INCORRECT INVERSE PROBLEM CONECTED WITH THE PARAMETER IDENTIFICATION OF THE HEAT AND MASS TRANSFER MODELS

by

Christo BOYADJIEV

Original scientific paper
UDC: 536.24:519.876.2
BIBLID: 0354–9836, *6* (2002), 1, 23–28

A method for inverse problem solution by means of iterative regularization has been developed. A numerical algorithm for solving inverse incorrect problems based on the developed iterative regularization has been proposed.

Introduction

The main problem of the modelling is of the heat and mass transfer processes the build-up of the structures of the mathematical descriptions of the processes on the basis of hypothesises (knowledge) concerning their physical mechanisms. Moreover the procedure needs an identification of the parameters of that mathematical description laying mainly on experimental data. The second problem is usually incorrect and the solution is very sensible with respect some errors of data derived from the experiment [1].

Problem formulation

Let's concern a numerical model expressed as

$$y = f(\mathbf{x}, \mathbf{b}) \tag{1}$$

where f is an objective function; $\mathbf{x} = (x_1, \ldots, x_m)$ is a vector of independent variables, $\mathbf{b} = (b_1, \ldots, b_J)$ – vector of parameters, *i. e.* numerical values of the objective function (y) may be calculated for various values of the independent variables ($\mathbf{x}$) and parameters ($\mathbf{b}$).

The parameters of the model (1) will be determined by means of N experimental values of the objective function $\hat{\mathbf{y}} = (\hat{y}_1, \ldots, \hat{y}_n)$. This requires the introduction of an error function

$$Q(\mathbf{b}) = \sum_{n=1}^{N} (y_n - \hat{y}_n)^2 \tag{2}$$

where $y_n = f(\mathbf{x}_n, \mathbf{b})$ are the calculated values of the objective function of the model (1) for $n = 1, \ldots, N$; $\mathbf{x}_n = (x_{1n}, \ldots, x_{mn})$ are the values of the independent variables from the experiments $n = 1, \ldots, N$.

The parameters of the model (1) can be determined from the conditions imposed by the minimum of the function $Q = (b_1, \dots, b_J)$ with respect to the parameters $\mathbf{b} = (b_1, \dots, b_J)$.

The solution of the inverse identification problem, *i. e.* the determination of the of **b** faces many troubles dues to the incorrectness of the problem. The incorrectness follows from the sensibility of the solution with respect the experimental errors associated with the determination of $\hat{y}$. The problem can be avoided by the application of regularization methods that make the problem conditionally correct.

In the cases when the minimum of $Q(\mathbf{b})$ can be determined by interative methods the problem needs the application of the so-called iterative regularization. The latter means a build-up of algorithms based of iterative methods for the minimization of $Q(\mathbf{b})$. In these cases the number of the iteration plays the role of the regularization parameter [2].

Regularization of the iterative method for parameter identification

Various iterative methods for a minimum search (the gradient ones too) are stable with respect the experimental errors of the objective functions. However, after a certain number of iterations the errors of calculation might grow due to the accumulation of experimental errors. This needs a stop of the iterative procedure at the particular iteration. The result is a stable approximation of the minimum of $Q(\mathbf{b})$, while the number of the last iteration is the regularization parameter. The determination of the minimum of $Q(\mathbf{b})$ could be done by gradient method [3].

Let the iteration starts with $\mathbf{b}_0 = (b_{10}, \dots, b_{J0})$ as an initial approximation. The value of $\mathbf{b}_i = (b_{i0}, \dots, b_{Ji})$ corresponding to each the iterations ($i = 1, 2, \dots$) follows directly from the conditions imposed by movement towards the anti-gradient of the function $Q(\mathbf{b})$:

$$b_{ji} = b_{j(i-1)} - \beta_{j(i-1)} \left(\frac{\partial Q}{\partial b_j} \right)_{i-1}, \quad j = 1, \dots, J; \quad i = 1, 2, \dots \tag{3}$$

Here β_{ji} is the step of the iteration and $b_{j0} = (b_{10}, \dots, b_{J0})$ is initial step. The gradient of $Q(\mathbf{b})$ follows from (2):

$$\left(\frac{\partial Q}{\partial_{bj}} \right)_{(i-1)} = 2 \sum_{n=1}^{N} [f(\mathbf{x}_n, \mathbf{b}_{i-1}) - \hat{y}_n] \left(\frac{\partial f(\mathbf{x}_n, \mathbf{b})}{\partial b_j} \right)_{(i-1)}, \quad j = 1, \dots, J; \; i = 1, 2, \dots \tag{4}$$

where $\partial f / \partial b_j$, $j = 1, \dots, J$, are calculated numerically.

The iterative step is successful if the following condition will be satisfied:

$$Q_{i-1} - Q_i = \sum_{n=1}^{N} \beta_{j(i-1)} \left[2f(\mathbf{x}_n, \mathbf{b}_{i-1}) - 2\hat{y}_n\right] \beta_{j(i-1)} \sum_{j=1}^{J} \left(\frac{\partial Q}{\partial b_j}\frac{\partial f}{\partial b_j}\right)_{i-1}$$

$$\sum_{j=1}^{J} \left(\frac{\partial Q}{\partial b_j}\frac{\partial f}{\partial b_j}\right)_{i-1} > 0, \quad i = 1, 2, \ldots \tag{5}$$

If the step is successful it can be enlarged ($\beta_{ji} = 2\beta_{j(i-1)}$)twice . However, if the step is unsuccessful ($Q_{i-1} - Q_i < 0$) it must be reduced ($\beta_{ji} = 1/2\beta_{j(i-1)}/2$) and the iteration must start again. The iterations continue till the parameters $\beta_{ji}(j = 1, ..., J; i = 1, 2, ...)$ approach to the their true values, *i. e.*

$$(b_{j(i-1)} - \bar{b}_j)^2 - (b_{ji} - \bar{b}_j)^2 = \beta_{j(i-1)} \left[2(b_{j(i-1)} - \bar{b}_j) - \beta_{j(i-1)} \left(\frac{\partial Q}{\partial b_j}\right)_{i-1}\right]$$

$$\left(\frac{\partial Q}{\partial b_j}\right)_{i-1} > 0, \quad j = 1, \ldots, J; \quad i = 1, 2, \ldots \tag{6}$$

Where $\bar{b}_j$, $j = 1, ..., J$, are the co-ordinates of the minimum point of $Q(\mathbf{b})$, *i. e.*, the exact values of the parameters of the model. These values are unknown but they may be substituted for admissible errors of the parameter identification (Δ_j), which are preliminary known:

$$\Delta_j^2 \geq (b_j - \bar{b}_j)^2, \quad j = 1, \ldots, J \tag{7}$$

It is clear that (6) yields:

$$\beta_{j(i-1)} < \frac{2(b_{j(i-1)} - \bar{b}_j)}{\left(\frac{\partial Q}{\partial b_j}\right)_{i-1}}, \quad j = 1, \ldots, J; \quad i = 1, 2, \ldots \tag{8}$$

where may to replace $\left|b_{j(i-1)} - \bar{b}\right|_i \leq \Delta_j$, $j = 1, \ldots, J$; $i = 1, 2, \ldots$, and the result is:

$$\beta_{j(i-1)} < \frac{2\Delta_j}{\left|\left(\frac{\partial Q}{\partial b_j}\right)_{i-1}\right|}, \quad j = 1, \ldots, J; \quad i = 1, 2, \ldots \tag{9}$$

The change of the inequality direction (9) for a particular parameter $j = j_0$ at an iteration $i = i_0$ means that this parameter is already reached the searched value $b_{j_0 i_0}$ and after that it remains constant, *i. e.* $\beta_{j_0 i_0} = 0$.

The iteration procedure stops when

$$\beta_{ji} \quad 0; \; j \quad 1,\ldots,J; \; i \quad i_0, i_1, \ldots \tag{10}$$

The results permit to create an algorithm 4 for a solution of the inverse identification problem of the model (determination of the model parameters) expressed as function of several variables.

Iterative algorithm

1. The accuracy of calculations is defined in accordance with the parameters of the model

$$\Delta_{j0}, \; j = 1, \ldots, J, \text{ where } J \text{ is the number of parameters.}$$

2. The initial approximation is defined as

$$\beta_{j0}, b_{j0}, \; j = 1, \ldots, J \text{ and put } i = 1.$$

3. Calculate the function (1) for iteration i:

$$y_{ni} = f\,(x_{1n}, \ldots x_{mn}), (b_{1(i-1)}, \ldots, b_{J(i-1)}) \,, \quad n = 1, \ldots, N$$

4. Calculate numerically

$$f_{ji} \quad \frac{\partial f}{\partial b_j}_{\,i} \,, \; j \quad 1, \ldots J$$

5. Calculate the function by the help of the eq. (2)

$$Q_i(b_{1(i\;\;1)}, \ldots b_{J(i\;\;1)}) \quad \sum_{n\;1}^{N} (y_{ni} \quad \hat{y}_n)^2$$

6. Calculate $\frac{\partial Q}{\partial b_j}_{\,i}$ from eq. (4)

$$\frac{\partial Q}{\partial b_j}_{\,i} \quad 2 \sum_{n\;1}^{N} [f(x_{1n}, \ldots, x_{mn}, b_{i(i\;\;1)}, b_{J(i\;\;1)}) \hat{y}_n]$$

$$\frac{\partial f(x_{1n}, \ldots, x_{mn}, b_{1(i\;\;1)}, b_{j(i\;\;1)}}{\partial b_j}_{\,i} \,, \; j \quad 1, \ldots, J; \quad i \quad 1, 2 \ldots$$

7. Check if $i = 1$?
- Yes, then go to 8;
- No, then go to 10.

8. Calculate

$$b_{ji} \quad b_{j(i\ \ 1)} \quad \beta_{j(i\ \ 1)} \frac{\partial Q}{\partial b_j}\Big._{i} , \Delta_{ji} \quad b_{ji}\Delta_{j0}; \quad j \quad 1,\ldots,J; \quad i \quad 1,2,\ldots$$

9. Put $i = i + 1$ and then go back to 3.

10. Check if $Q_i - Q_{i-1} \leq 0$?
- Yes, then go to 11;
- No, then go to 12.

11. Put $\beta_{ji} = 2\beta_{ji}$ and go to 13.
12. Put $\beta_{ji} = \beta_{ji}/2$ and go to 13.

13. Check if $\beta_{ji} \quad \dfrac{2\Delta_{j(i\ \ 1)}}{\left|\dfrac{\partial Q}{\partial b_j}\right|_i}, \quad j \quad 1,\ldots,J; \quad i \quad 1,2,\ldots$?
- Yes,then go to 8;
- No, then go to 14.

14. Put for $\beta_{ji} \quad 0$ for $j \quad j_0$ when $\beta_{j_0 i} \quad \dfrac{2\Delta_{j_0(i\ \ 1)}}{\left|\dfrac{\partial Q}{\partial b_{j_0}}\right|_i}$

15. Check $\beta_{ji} \quad 0, \ j \quad 1,\ldots,J; \ i \quad 1,2,\ldots$?
- Yes,then go to 8;
- No,then go to 16.

16. Stop. End of the iteration procedure.

This numerical algorithm allows modelling of wide number of heat and mass transfer processes. The mathematical descriptions must be numerical models (subject function as a result of the numerical solution of the model equations).

Conclusions

The numerical method for incorrect inverse problems solution conceived here stresses on parameter identification and allows modelling of a wide number of processes. The mathematical descriptions must be numerical model (subject function as a result of the numerical solution of the model equations).

References

1 Tikhonov, A. N, Arsenin, V. I., Methods for Solutions of Incorrect Problems (in Russian), Nauka, Moscow, 1979
2 Tikhonov, A. N, Kal'ner, V. D., Glasko, V. B., Mathematical Modelling of Technological Processes and Method of Inverse Problems (in Russian), Mashinostroenie, Moscow, 1990
3 Boyadjiev, Chr., Fundamentals of Modeling and Simulation in Chemical Engineering and Technology (in Bulgarian), Bulg. Acad. Sci., Inst. Chem. Eng., Sofia, 1993
4 Boyadjiev, Chr., On the Model Parameter Identification and the Incorrectness of the Invers Problems, *Proceedings*, Bourgas'2001, 6th Workshop on "Transport Phenomena in Two–Phase Flow", Sept. 11-16, Bulgaria, 2001

Author's address:

Chr. B. Boyadjiev
Bulgarian Academy of Sciences, Institute of Chemical Engineering
Acad. G. Bontchev Str., Bl.103, 1113 Sofia, Bulgaria
E-mail CHBOYADJ@BAS.BG

Paper submited: January 28, 2002
Paper revised: February 1, 2002
Paper accepted: February 15, 2002