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AN INVERSE PROBLEM OF HEAT AND MASS BIOT ESTIMATION

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Abstract. In the present work we apply a deterministic, an stochastic and a hybrid method for the estimation OF the Biot numbers in the problem of simultaneous heat and mass transfer in a porous media. The direct problem is modeled by the Luikov's system of partial differential equations, which is solved using the finite difference method. A sensitivity analysis is performed and test case results with synthetic data are presented.

Keywords. Luikov equations, drying, inverse problem, simulated annealing, Levenberg-Marquardt

1. Introduction

The analysis of the simultaneous heat and mass transfer phenomena in porous media has several relevant applications in different areas such as mechanical, biomedical, food and environmental engineering (Mikhailov and Özisik, 1994; Ekechukuwu, 1999; Neményi et al., 2000; Pavón-Melendez et al., 2002). In most cases the mathematical model is based on the Luikov's equations (Mikhailov, and Özisik, 1994; Luikov and Mikhailov, 1965; Luikov, 1975; Mikhailov and Shishendjiev, 1975; Pandey et al., 1999; Chang and Wang, 2000; Pandey et al., 2000).

More recently the inverse problem of simultaneous heat and mass transfer has attracted the attention of several researchers (Kanavce et al., 2002; Kanevce et al., 2002; Huang and Yeh, 2002; Dantas et al., 2002-2003; Lugon and Silva Neto, 2003a-2003b). The Levenberg-Marquardt (LM) method (Marquardt,1963) was used by many researchers (Kanavce et al., 2002; Kanevce et al., 2002; Lugon and Silva Neto, 2003a and 2003b) and the Alifanov's Iterative Regularization method (for details see Alifanov et al., 1995) was used by Dantas et all, 2002 and 2003. Hunag and Yet (2002) used the using Alifanov's iterative regularization method (Alifanov et al, 1995) to estimate the heat and mass Biot. In Lugon and Silva Neto, 2003a, a stochastic method, SA-Simulated Annealing, was used to estimate the dimensionless numbers of Luikov and Possnov. The studies were extended by Lugon and Silva Neto (2003b) including a hybrid solution, SA-LM, for the estimation of the Luikov and Possnov dimensionless numbers.

Lugon and Silva Neto (2004) studied the same problem including a hybrid solution, SA-LM (Silva Neto and Soeiro, 2003), for the estimation of the Luikov, Possnov and Kossovitch dimensionless numbers. In the present work we proceed the analysis of the same problems, investigating the estimation of the Biot numbers of heat and mass transfer in Luikov's formulation for simultaneous heat and mass transfer in a porous medium.

2. Mathematical Formulation and the Solution of the Direct Problem

Consider the problem of simultaneous heat and mass transfer in a one-dimensional porous media in which heat is supplied to the left surface of the porous media, at the same time that dry air flows over the right surface.

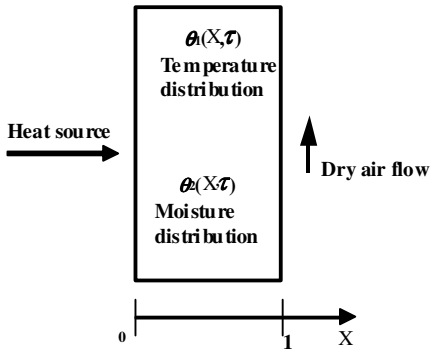

Figure 1 – Drying process schematic representation

The mathematical formulation of the direct heat and mass transfer problem considered, in the dimensionless form, is given by Mikhailov and Özisik (1994) and by Cotta (1993)

$$\frac{\partial \theta_1(X,\tau)}{\partial \tau} = \alpha \frac{\partial^2 \theta_1}{\partial X^2} - \beta \frac{\partial^2 \theta_2}{\partial X^2}, \quad 0 < X < 1, \quad \tau > 0 \tag{1}$$

$$\frac{\partial \theta_2(X,\tau)}{\partial \tau} = Lu \frac{\partial^2 \theta_2}{\partial X^2} - Lu\, Pn \frac{\partial^2 \theta_1}{\partial X^2}, \; 0 < X < 1, \quad \tau > 0 \tag{2}$$

subject to the initial conditions

$$\theta_1(X,0) = 0, \qquad 0 \le X \le 1 \tag{3}$$

$$\theta_2(X,0) = 0, \qquad 0 \le X \le 1 \tag{4}$$

and to the boundary conditions

$$\frac{\partial \theta_1(0,\tau)}{\partial X} = -Q, \quad \tau > 0 \tag{5}$$

$$\frac{\partial \theta_2(0,\tau)}{\partial X} = -Pn\, Q, \quad \tau > 0 \tag{6}$$

$$\frac{\partial \theta_1(1,\tau)}{\partial X} + Bi_q \theta_1(1,\tau) = Bi_q - (1-\varepsilon) Ko\, Lu\, Bi_m [1 - \theta_2(1,\tau)] = 0, \quad \tau > 0 \tag{7}$$

$$\frac{\partial \theta_2(1,\tau)}{\partial X} + Bi_m^* \theta_2(1,\tau) = Bi_m^* - Pn\, Bi_q [\theta_1(1,\tau) - 1], \quad \tau > 0 \tag{8}$$

where

$$\alpha = 1 + \varepsilon\, Ko\, Lu\, Pn \tag{9}$$

$$\beta = \varepsilon\, Ko\, Lu \tag{10}$$

$$Bi_m^* = Bi_m [1 - (1-\varepsilon) Pn\, Ko\, Lu] \tag{11}$$

the dimensionless variables are defined as

$$\theta_1(X,\tau) = \frac{T(x,t) - T_0}{T_s - T_0}, \text{ temperature} \tag{12}$$

$$\theta_2(X,\tau) = \frac{u_0 - u(x,t)}{u_0 - u^*}, \text{ moisture} \tag{13}$$

$$X = \frac{x}{l}, \text{ spatial coordinate} \tag{14}$$

$$\tau = \frac{at}{l^2}, \text{ time} \tag{15}$$

$$\mathrm{Lu} = \frac{a_m}{a}\text{, Luikov number} \tag{16}$$

$$\mathrm{Pn} = \delta \frac{T_s - T_0}{u_0 - u^*}\text{, Possnov number} \tag{17}$$

$$\mathrm{Ko} = \frac{r}{c}\frac{u_0 - u^*}{T_s - T_0}\text{, Kossovitch number} \tag{18}$$

$$\mathrm{Bi}_q = \frac{hl}{k}\text{, heat Biot} \tag{19}$$

$$\mathrm{Bi}_m = \frac{h_m l}{k_m}\text{, mass Biot} \tag{20}$$

$$Q = \frac{ql}{k(T_s - T_0)}\text{, heat flux} \tag{21}$$

and a represents the thermal diffusivity of the porous medium, a_m the moisture diffusivity of the porous media, c the specific heat of the porous medium, h the heat transfer coefficient between the porous medium and the air, h_m the mass transfer coefficient between the porous medium and the air, k the thermal conductivity, k_m the moisture conductivity, l the width of the medium, q the thermal flux supplied to the porous medium at the left side (see Fig. 1), r the latent heat of evaporation, T_0 the initial uniform temperature of the porous medium, T_s the dry air initial temperature, u_0 the initial moisture content, u^* the moisture content of the surrounding air, X the spatial coordinate axis, ε the phase change criterion (*i.e.*, $\varepsilon = 1$, vapor, $\varepsilon = 0$, liquid) and δ is the thermogradient coefficient.

When the geometry, the initial and boundary conditions, and the medium properties are known, the system of equations (1-8) can be solved yielding the temperature and moisture distribution in the media. The finite difference method was used for that purpose. We first choose initial guesses for θ_1 and θ_2. Then we solve Eqs. (1),(3),(5) and (7), with θ_2 fixed, in order to obtain a new estimate for θ_1. Then θ_1 is fixed and we solve Eqs. (2), (4), (6) and (8) to obtain a new estimate for θ_2. Such procedure is repeated until a convergence criterion related to the values of θ_1 and θ_2 is satisfied.

3. Mathematical Formulation and Solution of the Inverse Problem

3.1 Inverse Problem Formulation

In the present work we focus on the determination of parameters associated with Luikov's model, in particular the heat and mass Biot numbers, using a deterministic and a stochastic method. A hybrid approach combining the deterministic and stochastic method is also analyzed. For that purpose it is considered that transient temperature measurements, $Y_i, i = 1, 2, ...M$, are taken at one location of the medium.

Since the number of experimental data, M, is larger than the number of unknowns to be estimated, the inverse problem is implicitly formulated (Silva Neto and Soeiro, 2003) as a finite dimensional optimization problem where we seek for the minimization of the functional of squared residues

$$S(\vec{P}) = \sum_{i=1}^{M} \left[\theta_{1i}(\vec{P}) - Y_i\right]^2 = \vec{F}^T \vec{F} \tag{22}$$

where Y_i represents the dimensionless temperature measured in the porous media, $\theta_{1i}\left(\vec{P}\right)$ the calculated temperature, $\vec{P}$ is the vector of unknowns, and $F_i = \theta_{1i}(\vec{P}) - Y_i, i = 1,2,..., M$, are the elements of the vector of residues $\vec{F}$.

3.2 Sensitivity Analysis

The sensitivity analysis plays a major role in several aspects related to the formulation and solution of an inverse problem. Such analysis may be performed with the study of the sensitivity coefficients. Here we use the modified or scaled, sensitivity coefficients

$$SC_{P_j}(X,\tau) = P_j \frac{\partial V(X,\tau)}{\partial P_j}, \qquad j = 1, 2, \cdots, N_p \tag{23}$$

where V is the observable state variable (which can be measured), P_j, is a particular unknown of the problem and N_p is the total number of unknowns.

In the following table we have the reference values examined in this investigation for a wood sample, in all cases we considered forced convection, and studied changes in width, dry air temperature and heat flux (Dantas et al., 2003).

Table 1 – Reference values for experiments examined

Physical variables	Experiment 1	Experiment 2	Experiment 3
l (m)	0.01	0.01	0.025
ρ_0 (kg/m^3)	370	370	370
h_q (W/m^2 M)	22.5	22.5	22.5
h_m (W/m^2 s^o M)	2.5 x 10^{-6}	2.5 x 10^{-6}	2.5 x 10^{-6}
k_q (W/m K)	0.65	0.65	0.65
k_m (kg/m s^o M)	2.2 x 10^{-8}	2.2 x 10^{-8}	2.2 x 10^{-8}
δ (^{o} M/K)	2.0	2.0	2.0
c_p (J/kg K)	2500	2500	2500
c_m (kg/kg ^{o} M)	10^{-2}	10^{-2}	10^{-2}
λ (J/kg)	2.5 x 10^{-6}	2.5 x 10^{-6}	2.5 x 10^{-6}
T_0 (^{o} C)	24	24	24
T_s (^{o} C)	36	26	36
u_0 (^{o} M)	86	86	86
u^* (^{o} M)	8	8	8
Bi_q	0.34	0.34	0.85
Bi_m	1.14	1.14	2.85
Lu	0.008	0.008	0.008
Pn	0.3	0.05	0.3
Ko	65	390	65
ε	0.2	0.2	0.2
Q	5.0	5.0	5.0

In the present work the state variable is the temperature θ_1, and we are interested in investigating the estimation of Lu, Pn, Ko, Bi_q and Bi_m.

Here we have used a central finite difference approximation for the computation of the scaled sensitivity coefficients given by Eq. (23) with respect to the unknowns listed in the previous paragraph.

As a general guideline the sensitivity of the observable state variable with respect to the parameter we want to estimate must be high enough to allow an estimate within reasonable confidence bounds. Moreover, when two or more

parameters are simultaneously estimated, their effects on the state variable must be independent (uncorrelated). Therefore, when represented graphically the sensitivity coefficients should not have the same shape. If they do, it means that two or more different parameters affect the observable state variable in a similar way, being therefore difficult to distinguish their influences separately, which yields to poor estimations.

In Fig. 2 and 3 are represented the sensitivity coefficients with the same material, with characteristics and conditions described by the reference values in Table 1, experiments 1, 2 and 3, with respect to Lu, Pn, Ko, Bi_q and Bi_m. It must be said that the heat and mass Biot numbers depend on the width of the material and that the Pn and Ko numbers depend on the dry air temperature, so they were calculated accordingly.

It must be observed that the sensitivity coefficients depend in general on the values of the unknowns we want to determine, e.g. Bi_q and Bi_m. Therefore, they could be calculated only after we solve the inverse problem, and then it may be too late to find out that the sensitivity to a particular unknown is to small or that there is a correlation of that unknown with another one we are trying to estimate simultaneously. Nonetheless, we may use reference values for the unknowns and then we may perform the sensitivity analysis. In the present analysis we use the values presented in Table 1.

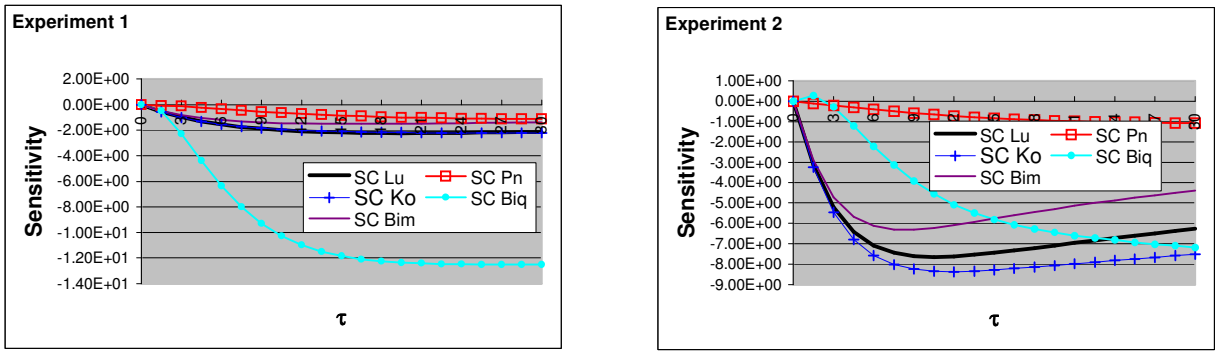

Figure 2 – Sensitivity coefficients for Lu, Pn, Ko, Bi_q and Bi_m for experiments 1 and 2

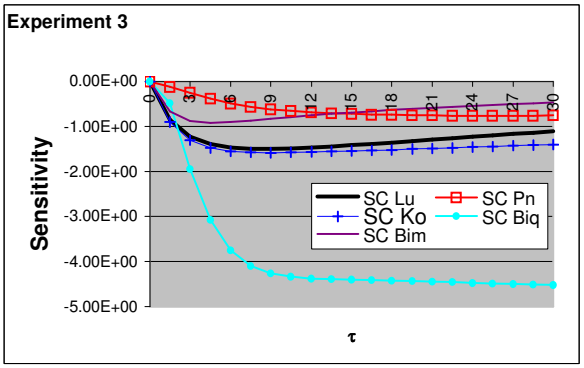

Figure 3 – Sensitivity coefficients for Lu, Pn, Ko, Bi_q and Bi_m for experiment 3

In the case of experiment 1, the sensitivity to Bi_q is higher than all others and in the interval $0 < \tau < 15$ it seems to be high enough to allow its estimation. The sensitivity to Lu, Ko and Bi_m in experiment 2 are uncorrelated in the range $6 < \tau < 15$ and are high enough to allow the estimation. In experiments 1 and 2, $\tau = 15$ correspond to $t = 5\,hours$ of real time for a sample with $l = 1\,cm$. To estimate Pn the best experiment is number 3 using $\tau_f = 15$, that is $t = 30\,hours$ for a sample with $l = 2.5\,cm$.

3.3 Inverse Problem Solution

Here we are interested in using a deterministic method (LM-Levenberg-Marquardt), an stochastic method (SA-Simulated Annealing) and a hybrid method (SA-LM) for the minimization of the cost functional given by Eq. (22).

3.3.1 The Simulated Annealing Method (SA)

Based on statistical mechanics reasoning, applied to a solidification problem, Metropolis (1953) introduced a simple algorithm that can be used to accomplish an efficient simulation of a system of atoms in equilibrium at a given temperature. In each step of the algorithm a small random displacement of an atom is performed and the variation of the energy ΔE is calculated. If $\Delta E<0$ the displacement is accepted, and the configuration with the displaced atom is used as the starting point for the next step. In the case of $\Delta E>0$, the new configuration can be accepted according to Boltzmann probability

$$P(\Delta E) = \exp(-\Delta E / k_B T) \tag{24}$$

A uniformly distributed random number p in the interval [0,1] is calculated and compared with $P(\Delta E)$. Metropolis criterion establishes that the new configuration is accepted if $p<P(\Delta E)$, otherwise it is rejected and the previous configuration is used again as a starting point.

Using the objective function $S(\vec{P})$, given by Eq. (22), in place of energy and defining configurations by a set of variables $\{P_i\}, i = 1,2,..N_p$, where N_p represents the number of unknowns we want to estimate, the Metropolis procedure generates a collection of configurations of a given optimization problem at some temperature T. This temperature is simply a control parameter. The simulated annealing process consists of first "melting" the system being optimized at a high "temperature", then lowering the "temperature" until the system "freezes" and no further change occurs.

The main control parameters of the algorithm implemented ("cooling procedure") are the initial "temperature", T_0, the cooling rate, r_t, number of steps performed through all elements of vector $\vec{P}$, N_s, number of times the procedure is repeated before the "temperature" is reduced, N_t, and the number of points of minimum (one for each temperature) that are compared and used as stopping criterion if they all agree with a tolerance ε, N_ε. For more details see references (Goffe et al., 1994; Silva Neto and Soeiro, 2003; Metropolis et al., 1953; Silva Neto and Soeiro, 2002).

3.3.2 The Levenberg-Marquardt Method (LM)

The Levenberg-Marquardt is a deterministic local optimizer method based on the gradient. In order to minimize the functional S we first write

$$\frac{dS}{d\vec{P}} = \frac{d}{d\vec{P}}\left(\vec{F}^T \vec{F}\right) = 0 \quad \rightarrow \quad J^T \vec{F} = 0 \tag{25}$$

where J is the Jacobian matrix, with the elements $J_{ps} = \partial \theta_{1p} / \partial P_s$ being $p = 1,2,...M$, and $s = 1,2,...N_p$. Observe that the elements of the Jacobian matrix are related to the scaled sensitivity coefficients presented in section 3.2.

Using a Taylor's expansion and keeping only the terms up to the first order,

$$\vec{F}(\vec{P} + \Delta\vec{P}) \cong F(\vec{P}) + J\Delta\vec{P} \tag{26}$$

Introducing the above expansion in Eq. (25) results

$$J^T J\Delta\vec{P} = -J^T \vec{F}(\vec{P}) \tag{27}$$

In the Levenberg-Marquardt method it is added to the diagonal of matrix $J^T J$ a damping λ^n factor to help to achieve convergence (Marquardt, 1963).

Equation (27) is written in a more convenient form to be used in the iterative procedure,

$$\Delta\vec{P}^{n} = -\left[\left(J^{n}\right)^{T} J^{n} + \lambda^{n}\breve{I}\right]^{-1}\left(J^{n}\right)^{T}\vec{F}\left(\vec{P}^{n}\right) \tag{28}$$

where $\breve{I}$ is the identity matrix and n is the iteration counter

The iterative procedure starts with an estimate for the unknown parameters, $\vec{P}^{0}$, being new estimates obtained with $\vec{P}^{n+1} = \vec{P}^{n} + \Delta\vec{P}^{n}$, while the corrections $\Delta\vec{P}^{n}$ are calculated with Eq. (28). This iterative procedure is continued until a convergence criterion such as

$$\left|\Delta P_{k}^{n} / P_{k}^{n}\right| < \varepsilon, \qquad n = 1,\ 2, \cdots, N_{p} \tag{29}$$

is satisfied, where ε is a small number, e.g. 10^{-5}.

The elements of the Jacobian matrix, as well as the right side term of Eq. (8), are calculated at each iteration, using the solution of the problem with the estimates for the unknowns obtained in the previous iteration.

3.3.3 Combination of the Gradient Based Local Optimizer (LM) and the Stochastic Global Optimizer (SA)

Due to the complexity of design space if convergence is achieved with a gradient based method it may in fact lead to a local minimum. Therefore, global optimization methods are required in order to reach the global minimum. The main disadvantage of these methods is that the number of function evaluations is high, becoming sometimes prohibitive from the computational point of view (Silva Neto and Soeiro, 2003; Metropolis et al., 1953; Silva Neto and Soeiro, 2002).

Trying to keep the best feature of each method, we have combined the SA and LM methods (SA-LM). We allow the stochastic method to run for a while, say 15 minutes corresponding to 1000 evaluations, obtaining quite quickly an initial guess for the LM. We then run the LM, reaching within a few iterations a point of minimum. After that we run again the SA. If the same solution is reached, it is likely that a global minimum was reached, and the iterative procedure is interrupted. If a different solution is obtained it means that the previous one was a local minimum. In that case we run again the LM and SA until the global minimum is reached.

3.4 Confidence bounds

The confidence bounds to the estimates $\vec{P}^{n}$ are calculated using the procedure developed by Gallant (1987)

$$\sigma_{\vec{P}} = \sigma\left\{\mathrm{diag}\left[J^{T} J\right]^{-1}\right\}^{1/2} \tag{30}$$

Assuming a normal distribution on the experimental data error, and 99 % of confidence, the limits of the confidence bounds to the estimates P_{s}, $s = 1,2,...,M$, are calculated by Flach and Özisik (1989) as,

$$\left(P_{s} - 2{,}576\,\sigma_{Ps}, P_{s} + 2{,}576\,\sigma_{Ps}\right), \quad s = 1,2,..,M \tag{31}$$

4. The computer codes

The Simulated Annealing code used in this work is the same used in "Global Optimization of Statistical Functions with Simulated Annealing" by Goffe et al., 1994, that was coded in Fortran. The direct problem solver was coded in Delphi as a DLL function that is called from the Fortran routine each time it is needed. Basically the Fortran routine calls the Delphi DLL function passing the tentative values for parameters we want to estimate. The Delphi DLL routine uses the parameters to solve the direct problem, read values of the experimental data from an ASCII file, calculates the value of the cost function *S,* given by Eq. (22), and finally returns the value of the cost function to the Fortran routine.

The routine used for the Levenberg-Marquardt method was fully implemented in Delphi by Lugon and Silva Neto, 2003.

5. Numerical Results and Discussion

5.1 Synthetic data

As real data were not available we have generated synthetic data with

$$Y_{meas_i} = \theta_{1_{exact_i}} + e\sigma \qquad , \quad i = 1, 2, ..., M \tag{32}$$

where *e* is a random number and σ is the standard deviation of measurement errors.

5.2 Test case results

Although the Simulated Annealing method is independent of the gradient, to keep the compatibility with the Levenberg-Marquardt method that is based in the gradient, we used data for which the sensitivity is the highest (see section 3.2). So, we have used of temperature measures obtained from experiment 2, considering just one temperature sensor located at $X = 0$, acquiring data starting at $\tau_0 = 0.0$, at every interval $\Delta\tau = 0.15$, up to the final time of observation $\tau_f = 15$. In this particular physical case, the drying of wood (Luikov, A.V. and Mikhailov, Y.A, 1965), such dimensionless time corresponds to 5 hours of experiment, taking measurements in a frequency of every 3 minutes.

In order to perform the validation of the methodology we have solved the inverse problem with noiseless data, i.e. $\sigma = 0$ in Eq. (32). Both heat and mass transfer Biot numbers were simultaneously estimated and the results obtained are shown in Table 2 (test cases 1 and 4).

Initial guesses were made with a deviation up to 50% with respect to the exact values.

To solve a more realistic problem we considered noisy data, i.e. we used synthetic data with $\sigma = 0.25$ and $\sigma = 0.62$ resulting in approximately 2% and 5% of measurement error respectively. The results obtained are also shown in Table 2 (test cases 2, 3, 5 and 6).

Observe that LM presented no difficult at all to estimate the parameters, both with and without error in data. No problem is noticed when we change the initial guess.

Table 2 – Test case results using Levenberg-Marquardt method

	% error	Inform.	Bi_q	Bi_m	Time
1	0%	Initial Guess	0.300	1.250	2 min.
		Result	0.340	1.140	
2	2%	Initial Guess	0.300	1.250	2 min.
		Result	0.339	1.140	
3	5%	Initial Guess	0.300	1.250	2 min.
		Result	0.324	1.196	
4	0%	Initial Guess	0.170	1.710	2 min.
		Result	0.340	1.140	
5	2%	Initial Guess	0.170	1.710	2 min.
		Result	0.339	1.140	
6	5%	Initial Guess	0.170	1.710	2 min.
		Result	0.332	1.184	

Exact values: $Bi_q = 0.340$ and $Bi_m = 1.140$

But in the real case, we do not know the material properties, so we can not fix the dimensionless numbers of Luikov, Possnov and Kossovitch (Lu, Pn and Ko). In Lugon and Silva Neto, 2003 we successfully estimated Lu, Pn and Ko using an hybrid SA-LM method.. The association of SA and LM proved to be very effective, the global minimum was found within a reasonable computation time and accuracy. So now we study a little further this possibility, applying again an hybrid SA-LM method, to estimate Lu, Pn, Ko, Bi_q and Bi_m.

First we run the SA method using data from experiment 2 for estimating Lu, Pn , Ko, Bi_q and Bi_m. These estimates are called $\vec{Z}_{SA}$, which are used as the initial guess for the LM method, i.e. $\vec{Z}^0_{LM} = \vec{Z}_{SA}$. The LM method is

used first taking data from experiment 1 for estimating Bi_q, then using data from experiment 2 for estimating Lu, Ko and Bi_m, then finally with data from experiment 3 to estimate Pn. In all experiment we used $\tau_f = 15$. Only 5 iterations of each LM method are needed. We repeated the procedure until a convergence criteria is achieved, i.e. $\vec{Z}_{SA} = \vec{Z}_{LM}$. Therefore, this is probably a good estimate to the global minimum. In Fig. 2 we have a diagram describing this procedure.

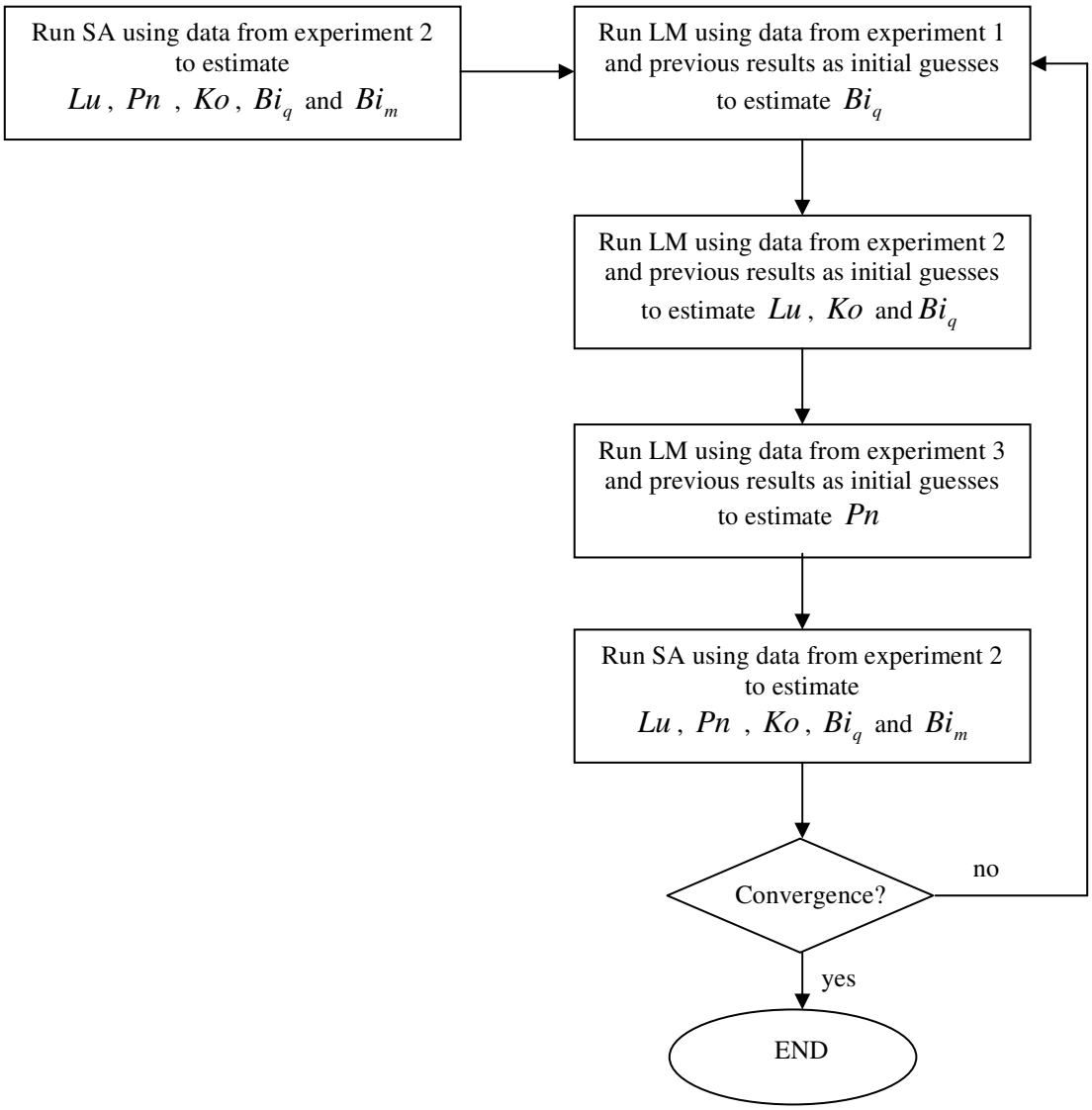

Fig 2 – Diagram describing the hybrid SA-LM estimation process

It can be observed from Table 3 that both LM and SA methods isolated performed poorly. The LM does not succeed to simultaneously estimate the 5 parameters within a reasonable number of iterations, that is, within a reasonable time, even when no error is present in the data and with initial guess near the exact values, see test cases 1-3 in Table 3. The SA needs a large number of function evaluations, therefore requires a great computational effort (see test case 4).

Table 3 – Test case results using SA, LM and SA-LM.

	Method	% error	Information	Lu	Pn	Ko	Bi_q	Bi_m	Time and Iterations
1	LM – experiment 2	0%	Guess	0.0040	0.0750	195	0.170	1.710	4 min.
			Result	0.0056	0.0770	267	0.400	2.730	5 iterations
2	LM – experiment 2	2%	Guess	0.0040	0.0750	195	0.170	1.710	3 min.
			Result	0.0054	0.0714	245	0.419	3.012	5 iterations
3	LM – experiment 2	2%	Guess	0.0070	0.0550	350	0.300	1.250	3 min.
			Result	0.0076	0/0719	359	0.341	1.289	5 iterations
4	SA – experiment 2 20.000 eval.	2%	Guess	0.0040	0.0750	195	0.170	1.710	336 min.
			Result	0.0082	0.0446	380	0.346	1.150	
5	SA-LM SA - experiment 2 (1.000 eval. SA) LM – experiment 1,2 and 3	2%	Guess	0.0040	0.0750	195	0.170	1.710	35 min.
			$\vec{Z}_{LM}^{0}$	0.0078	0.0620	316	0.354	1.500	
			Result	0.0078	0.0568	392	0.336	1.140	

Exact values: $Lu = 0.008$, $Pn = 0.05$, $Ko = 390$, $Bi_q = 0.340$ and

The confidence bounds, calculated with the procedure developed by Gallant in test case 5 (section 3.4), are shown in Table 4. We observe that the estimated values are near the exact values and within the confidence bounds.

Table 4 – Confidence bounds calculated for test case 5

	P_s estimate	P_s min	P_s max	P_s exact
Lu	**0.0078**	0.0076	0.0080	0.0080
Pn	**0.0568**	0.0500	0.0636	0.0500
Ko	**392**	389	395	390
Bi_q	**0.336**	0.332	0.340	0.340
Bi_m	**1.140**	0.905	1.375	1.140

6. Conclusions

The use of the SA method is effective in avoiding local minima but requires a great computational effort and did not achieve the global minimum with the desired accuracy. The LM did not work even for initial guesses near the global minimum and with no error in the data within a reasonable number of iterations, that is a reasonable time.

So, each method separately performed poorly, but the hybrid combination considered (SA-LM) yielded satisfactory results.

7. Acknowledgements

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