION



Simultaneous estimation of $Bi_m(\tau)$ and $Bi_q(\tau)$ by using temperature and moisture content measurements

4. FUNCTION ESTIMATION

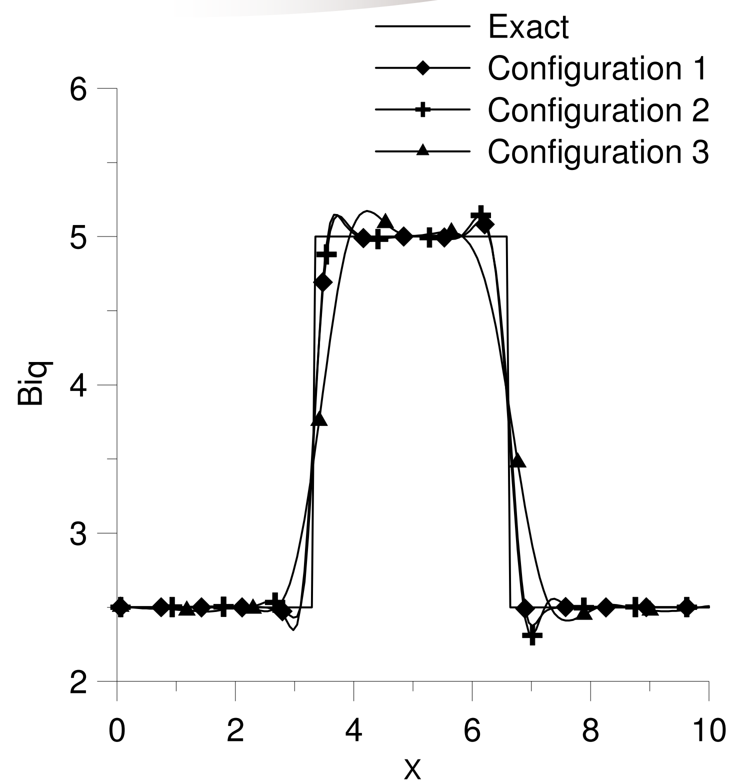


4. FUNCTION ESTIMATION

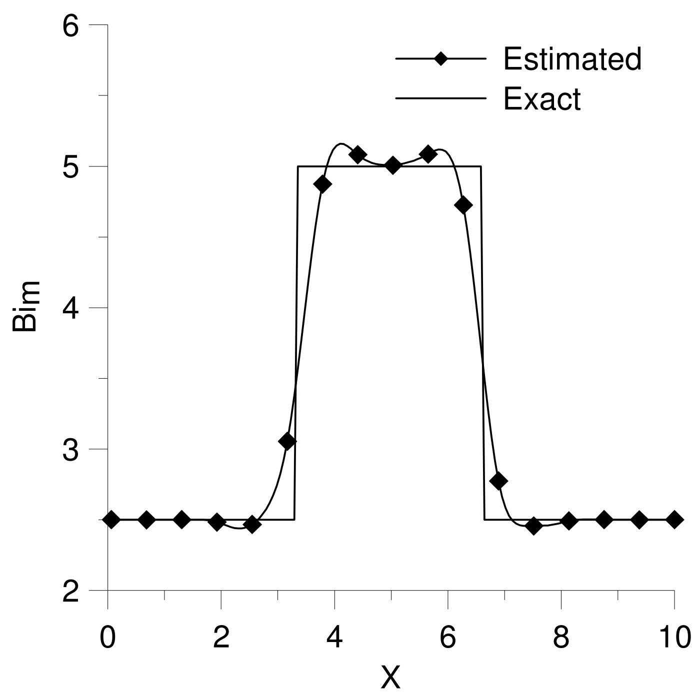
TEMPERATURE SENSORS

Table . Sensor configurations used for the estimation of $Bi_q(X)$ with known $Bi_m(X)$.

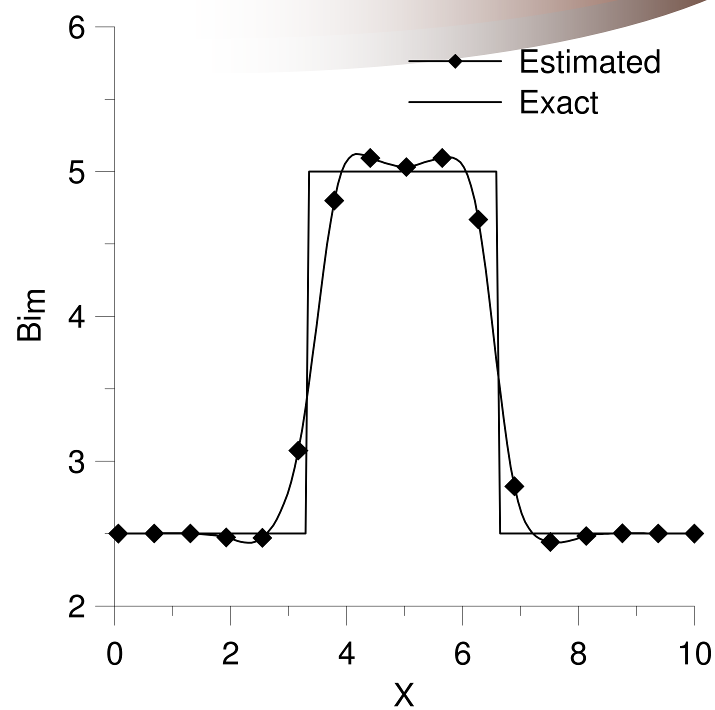
Config.	Number of Sensors	*Y* Location	*RMS Error*
1	33	0.925	4.38×10^{-2}
2	33	0.850	4.58×10^{-2}
3	*13*	0.850	1.11×10^{-1}



4. FUNCTION ESTIMATION



Results obtained for $Bi_m(X)$ with known $Bi_q(X)$ by using temperature measurements of 17 sensors equally spaced

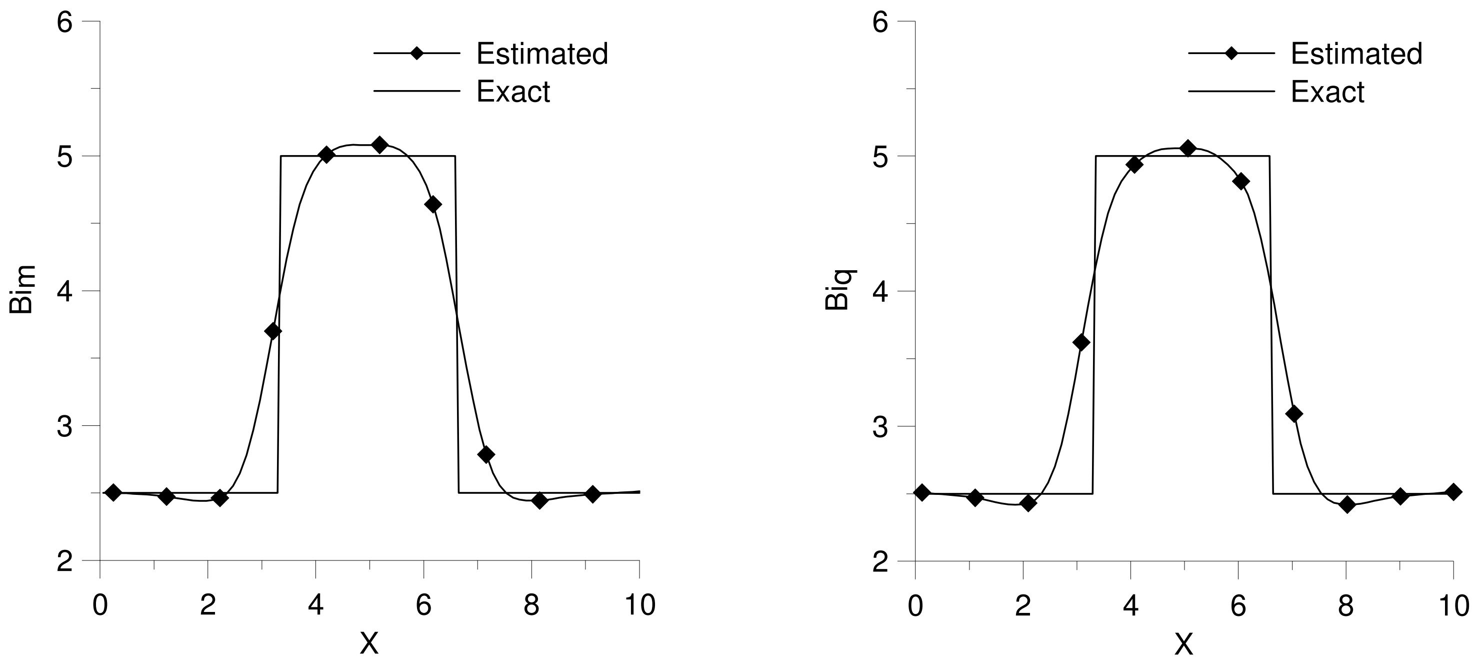


Results obtained for $Bi_m(X)$ with known $Bi_q(X)$ by using moisture content measurements of 17 sensors equally spaced

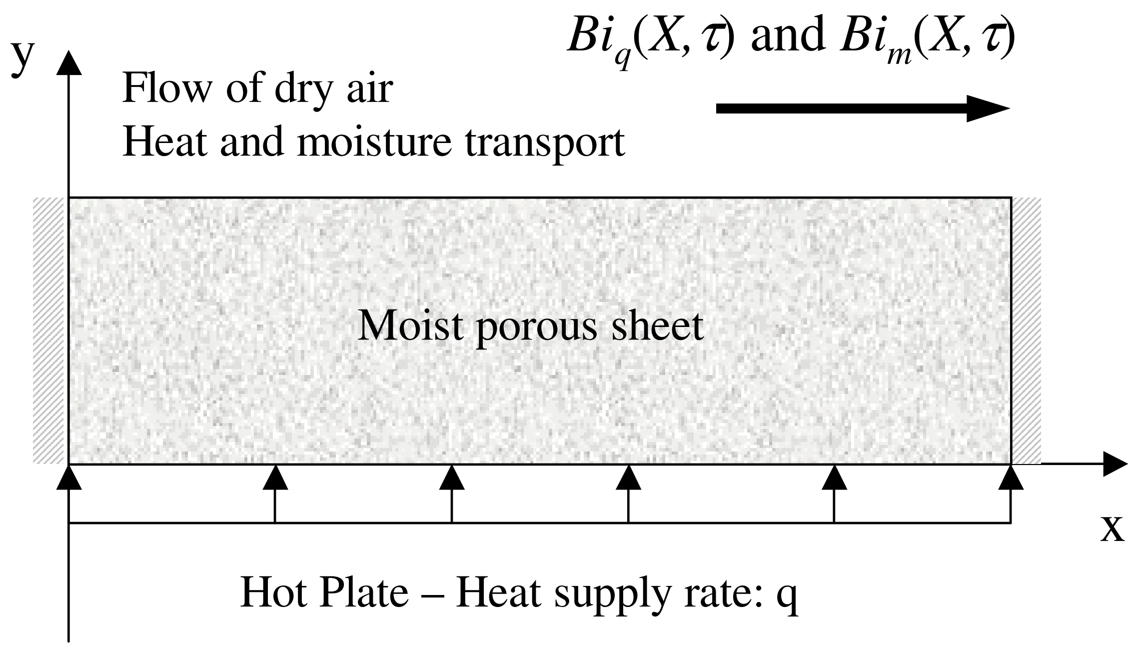
4. FUNCTION ESTIMATION

Simultaneous estimation of $Bi_q(X)$ and $Bi_m(X)$:

14 temperature sensors and 15 moisture content sensors

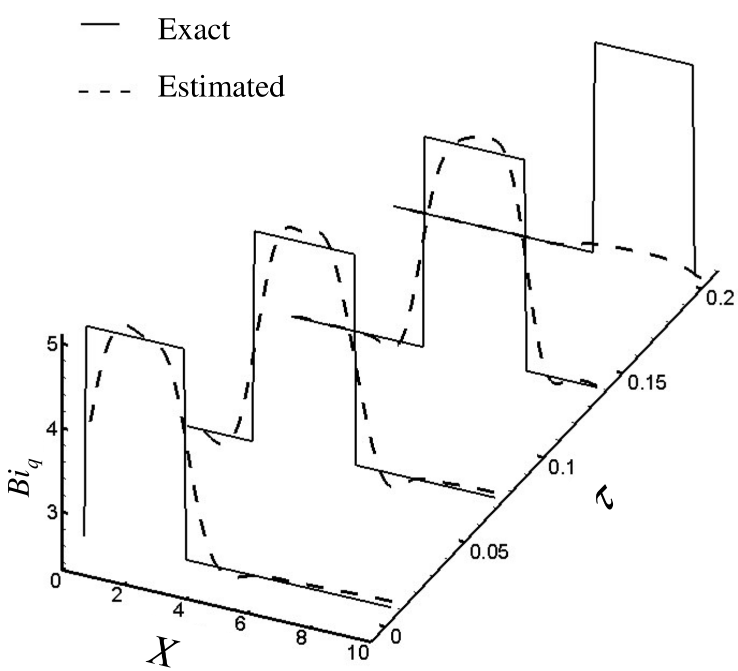


4. FUNCTION ESTIMATION

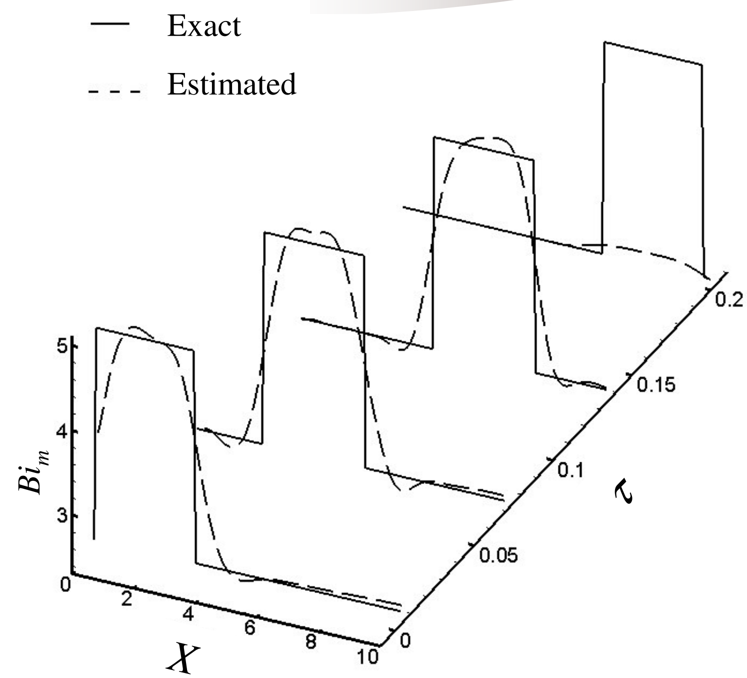


4. FUNCTION ESTIMATION

13 sensors at $Y = 0.85$

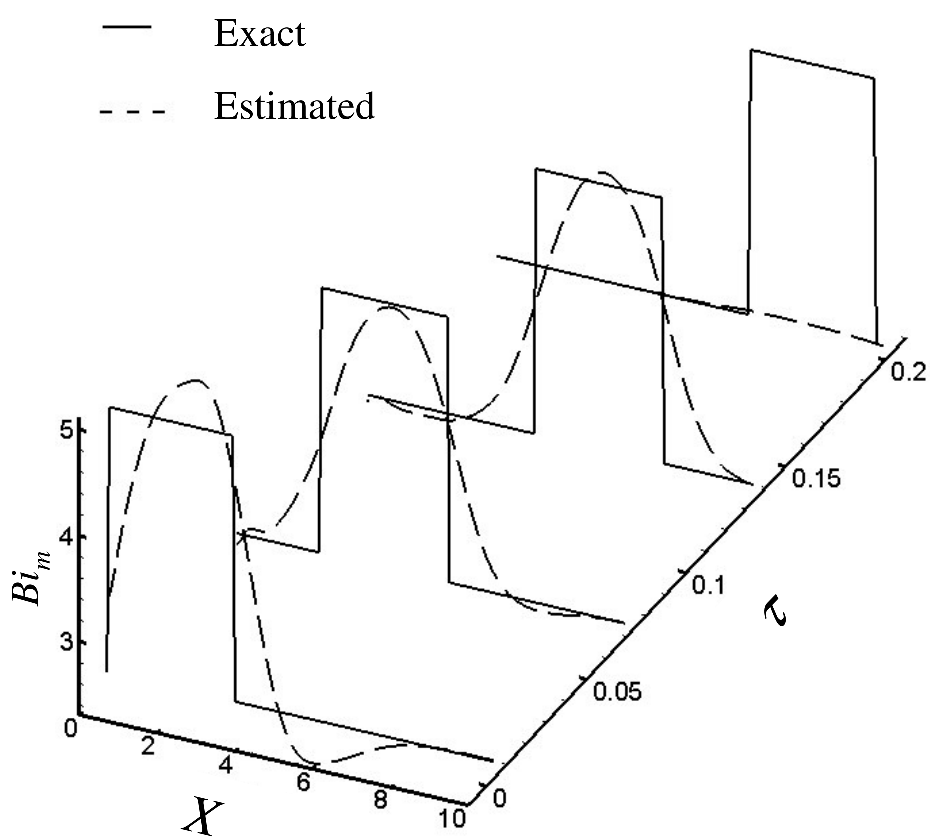


Results obtained for $Bi_q(X,\tau)$ with known $Bi_m(X,\tau)$ by using temperature measurements



Results obtained for $Bi_m(X,\tau)$ with known $Bi_q(X,\tau)$ by using temperature measurements

4. FUNCTION ESTIMATION

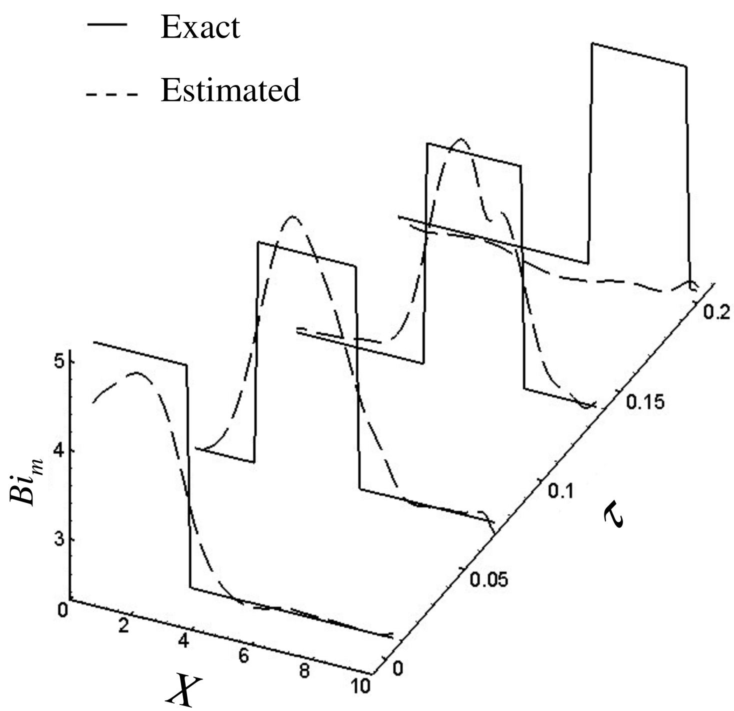


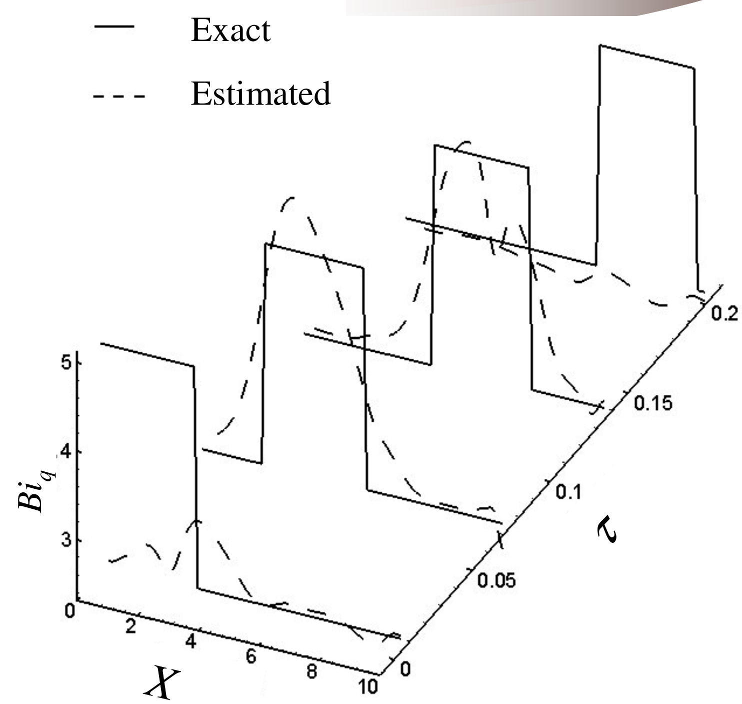
13 sensors at $Y = 0.85$

Results obtained for $Bi_m(X, \tau)$, with known $Bi_q(X, \tau)$, by using moisture content measurements

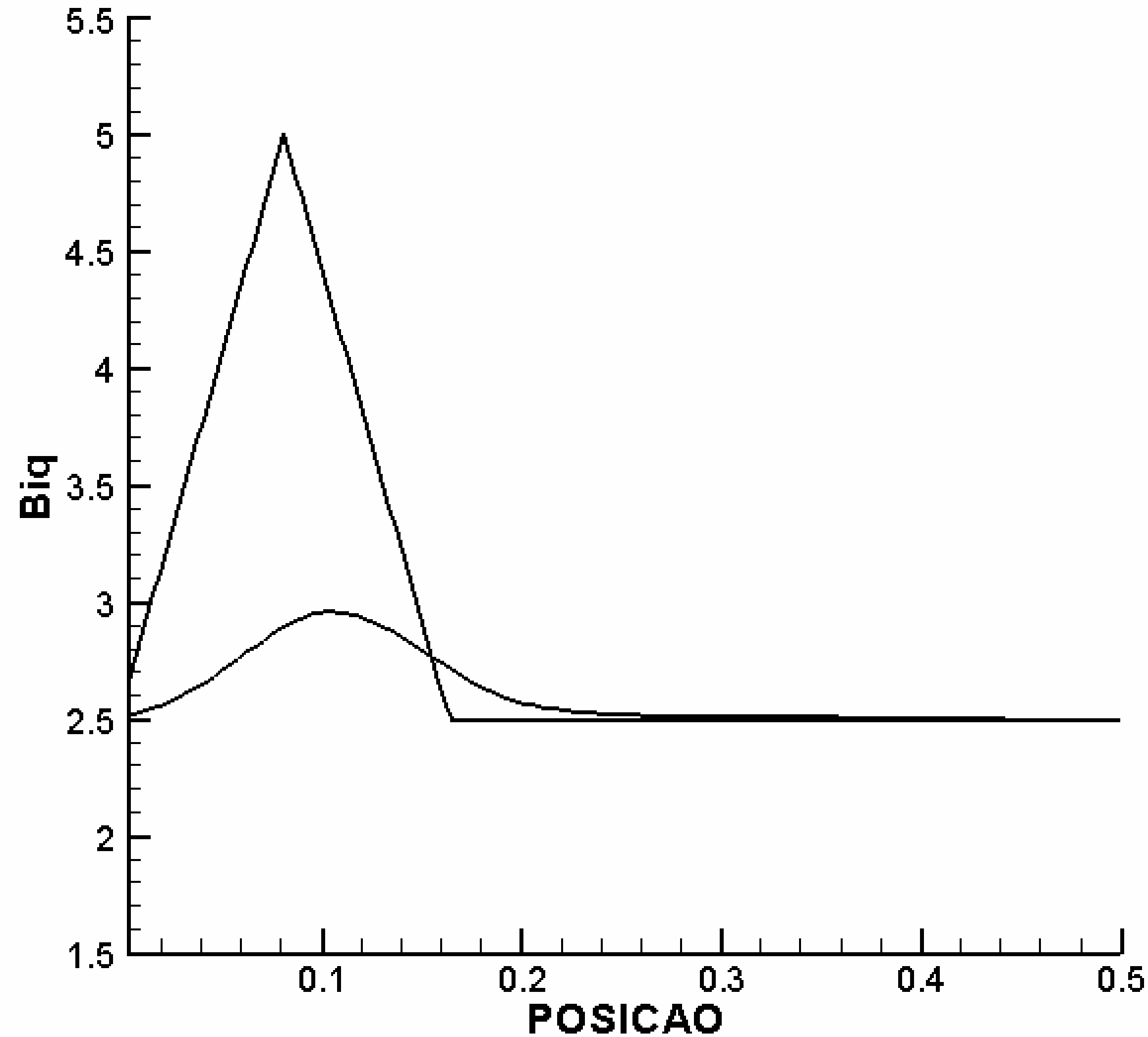
4. FUNCTION ESTIMATION

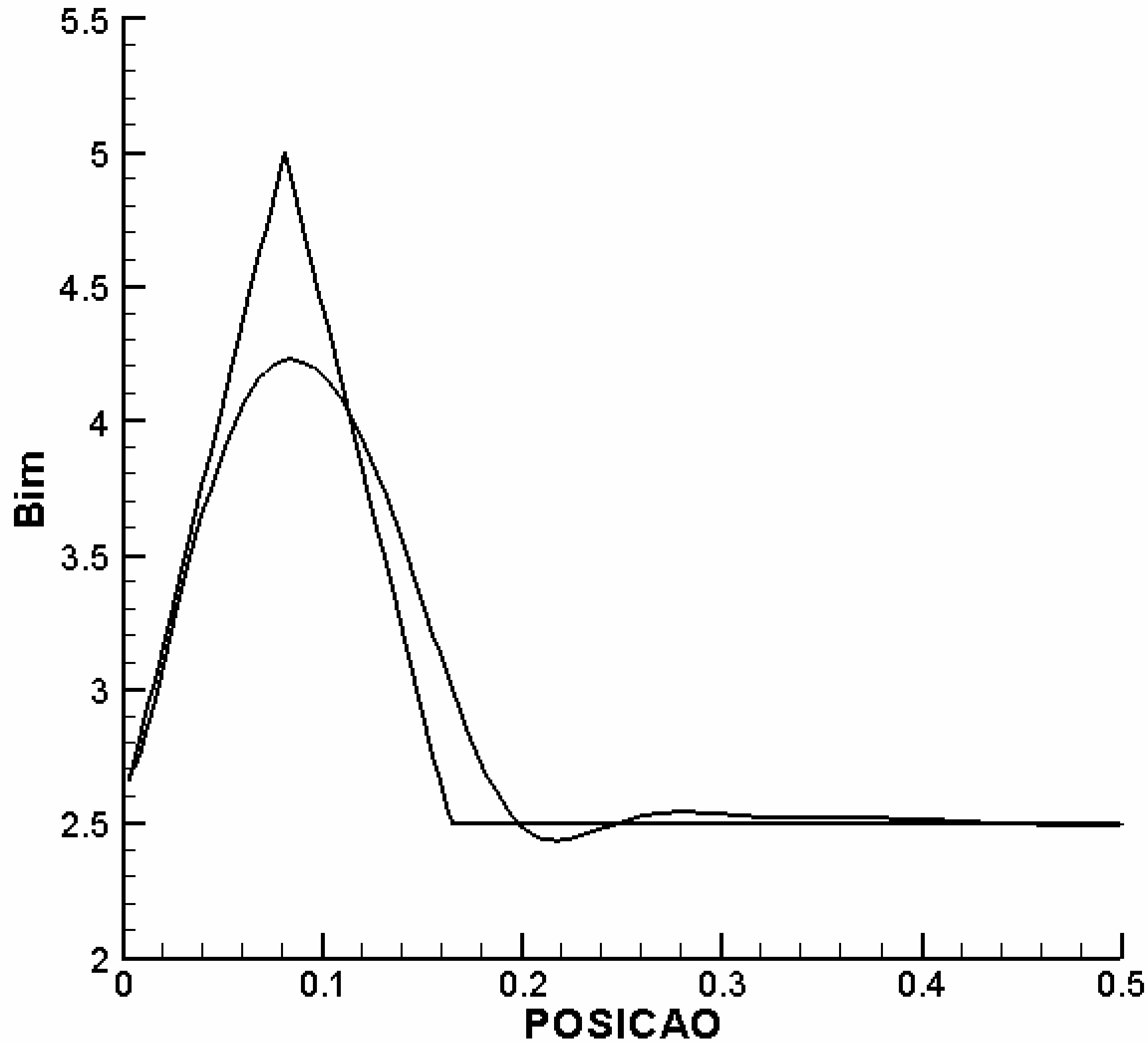
13 temperature sensors and 13 moisture content sensors





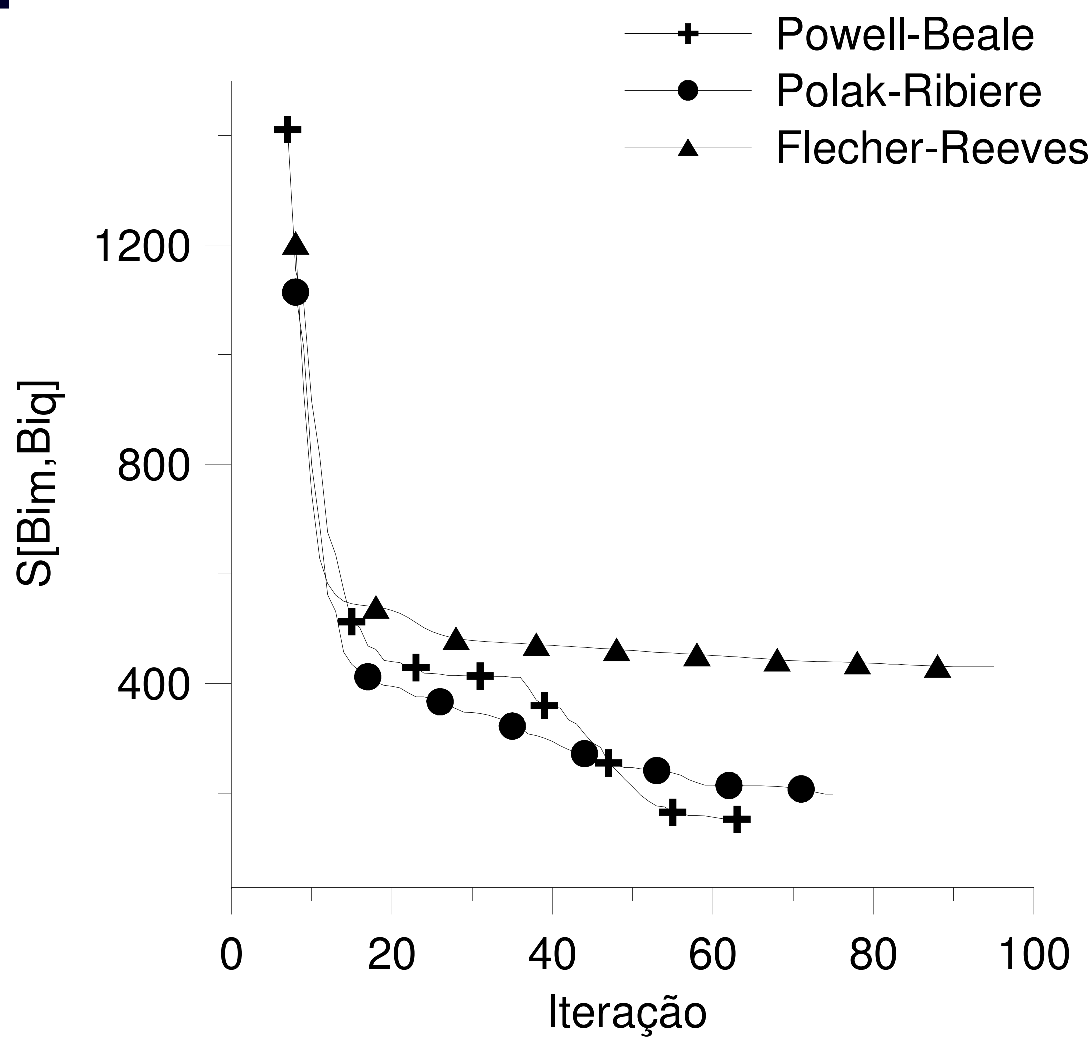
Results using temperature and moisture content measurements - simultaneous estimation of $Bi_m(X,t)$ and $Bi_q(X,t)$


Biq
5.5
5
4.5
4
3.5
3
2.5
2
1.5
0.1
0.2
0.3
0.4
0.5
POSICAO



Bim
POSICAO
5.5
5
4.5
4
3.5
3
2.5
2
0
0.1
0.2
0.3
0.4
0.5

4. FUNCTION ESTIMATION



4. FUNCTION ESTIMATION

Method	# Iterations	Final Functional	RMS Error (Bi_m)	RMS Error (Bi_q)
Powell - Beale	63	151.936	4.379×10^{-1}	6.892×10^{-1}
Polak - Ribiere	75	197.790	5.117×10^{-1}	7.087×10^{-1}
Fletcher - Reeves	95	430.310	5.748×10^{-1}	8.378×10^{-1}

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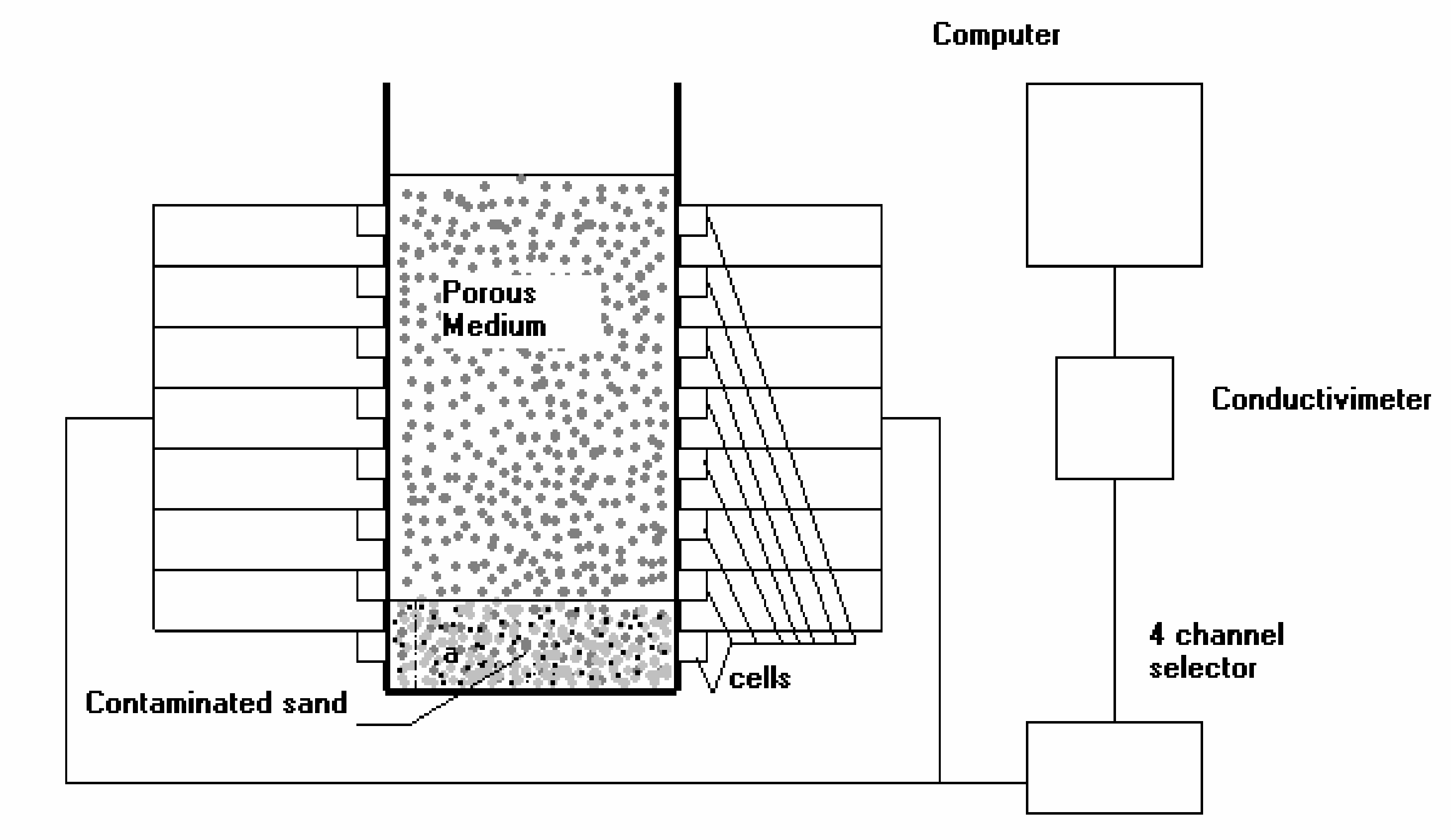
Estimation of Diffusion Coefficient



Estimation of Diffusion Coefficient

$$\frac{\partial C}{\partial t} = D^* \frac{\partial^2 C}{\partial z^2} \qquad \text{for t > 0 and z > 0}$$

$$\frac{\partial C}{\partial z} = 0 \qquad \text{at z = 0 , for t > 0}$$

$$C = f(z) = \begin{cases} C_0 & \text{for } t = 0 \quad \text{and} \quad 0 < z < a \\ 0 & \text{for } t = 0 \quad \text{and} \quad z > a \end{cases}$$

$$C^*(z,t) = \frac{C(z,t)}{C_0} = \frac{1}{2}\left[erf\left(\frac{a+z}{2\sqrt{D^* t}} \right) + erf\left(\frac{a-z}{2\sqrt{D^* t}} \right) \right]$$

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Inverse Problem: Estimate **P** = [D^* , a] by using concentration measurements.

Minimization of: $S(\mathbf{P}) = [\mathbf{Y} - \mathbf{C}(\mathbf{P})]^T [\mathbf{Y} - \mathbf{C}(\mathbf{P})]$

Levenberg-Marquardt's method: $\mathbf{P}^{k+1} = \mathbf{P}^k + (\mathbf{J}^T \mathbf{J} + \mu^k \Omega^k)^{-1} \mathbf{J}^T [\mathbf{Y} - \mathbf{C}(\mathbf{P}^k)]$

- Mass diffusion coefficient of KBr in sand
- 4 conductivity cells located at z = 2.5 , 22.5, 32.5 and 42.5 mm
- Measurements were taken until 90 hours after the beginning of the experiment
- Frequency of 1 measurement per cell every 20 minutes.

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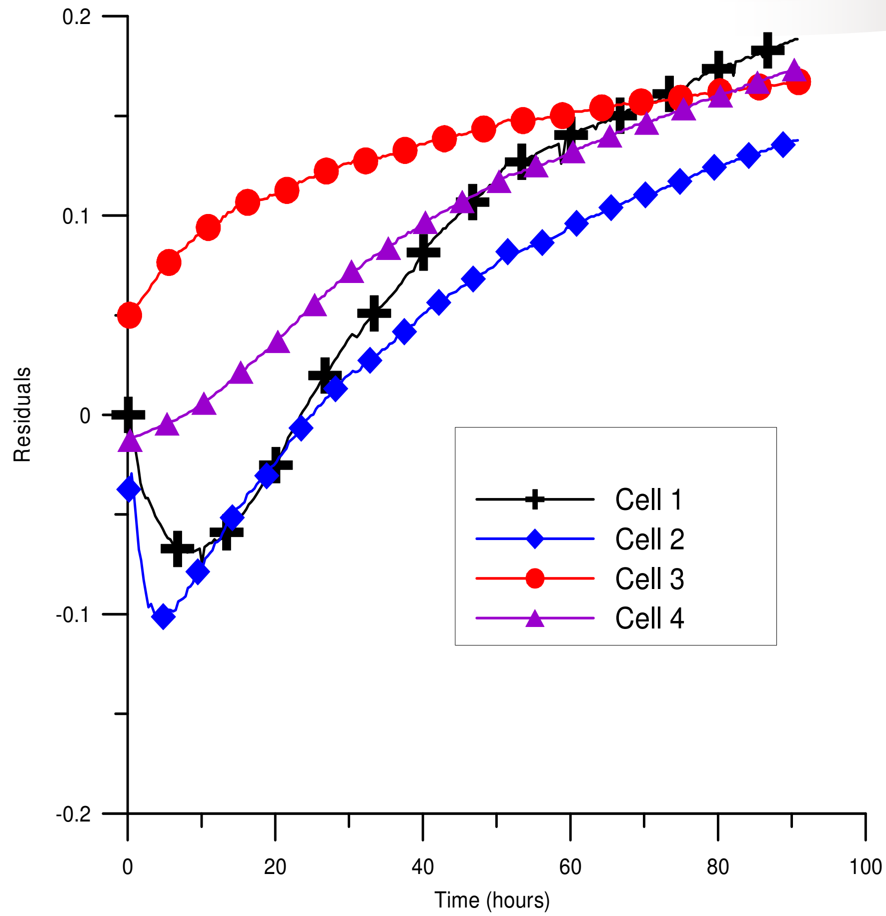
$D^* = 8.29 \times 10^{-6}$ cm²/s

8.06×10^{-6} cm²/s $< D^* < 8.53 \times 10^{-6}$ cm²/s



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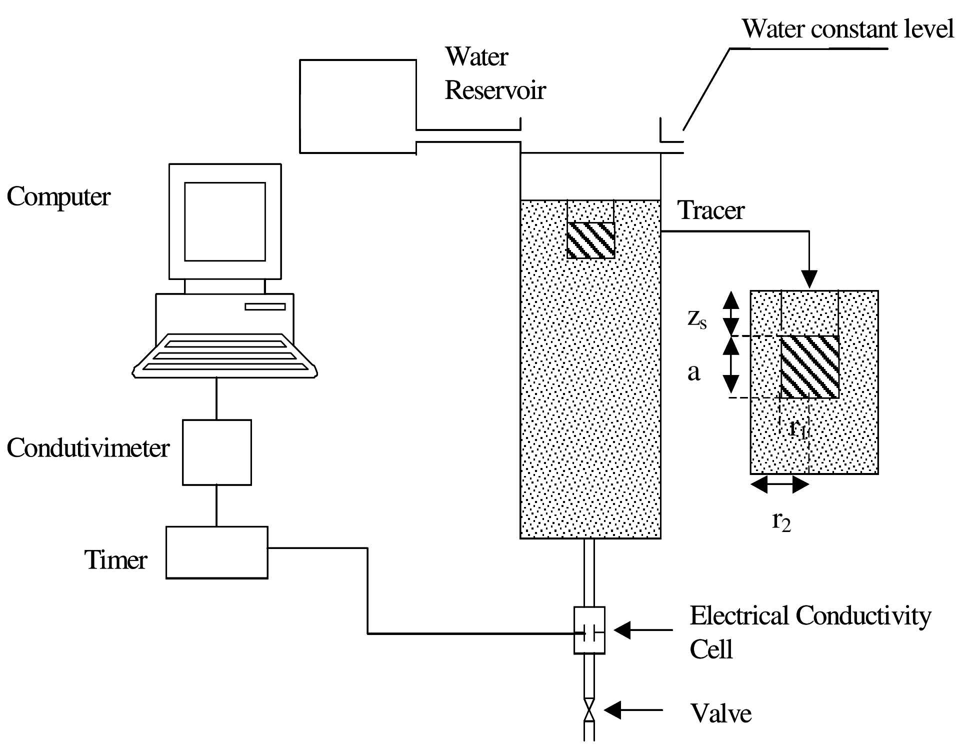
Estimation of Dispersion Coefficient



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

$$c(z,0) = \begin{cases} C_b, & em \quad 0<z<z_s \\ C_0, & em \quad z_s<z<a+z_s \\ C_b, & em \quad z_s+a<z<L \end{cases} \qquad \text{for} \quad t=0$$

$$c(0,t) = C_b \qquad \text{in} \quad z=0 \quad and \quad t>0$$

$$D\frac{\partial c(L,t)}{\partial z} + h_m c(L,t) = h_m C_b \qquad \text{in} \quad z=L \text{ and } t>0$$

where D is the dispersion coefficient, R is the retardation factor, V is the porous velocity and L is the column length

Inverse Problem: Estimate **P** = [D , R , h_m] by using outflow concentration measurements.

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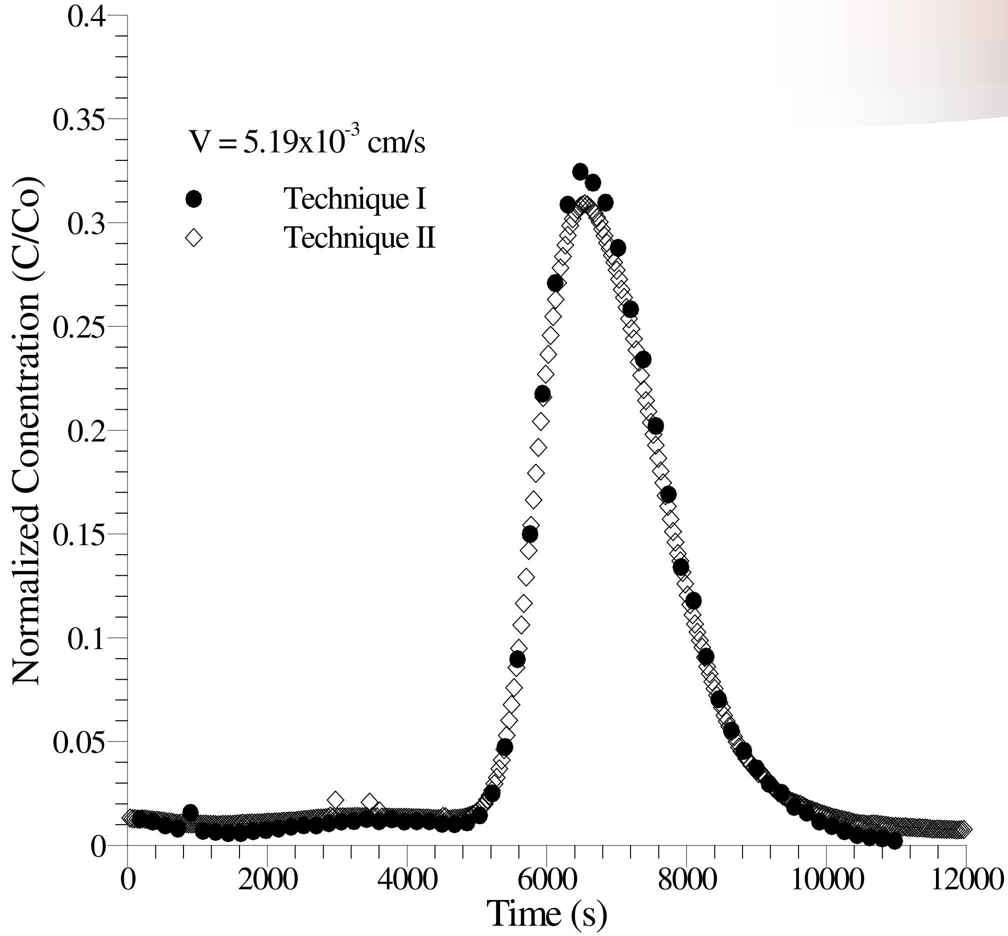

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