INCORRECT INVERSE PROBLEM SOLUTION METHOD FOR PARAMETER IDENTIFICATION OF TRANSPORT PROCESSES MODELS

by

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A method for model parameter identification on the bases of minimization of the least square function has been proposed. An iterative regularization procedure and a numerical algorithm have been developed for incorrect (ill-posed) or essentially incorrect inverse problem solution. The method has been tested with one and two-parameter models, when the relations between objectives function and parameters are linear and non-linear. The "experimental" data for parameters identification are obtained from the model and a generator for random numbers. The effects of the initial approximations of the parameter values and the regularization parameter values have been investigated. A statistical approach has been proposed for the analysis of the model adequacy.
It is demonstrated that in the cases of essential incorrectness, the least square function do not reach minima. A criterion for the incorrectness of the inverse problem was proposed.

Key words: *model parameter identification, incorrect inverse problems, iterative method, regularization, model adequacy*

Introduction

The main problem of the modelling of the hydrodynamic, heat and mass transfer processes is the build-up mathematical structure, describing the processes based on the hypothesis (knowledge) concerning to their physical mechanisms. Moreover, the procedure needs of the parameters identification of the mathematical description, based on experimental data. The inverse identification problem is often an incorrect (ill-posed), *i. e.* the solution is sensible with respect to the errors of the experimental data [1-5]. The main cause is small parameters – pre-factors of the high-ranking (second) derivatives – in the parabolic partial differential equations in the hydrodynamic, heat and mass transfer models (viscosity, diffusivity, conductivity).

The solution of the parameters identification problem can be obtained by the minimization of the functional of variances (least square function), *i. e*. from the condition for a minimal difference between calculated and experimental data [5-10].

There are different methods (selection, quasi-solution, substitution of equation) permitting to obtain solutions of the incorrect inverse problems in the cases of a presence of the additional information about the functional minima [4, 5, 10].

In many cases the inverse problems are essential incorrect and a regularization operator permits to obtain the solution [5, 6, 10]. The problem regularization use variational or iterative approaches. Further the gradient methods are employed for a minima search [6, 7, 11-14]. The iterative procedure stops when the iterative solution moves away from the exact solution and the number of the last iteration is accepted as a regularization parameter of the inverse problem solution.

In many cases, this approach generates a large deviation of the iterative solution from the exact solution. In the present paper, the new proposed iterative algorithm permits minimization of the difference between iterative and exact solutions.

Problem formulation

Let us consider a numerical model:

$$y \quad f(\vec{x}, \vec{b}) \tag{1}$$

where f is an objective function, expressed analytically, numerically or through an operator (algorithm); $\vec{x} = (x_{1, ..., } x_m)$ is a vector of independent variables, $\vec{b} = (b_{1, ..., } b_J)$ – vector of parameters.

The parameters of the model (1) should be determined by means of N experimental values of the objective function $\hat{y} \quad (\hat{y}_1, ..., \hat{y}_N)$. This requires the introduction of a least square function:

$$Q(\vec{b}) \quad \sum_{n\ 1}^{N} (y_n \quad \hat{y}_n)^2 \tag{2}$$

where $y_n = f(\vec{x}_n, \vec{b})$ are the calculated values of the objective function of the model (1), while $\vec{x}_n = (x_{1n}, ..., x_{mn})$ are the values of the independent variables from the different experimental conditions (regimes), $n = 1, ..., N$.

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

The determination of $\vec{b}$ faces many troubles due to the incorrectness of the problem. They are a result of the sensibility of the solution with respect to the experimental errors associated with the determination of $\hat{y}$. They can be avoided by applications of regularization methods that make the problem conditionally correct.

Incorrectness of the inverse problem

Let us consider the one-parameter model:

$$y = 1 - \exp(-bx) \tag{3}$$

where y is an objective function, x is an independent variable and b is an parameter.

In the fig. 1 is shown a dependence of the objective function from the model parameter at a constant value of the independent variable $x = x_0$. The relation between the

objective function and the parameter in the fig. 1 is typical in the cases of small parameter (viscosity, diffusivity, conductivity) as a pre-factor of the second derivative in many models of hydrodynamic, heat and mass transfer processes.

The fig. 1 permits to obtain objective function y_0 for a given parameter value b_0, *i. e*. this is the direct problem solution. The inverse problem is an obtaining of the parameter value b_0 if the experimental value of the objective function y_0 is known.

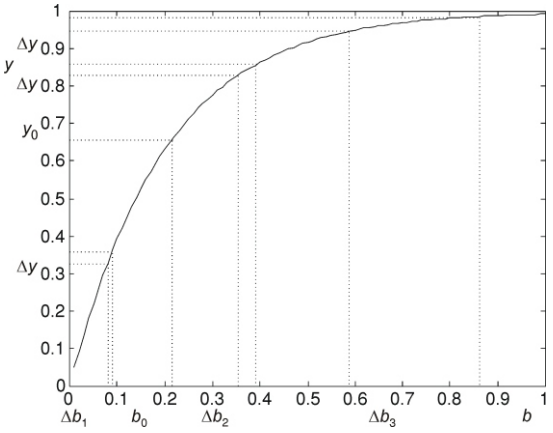

Figure 1. Objective function *y* for different values of the model parameter *b* at $x = x_0 = \text{const}$.

Let y is an experimental error of the objective function. In the fig. 1 is seen, that the error of the parameter identification is different for small and large objective function values. For the small objective function values the error b_1 is small and the inverse identification problem is correct. If the objective function values are large, the error b_2 is large too and the inverse problem is incorrect (ill-posed). In the case of very large objective function values, b_3 is very large and the inverse identification problem is essentially incorrect.

The results in the fig. 1 show that inverse method incorrectness is not result of the error size and the cause is the parameter sensitivity with respect to the experimental errors of the objective function.

Incorrectness of the least square function method

Let us consider the two-parameter model:

$$y = 1 - b_1 \exp(-b_2 x) \tag{4}$$

where $\overline{b}_1 \quad 1$ and $\overline{b}_2 \quad 5$ are exact parameter values.

The parameter identification problem will be solved by the help of the "experimental" data, obtained by a generator of random numbers:

$$\hat{y}_n^{(1)} \quad (0.95 \quad 0.1A_n)\, y_n\,, \quad \hat{y}_n^{(2)} \quad (0.9 \quad 0.2A_n)\, y_n \tag{5}$$

Here, A_n are random numbers at the interval [0, 1], and y_n is obtained from the model (5) for $x = 0.01n$ $(n = 1,\ldots,100)$. Obviously, the maximum relative errors of the

"experimental" data ($\Delta\hat{y}$) are 5% and 10%. The values of y_n, $\hat{y}_n^{(1)}$ and $\hat{y}_n^{(2)}$ are shown in fig. 2.

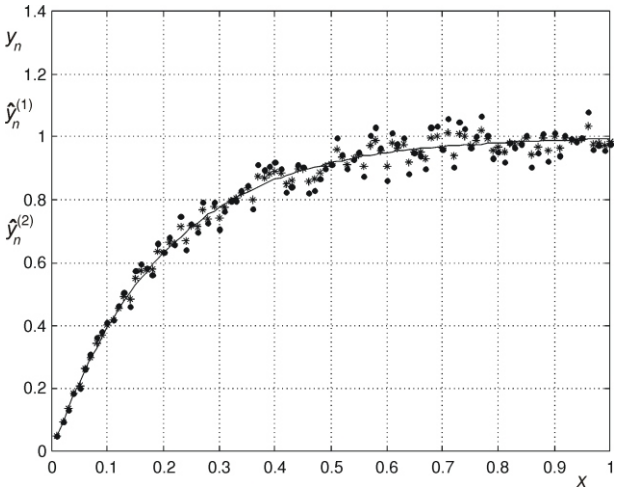

Figure 2. Mathematical model and "experimental" data
[*] – $\hat{y}_n^{(1)}$ values of y with a maximal "experimental" error of 5%;
[ ] – $\hat{y}_n^{(2)}$ values of y with a maximal "experimental" error of ±10%;
[—] – y = 1 – exp(–5x)

In the fig. 2 is seen that inverse identification problem is correct when $0 < x < 0.3$, incorrect if $0.31 < x < 0.65$, and essentially incorrect when $0.66 < x < 1$.

In the figs. 3-5, are seen the horizontals of the least square function (2) in the cases of 5% relative experimental data error and different interval of x, when inverse problem is correct (fig. 3), incorrect (fig. 4), and essentially incorrect (fig. 5). These results show that the least square method is correct when the differences between exact parameter values in the model and the coordinates of the least square function minimum are very small (fig. 3). These differences are too large, when the inverse problem is incorrect (fig. 4). In the case, when inverse problem is essentially incorrect the least square function has not a minimum (fig. 5).

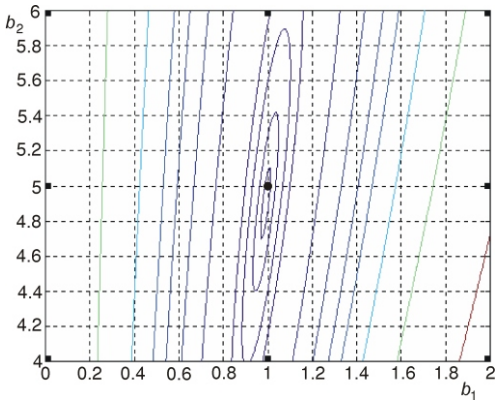

Figure 3. The horizontals of the least square function *Q*
(n = 1-30; Δ ŷ [%] = ±5); [ ] – b = [1; 5];

The results obtained show (figs. 3-5), that in the cases of incorrect inverse problems, the least square function minimization is not lead to solution of the inverse problem and for the problem solution must be use additional conditions.

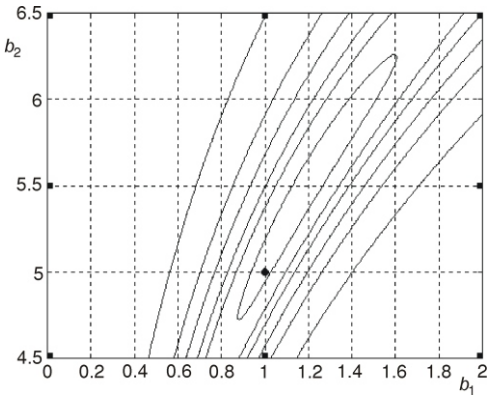

Figure 4. The horizontals of the least square function *Q*
(n = 31-65; Δ ŷ[%] = ±5); [ ] – b = [1; 5];

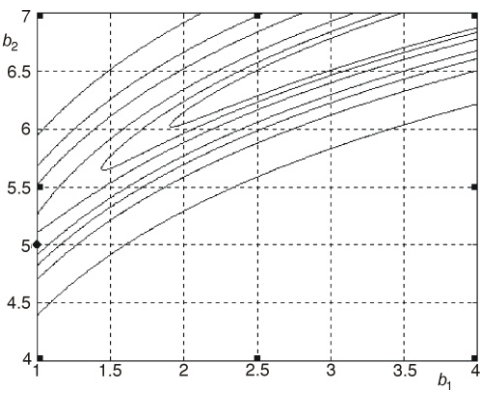

Figure 5. The horizontals of the least square function *Q*
(*n = 66-100; Δ ŷ [%] = ±5); [ ] – b = [1; 5]*

Regularization of the iterative method for parameter identification

Various iterative methods for a minimum search (the gradient ones too) are stable with respect to the experimental errors of the objective functions. However, after certain number of iteration an increasing of the difference between iterative and exact values of the parameters start. That is why in each step must be checked the increasing of this difference.

The present paper proposes a method with a preliminary defined accuracy of the parameters identification. The minimum of $Q(\vec{b})$ is determined by a gradient method, controlling the difference between iterative and exact parameter values in each iteration step.

Let the iteration procedure starts with an initial approximation $\vec{b}^{(0)}$ $(b_1^{(0)},\ldots,b_J^{(0)})$. The values of $\vec{b}_i = (b_{1i}, \ldots, b_{Ji})$, where i is iteration number, are result of the conditions imposed by the movement towards the anti-gradient of the function $Q(\vec{b})$:

$$b_{ji} = b_{j(i-1)} - \beta_{(i-1)} R_{j(i-1)}, \quad j = 1, \ldots, J \tag{6}$$

where

$$R_{j(i\ 1)} \quad \frac{\dfrac{\partial Q}{\partial b_j}_{(i\ 1)}}{\sqrt{\displaystyle\sum_{j\ 1}^{J} \left(\frac{\partial Q}{\partial b_j}_{(i\ 1)}\right)^2}}, \quad j \quad 1,\ldots,J \tag{7}$$

Here β_i is the iteration step and $\beta_0 = 10^{-2}$ (arbitrary small step value).
Each iteration step is successful if two conditions are satisfied:

$$Q_{i+1} - Q_i = \sum_{n=1}^{N} \beta_{(i+1)} \left[2f(\vec{x}_n, \vec{b}_{(i+1)}) - 2\hat{y}_n \right] \beta_{(i+1)} \sum_{j=1}^{J} R_j \left(\frac{\partial f}{\partial b_j} \right)_{(i+1)} \sum_{j=1}^{J} R_j \left(\frac{\partial f}{\partial b_j} \right)_{(i+1)} < 0 \tag{8}$$

$$(b_{j(i+1)} - \bar{b}_j)^2 - (b_{ji} - \bar{b}_j)^2 - \beta_{(i+1)} [2(b_{j(i+1)} - \bar{b}_j) - \beta_{(i+1)} R_{j(i+1)}] R_{j(i+1)} < 0$$
$$j = 1, \ldots, J$$

The first condition in (8) indicates that iterative solution ($\vec{b}_i$) approaches the solution at the minimum ($\vec{b}^*$), while the second condition in (8) concerns the approach of the iterative solution ($\vec{b}_i$) towards the exact solution ($\bar{b}$). Obviously, it is due to the effect of the problem incorrectness $\bar{b} - \vec{b}^*$ (see figs. 3-5).

The results obtained permit to create an algorithm for solution of the inverse identification problems [18, 19].

Correct problem solution

The literature sources [5, 6, 10, 11], teach that every method for solving of incorrect problems must solving a correct ones. Therefore, the first solution of the inverse problem corresponds to the interval $0 < x < 0.3$.

The proposed algorithm was used for the solution of the identification problem and results are shown on the tab. 1.

Table 1. One and two-parameter model solutions

$\Delta\hat{y}$ [%]	b^*	i	b_1^*	b_2^*	i
5	4.9678	337	1.0025	5.0674	128
10	4.9351	339	0.99401	4.9218	172

Incorrect problem solution

The parameters identification problem will be solved by minimization of the least square function (2), where $x_n = 0.01n$, $n = 31, \ldots, 65$, *i. e.* $0.31 \quad x \quad 0.65$.

The incorrect problem solution for the one-parameter model ($b^{(0)} = 6$, $\gamma = 0.5$) and two-parameter model ($b_1^{(0)} = 1.1$, $b_2^{(0)} = 6$, $\gamma = 0.05$) are shown on the tab. 2.

Table 2. Incorrect problem solution

$\Delta\hat{y}$ [%]	b^*	i	b_1^*	b_2^*	i
5	5.0614	1213	1.1797	5.4666	642
10	5.1232	1217	1.3778	5.9106	416

The results from tab. 2 show that differences between the exact and the obtained values of the parameters are significant. The correctness of the parameter identification will be tested through the model adequacy as a criterion [15-17].

Statistical analysis of model adequacy

The model is adequate if the variance of the experimental data error (S_ε) is equal to the variance of the model error (S). The test needs to the experimental values of the objective function $\hat{y}_k$,($k = 1, ..., K$) upon identical technological conditions (regime) $x = \vec{x}^{(0)} = (x_1^{(0)}, \ldots, x_K^{(0)})$, where K =5-10. The experimental data variance requires estimation of the mathematical expectation of $y(\tilde{m}_y)$ [10, 15]:

$$\tilde{m}_y \quad \frac{1}{K} \sum_{k\ 1}^{K} \hat{y}_k \tag{9}$$

and as a result

$$S_\varepsilon^2 \quad \frac{1}{K \quad 1} \sum_{k\ 1}^{K} (\hat{y}_k \quad \tilde{m}_y)^2 \tag{10}$$

Thus, the variance of the model error [10] is:

$$S^2 \quad \frac{1}{N \quad J} \sum_{n\ 1}^{N} (y_n \quad \hat{y}_n)^2 \quad \frac{Q}{N \quad J} \tag{11}$$

where N is experimental data number and J – the parameters number.

The model adequacy is defined by the variance ratio:

$$F \quad \frac{S^2}{S_\varepsilon^2} \tag{12}$$

where $S^2 \quad S_\varepsilon^2$, if S contains the error effect of the both model and experimental data. The value of F is compared to the tabulated values (F_J) of the Fisher's distribution (criteria) [15]. The condition of the model adequacy is:

$$F \quad F_J(\alpha, \nu, \nu_\varepsilon) \tag{13}$$

where $\nu = N - J$, $\nu_\varepsilon = K - 1$, and α = 0.01-0.1.

The statistical analysis of the one and two parameters model adequacy was tested for $0 \quad x \quad 0.30$ and the results are presented on tab. 3. For the test performed: N =

= 30, J = 1(2), K = 10, $x^{(0)}$ = 0.2, and α = 0.05. The results collected confirm the adequacy of the model.

Table 3. Statistical analysis of the model adequacy (0 x 0.3)

J	$\Delta\hat{y}$ [%]	b_1^*	b_2^*	γ	$S_\varepsilon \cdot 10^{-2}$	$S \cdot 10^{-2}$	F	F_J
1	5	–	4.9678	0.9	1.7933	1.7071	0.9061	2.24
1	10	–	4.9351	0.9	3.5867	3.4139	0.9059	2.24
2	5	1.0025	5.0674	0.9	1.7933	1.8354	1.0475	2.25
2	10	0.9940	4.9218	0.9	3.5867	3.4434	0.9217	2.25

The statistical analysis of the cases corresponding to incorrect inverse problem (0.31 x 0.65) was performed for N = 35, J = 1(2), K = 10, $x^{(0)}$ = 0.5, and α = 0.05 (see tab. 4). The models are adequate despite the large differences between the calculated and the exact values of the model parameters (see tab. 2).

Table 4. Statistical analysis of the model adequacy (0.31 x 0.65)

J	$\Delta\hat{y}$ [%]	b_1^*	b_2^*	γ	$S_\varepsilon \cdot 10^{-2}$	S$\cdot 10^{-2}$	F	F_J
1	±5		5.0614	0.5	2.6042	2.3588	0.8205	2.19
1	±10		5.1232	0.5	5.2083	4.7328	0.8257	2.19
2	±5	1.1797	5.4666	0.05	2.6042	2.3656	0.8252	2.20
2	±10	1.3778	5.9106	0.05	05.2083	4.7349	0.8265	2.20

Essentially incorrect problem

The parameters identification problem when inverse problem is essentially incorrect will be solved by minimization of the least square function (2), where n = 66, ..., 100.

The results in the tab. 5 are solutions of the identification problems for one- and two-parameter models.

Table 5. One and two-parameters model solutions (0.66 x 1)

$\Delta\hat{y}$ [%]	b*	i	b_1^*	b_2^*	i
5	5.1828	2066	2.1720	6.1731	54
10	5.3816	2156	4.9003	7.4004	128

The results in the tab. 5 show that the differences between obtained and exact parameters values are very large, but the differences between obtained and exact models exhibit just the opposite behavior.

Statistical analysis of the model adequacy in the cases of essential incorrectness of the inverse problem (0.66 x 1) was done for $N = 35$, $J = 1(2)$, $K = 10$, $x^{(0)} = 0.8$, and $\alpha = 0.05$. The results are collected in the tab. 6. The models employed in this paper are adequate independently despite the large differences between the calculated and the exact values of the model parameters (see tab. 5).

Table 6. Statistical analysis of the model adequacy (0.66 x 1)

J	$\Delta\hat{y}$ [%]	b_1^*	b_2^*	γ	$S_\varepsilon \cdot 10^{-2}$	$S \cdot 10^{-2}$	F	F_J
1	±5		5.1828	5	2.7850	2.5988	0.8707	2.19
1	±10		5.3816	5	5.5701	5.2482	0.8723	2.19
2	±5	2.1720	6.1731	5	2.7851	2.6221	0.8855	2.20
2	±10	4.9003	7.4004	5	5.5701	5.2482	0.8877	2.20

General case

It was shown, that if the "experimental" data were obtained upon conditions (regimes), corresponding to the interval 0 x 1, the parameter identification problem is correct, incorrect, and essential incorrect.

In practice, very often is possible to have experimental data in very large regime interval (for example 0 x 1). However, it is unknown which from the experimental data lead to correct or incorrect problem. That is why the parameter identification problem will be solved by minimization of the least square function, obtained in the very large experimental data interval:

$$Q(\vec{b}) \quad \sum_{n\ 1}^{100} (y_n \quad \hat{y}_n)^2 \tag{14}$$

where $y_n = f(x_n, \vec{b})$, $x_n = 0.01n$, $n = 1, ..., 100$, $b = (b_1, b_2)$.

In the tab. 7 the results of the parameter identification for one- and two-parameter model are shown. This results are obtained for initial approximation, $b^{(0)} = 6$, ($\gamma = 5$) and $b_1^{(0)}$ 1.1, $b_2^{(0)}$ 6 ($\gamma = 2$).

Table 7. One and two-parameters model solutions (0 x 1)

$\Delta\hat{y}$[%]	b*	i	b_1^*	b_2^*	i
5	5.0117	50	1.0106	5.1717	65
10	5.0231	50	1.0196	5.1721	66

Statistical analysis of the model adequacy in the cases of 0 x 1 was made for $N = 100$ and the results are shown in the tab. 8. They show that all of models are adequate due to $F < F_j$.

Table 8. Statistical analysis of the model adequacy (0 x 1), $K = 10$, for different regimes ($x_1^{(0)}$ 0.2, S_ε, F ; $x_2^{(0)}$ 0.5, S_ε, F ; $x_3^{(0)}$ 0.8, S_ε, F)

b_1^*	b_2^*	S_ε 10 ^{2}	S_ε 10 ^{2}	S_ε 10 ^{2}	$S \cdot 10^{-2}$	F	F	F	F_J
–	5.011	1.79	2.60	2.78	2.33	0.80	0.70	1.69	1.99
–	5.023	1.79	1.79	1.79	2.33	1.69	1.69	1.69	1.99
1.010	5.171	1.79	1.79	1.79	2.40	1.80	1.80	1.80	1.99
1.019	5.172	1.79	1.79	1.79	2.40	1.79	1.79	1.79	1.99

Incorrect inverse problem "diagnostics"

In all these cases the difference between correct and incorrect inverse identification problem is based on the distance between exact solution point and least square function minimum point. In practice however the exact parameter values are unknown and a criterion for the inverse problem "diagnostics" will be very useful.

On the tabs. 9 and 10 are shown the solutions of correct and incorrect inverse problems on the bases of different experimental data sets. It is seen that a criterion of the inverse problem incorrectness is the large difference between solutions which are obtained on the bases of different experimental data sets.

The results in the tabs. 9 and 10 show that the solution of the inverse problem $\vec{b}^*$ permit to calculate the objective function y_n $f(\vec{x}_n, \vec{b}^*)$ for different "experimental" conditions ($n = 1, \ldots, N$). If put this values (y_n) in eqs. (5), different sets of random num-

Table 9. Solutions of correct and incorrect problems using different "experimental" data sets

$b_1^{(0)}$ 1.1, $b_2^{(0)}$ 6					
Different "experimental" data		b_1^*	b_2^*	γ	i
0 x 0.3	1	1.0025	5.0674	0.9	128
	2	1.0115	5.1706	0.9	120
	3	1.0068	5.1881	0.9	179
0.31 x 0.65	1	1.1564	5.2675	0.05	798
	2	0.5789	3.7056	0.05	1803
	3	1.1723	5.2624	0.05	776

bers A_n permit to obtained different sets of "experimental" data $\hat{y}_n (n = 1, \ldots, N)$. The comparison of the inverse problem solutions, using different "experimental" data sets, will show the inverse problem correctness (incorrectness).

Table 10. Solutions of essentially incorrect problem and general case, using different "experimental" data sets

$b_1^{(0)}$ 1.1, $b_2^{(0)}$ 6					
Different "experimental" data		b_1^*	b_2^*	γ	i
$0.66 < x < 1$	1	4.5933	6.7246	5	680
	2	0.1161	2.3417	5	390
	3	2.7943	5.9219	5	133
$0 < x < 1$	1	1.0106	5.1716	2	66
	2	1.0100	5.1963	2	70
	3	1.0134	5.1913	2	76

Conclusions

The proposed iterative method and algorithm for model parameters identification in the cases when inverse problem is incorrect shows that a large difference between parameter values, obtained on the bases of different experimental data sets, is a criterion for inverse problem incorrectness.

The solution of the model parameters identification problem by the help of the least square function minimization manifests a large difference between the exact and calculated (as a function minimum) parameter values *i. e*. the minimization of the least square function is not a solution of the parameter identification problem. This difference is not result of the experimental data size and can be explained with the inverse problem incorrectness, *i. e*. the parameter value sensibility with respect to the experimental data errors.

An additional condition is introduced for the inverse problem regularization, which permits to use least square function minimization for a solution of the model parameter identification problem.

A statistical analysis of the model adequacy is a criterion for the applicability of the presented iterative method for the model parameters identification.

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