The condition number of a matrix as an optimality criterion in the problems of parametric identification of linear equations systems

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Abstract. When solving applied problems, an important aspect of the analysis is the stability of the obtained solution with respect to experimental data errors. Empirical experimental data, although a priori inaccurate, can be represented by intervals of their range of values. In some cases, the limits of their variation may also be known. Obviously, the degree of inaccuracy of input data influences the solution of the parametric identification problem. Therefore, in the case when this solution is not the only one, methods for assessing the influence of experimental error on the stability of each potential solution are of interest as they may provide additional arguments in favour of choosing one of them. In the case of models formalized in the form of systems of linear algebraic equations, a similar effect can be investigated using the condition number. In a case of quantitative analysis of multicomponent mixtures, the paper presents an approach to the parametric identification of linear models based on the calculation of the maximum permissible parameter estimates in combination with the study of the coefficient stability of the system.

1. Introduction

Square systems of linear algebraic equations

\begin{equation}
A \bar{x} = B
\end{equation}

are among the most well-studied objects in applied mathematics. In practical problems, the components of the coefficient matrix and the column vector are formed on the basis of experimental data, and therefore they should initially be considered as approximate estimates of the exact parameters of the system (1).

To solve system (1), many exact and approximate numerical methods have been developed. Due to the high sensitivity of the solutions of such systems to changes in the parameters included in them, it is rarely possible to obtain stable solutions. In this case, it is customary to distinguish between stability on the right-hand sides of the system and coefficient stability.
If the matrix $A$ is nondegenerate then the degree of variation of the solution depending on the matrix coefficients and the column vector can be estimated using the condition number of the matrix [1–3]:

$$\text{cond} \left( A \right) = \left| A \right| \left| A^{-1} \right|,$$

(2)

wherein $\left| \cdot \right|$ – the indication of the corresponding matrix norm. The larger $\text{cond} \left( A \right)$, the more significant the influence of errors in the parameters of system (1) on its solution may be. According to some estimates [4], if $\text{cond} \left( A \right) \geq 1000$, then the matrix is considered poorly conditioned, if $1 \leq \text{cond} \left( A \right) \leq 100$, then well-conditioned.

The following quantitative estimates are known for the relative errors of the exact solution $\vec{x}^*$:

- $\delta_{x^*} \leq \text{cond} \left( A \right) \cdot \delta_{B^*}$ – if there is an error in the column vector $B \left( B^* \right.$ – its exact value$)$;
- $\delta_{x^*} \leq \text{cond} \left( A \right) \cdot \delta_{A^*}$ – if there is an error in the matrix of coefficients $\left( A^* \right.$ – is the matrix of the true values of the system’ coefficients$)$;
- $\delta_{x^*} \leq \text{cond} \left( A \right) \cdot \left( \delta_{A^*} + \delta_{B^*} \right)$ – in the case of assignment with errors and coefficients of system (1), and its column vector components.

$\delta_{x^*}$ is the designation of relative errors, e.g. $\delta_{x^*} = \frac{\| \Delta \vec{x} \|}{\| \vec{x}^* + \Delta \vec{x} \|}$, where $\Delta \vec{x}$ is the disturbance of $\vec{x}^*$.

The task of parametric identification of model (1) is to process known experimental data for the matrix $A$ elements, column vector $B$, and vector of variables $\vec{x}$ determine the true values of all parameters of this system. Moreover, if point estimates of the desired parameters are obtained, then due to the high sensitivity of the solutions of systems of linear algebraic equations to small changes in the parameters, it is necessary that these point estimates coincide with the true ones, which, obviously, will require appropriate justification. Therefore, taking into account the inherent inaccuracy of the input data, it is appropriate to raise the question of determining the intervals of values for the elements of the matrix $A$ and vector $B$, which ensure the adequacy of the solutions of the direct problem (1). It is important to note that the requirements for the adequacy of the solution can often be represented in the form of conditions on the values of variables, consequent verification of which may require a large number of iterations to adjust the model.

In this regard, the development of parametric identification methods is relevant, the use of which will take into account all the requirements that are significant for a researcher determining interval parameter estimates. The advantage of this approach, among other things, is also explained by the fact that knowing the intervals of the maximum variation in the values of each parameter will allow us to estimate the error of the solution (and as such can be used to interpret the degree of uncertainty).

In the present work, it is proposed to use an approach based on the development of ideas expressed by L.V. Kantorovich as a method of parametric identification of model (1) regarding the problems of mathematical processing of observations [5]. The essence of this approach is to use a wide range of mathematical modelling methods to search not for point but rather interval estimates of the desired parameters, which provide acceptable qualitative characteristics of the description of experimental data. A clear advantage of this approach is the ability to determine the desired values, taking into account all significant available information about the object of study.

The interest in problems of this kind is explained by the practical relevance of the results [5–8]. However, the application of traditional approaches is rarely adequate: in some cases, due to physicochemical measurements errors [5, 8], in others, due to characteristic features of the applied mathematical methods [9]. This direction has been widely developed in relation to the problems of physical chemistry.
The paper presents the implementation of the described approach to one of the physical chemistry problems [10, 11], represented by linear models, namely, the task of quantitative analysis of multicomponent mixtures based on UV spectrometry data. Thus, the aforementioned factors determine the relevance of the present work, the primary objective of which is to develop a method for the parametric identification of the Vierordt equations used to identify quantitative characteristics of multicomponent mixtures [12, 13].

2. Problem statement
One of the methods for the quantitative analysis of multi-component solutions absorbing ultraviolet rays is the Vierordt method [12]. Its use is possible if the following two conditions are satisfied:

1) the light absorption of each component of the mixture obeys the Bouguer-Lambert-Beer law, described in logarithmic form as:

\[ \lg \left( \frac{I_0}{I} \right) = D = \varepsilon \lambda l c, \]  

(3)

where \( I_0 \) and \( I \) are the intensities of the incident and transmitted light flux, respectively, \( \varepsilon \lambda \) is the molar absorption coefficient corresponding to the wavelength \( \lambda \) (1·mol\(^{-1}\)·cm\(^{-1}\)), \( l \) is the thickness of the absorbing layer (cm), \( c \) is the concentration of the solution component (mol·l\(^{-1}\)), \( \lg \left( \frac{I_0}{I} \right) = D \) is the optical density that characterizes the absorption capacity of a substance in a solvent;

2) the entire mixture is performed additivity principle, according to which optical density of noninteracting component of a \( m \)-component mixtures, each of which obeys the Lambert-Bouguer-Beer’s law at a certain wavelength \( \lambda \), is equal to the sum of the individual components of the absorption at the same wavelength:

\[ D^\lambda = \sum_{i=1}^{m} D_i^\lambda = l \sum_{i=1}^{m} \varepsilon_i^\lambda c_i, \]  

(4)

where \( l \) is the thickness of the absorbing layer, \( \varepsilon_i^\lambda \) are the molar absorption coefficients at a specified wavelength \( \lambda \), \( c_i \) is component concentration in the mixture, \( i = 1, m \) is the component index. Relation (4) is called the Vierordt equation.

When considering a mixture of \( m \) components, via spectral analysis for each \( i \)th component, an analytical wavelength \( \lambda_i \) is defined as corresponding to maximum absorption, and \( m \) Vierordt equations are constructed, which leads to the system:

\[ D_i^\lambda = \varepsilon_i^\lambda c_i l + \ldots + \varepsilon_m^\lambda c_m l \]

\[ \ldots \ldots \ldots \ldots \ldots \]

\[ D_m^\lambda = \varepsilon_1^\lambda c_1 l + \ldots + \varepsilon_m^\lambda c_m l. \]  

(5)

In fact, (5) represents a square system of linear algebraic equations, the main purpose of which is to determine the concentration of the components of the mixture. And this requires the implementation of its parametric identification using experimentally obtained data on optical densities, molar absorption coefficients, as well as knowledge of the thickness of the absorbing layer.

It is known that solutions of systems of linear algebraic equations are extremely sensitive to changes in their parameters. In the case of system (5), all its coefficients are determined based on the processing of experimental data, and therefore are a priori inaccurate. This can cause a distortion of the solution. Moreover, the resulting solution may contain both positive and negative components, which, taking into account the physical meaning of the concentrations, is unacceptable. Therefore, an important aspect of the task of quantitative analysis of multicomponent mixtures using the Vierordt
method is related to verification of the resulting solution for adequacy, which, in turn, largely depends on the method of identifying system parameters (5) and on the optimality criterion for the resulting solution.

3. Methods, models, algorithms

We will introduce the following notations \( b_i = D^h_i, x_j = c_j, a_{ij} = \varepsilon_{ij}^h, A = (a_{ij}), B = (b_i), \bar{x} = (x_j), \) \( i, j = 1, m \) and write down the system (3) in a matrix form (1):

The molar absorption \( \varepsilon_{ij}^h \) coefficients, \( i, j = 1, m \) are characteristics of the mixture components and are independent of concentration value. Therefore, if mixed solutions of the same chemical components are being investigated, the elements of matrix \( A \) should be considered constants. This means that if the coefficient matrix of system (4) is identified, the quantitative composition of arbitrary mixtures composed of the same components will be determined based on the values of the elements of the column vector \( B \), which are established experimentally. In this situation, it is logical to identify matrix \( A \) based on the analysis of model mixtures.

When choosing the criteria according to which the identification of the system (1) should be carried out, the following should be taken into account. First, the accuracy of the model, which is understood as the proximity of the values of the left and right sides of system (1), should be acceptable. (This requirement is traditional for any parametric identification task.) Secondly, the coefficient matrix \( A \) should be suitable for the quantitative analysis of arbitrary mixtures, composed of the same components as model solutions. The reason for introducing this criterion is to neutralize the effect of errors that inevitably arises when determining the elements of the matrices \( A \) and \( B \). The criteria in the form of condition number (2) [1–4] satisfies these requirements, for which the smaller the value, the better. Indeed, due to the properties of the condition number of the matrix, if \( \text{cond} (A) \gg 1 \), then the matrix \( A \) is close to degenerate. Therefore, even very small errors made in the calculation of its elements, or the elements of the column vector \( B \), will lead to a significant distortion of the solution vector \( \bar{x} \). The minimum value of the condition number equal to 1 corresponds to the identity matrix \( A \), at which small changes in the parameters of system (1) obviously will not significantly change the solution \( \bar{x} \).

For parametric identification of the system of Vierordt equations, the following multi-stage procedure was developed and implemented based on the use of maximum permissible estimates of the unknown quantities and the condition number of the coefficient matrix.

**Step 1.** Based on UV spectrometry data analysis using appropriate mixtures of physicochemical methods for experimental data processing [12] to carry out the calculation of the matrix \( A \) elements and the column vector \( B \). Take the obtained values for the initial approximations of the parameters of the system of Vierordt equations (5).

**Step 2.** Introduce the matrix \( A' = (\gamma_{ij} a_{ij}) \) and column vector \( B' = (\delta_i b_i) \), where \( \gamma_{ij} \) and \( \delta_i \), \( i, j = 1, m \) are non-negative numbers.

The essence of each of which is to quantify how many times the corresponding experimental value of the molar absorption coefficients \( \varepsilon_{ij}^h \) and optical densities \( A^h \) should be changed and, so that the model (5) describes the available observations. (This allows us to consider \( \gamma_{ij} \) also \( \delta_i \) as estimates of the measurement errors of the corresponding experimental quantities.)

**Step 3.** Calculate the maximum permissible approximation error of the experimental data \( \xi \).

The value characterizes the maximum measurement error of the corresponding parameters of the Vierordt equation system, which provides a given correspondence of the left and right sides system (1) [8].

To implement this stage, the following model has been developed:
\[ \xi \to \min , \]
\[ |A^t x - B| \leq \bar{r} , \]
\[ |\delta_i - I| \leq 0.005 , \quad i = 1, m , \]
\[ |\gamma_{ij} - I| \leq \xi , \quad i, j = 1, m , \]
\[ \delta_i \geq 0 , \quad \gamma_{ij} \geq 0 , \quad \xi \geq 0 , \quad i, j = 1, m . \]

Here \( \bar{r} \) is a column vector whose components correspond to permissible errors in system (1). The condition \( |\delta_i - I| \leq 0.005 \) follows from the fact that the experimental determination of optical densities is carried out with an error not exceeding 0.5%.

**Step 4.** Calculate the maximum permissible estimates for the parameters \( \gamma_{ij} \) and \( \delta_j \), \( i, j = 1, m \) based on the use of the model:

\[ \gamma_{ij} \to \min \quad ( \gamma_{ij} \to \max , \quad \delta_i \to \min , \quad \delta_i \to \max , \quad i, j = 1, m ) , \]
\[ |A^t x - B| \leq \bar{r} , \]
\[ |\delta_i - I| \leq 0.005 , \quad i = 1, m , \]
\[ |\gamma_{ij} - I| \leq \xi^* , \quad i, j = 1, m , \]
\[ \delta_i \geq 0 , \quad \gamma_{ij} \geq 0 , \quad i, j = 1, m . \]

Here \( \xi^* \) is the optimal solution to problem (6).

The maximum permissible estimates of the parameters will be called the boundaries of the intervals \( [\gamma_{ij}^{\min}, \gamma_{ij}^{\max}] \) and \( [\delta_i^{\min}, \delta_i^{\max}] \), consisting of the values of \( \gamma_{ij} \) and \( \delta_i \), each of which preserves the compatibility of the system of inequalities \( |A^t x - B| \leq \bar{r} \) for some values of other parameters, and outside of the compatibility range this system is not provided by any set of parameter values. These intervals themselves will be called uncertainty intervals.

**Step 5.** Generate a set of uncertainty \( \Lambda \) in the form of a direct product of all intervals of

\[ \Lambda = [\gamma_{ij}^{\min}, \gamma_{ij}^{\max}] \times \ldots \times [\gamma_{ij}^{\min}, \gamma_{ij}^{\max}] \times [\delta_i^{\min}, \delta_i^{\max}] \times \ldots \times [\delta_i^{\min}, \delta_i^{\max}] . \]

It is evident that \( \Lambda \) is the external approximation of a set of parameter values \( \gamma_{ij} \) and \( \delta_j \), \( i, j = 1, m \) that form a solution set of (6).

**Step 6.** Implement a search on a set of uncertainty \( \Lambda \) to identify a set of parameter values \( \gamma_{ij} \) and \( \delta_j \) yielding the minimum value of the condition number of the coefficient matrix \( A' \).

4. Testing

As model mixtures for testing the developed approach, we considered three solutions with a known molar ratio of components. All model mixtures consist of low molecular weight individual products of mono- (I), di- (II), tri- (III) and tetra- (IV) addition of diallyl malone ester to \( C_{60} \) fullerene. All of these compounds were obtained in the laboratory for the synthesis of low molecular weight bioregulators of the Ufa Institute of Chemistry, Russian Academy of Sciences [14].
The first solution was a four-component equimolar mixture of substituted fullerenes I-IV, the second was a four-component non-equimolar mixture of substituted fullerenes I-IV, and the third was a five-component equimolar mixture of fullerene C$_{60}$ and substituted fullerenes I-IV (Table 1).

**Table 1.** The concentrations of the model mixtures components, $\cdot 10^{-6}$ mol·l$^{-1}$.

| Components of the mixture | Number of the mixture component (j) | $\bar{x}^1$ | $\bar{x}^2$ | $\bar{x}^3$ |
|---------------------------|------------------------------------|------------|------------|------------|
| C$_{60}$                  | 1                                  | –          | –          | 7.5        |
| I                         | 2                                  | 7.5        | 3.82       | 7.5        |
| II                        | 3                                  | 7.5        | 7.62       | 7.5        |
| III                       | 4                                  | 7.5        | 11.36      | 7.5        |
| IV                        | 5                                  | 7.5        | 14.97      | 7.5        |

The results of the first stage using physicochemical methods for model mixtures were determined by optical density column vectors $B^1$, $B^2$, and $B^3$

$$B^1 = \begin{bmatrix} 1.228 \\ 1.005 \\ 0.697 \\ 0.589 \end{bmatrix}, \quad B^2 = \begin{bmatrix} 1.481 \\ 1.249 \\ 0.899 \\ 0.715 \end{bmatrix}, \quad B^3 = \begin{bmatrix} 1.622 \\ 1.240 \\ 0.851 \\ 1.029 \end{bmatrix},$$

as well as the molar absorption coefficients of the matrix $A$:

$$A = \begin{bmatrix} 54000 & 30800 & 35800 & 28500 & 30900 \\ 30900 & 22800 & 28300 & 27900 & 28800 \\ 19600 & 21000 & 21800 & 18500 & 16050 \\ 50500 & 24370 & 17630 & 15070 & 11800 \\ 60780 & 24150 & 15350 & 13000 & 11700 \end{bmatrix}.$$

The condition number of the matrix $A$ was derived as $\text{cond}(A) = \|A\|\|A^{-1}\| = 146072.7 \cdot 0.00188 = 274.6$. It implies that the influence of the error parameters of the system (3) is significant. Additional confirmation of this was obtained by analyzing system (3) when all experimental data were substituted into it. The average relative deviation of the left parts of the model from the right for the first model mixture was 17.9%, for the second and third – 19.6% and 13.2% respectively.

Assuming the concentrations in system (1) to be unknown, and resolving it (i.e., using the expression $\bar{x} = A^{-1}B$), we can see (Table 2) that the calculated concentrations of the model mixtures differ significantly from the actual ones, and in two cases are generally negative. This makes it necessary to adjust the parameters of the system (1).

**Table 2.** Estimated concentrations of the model mixtures components, $\cdot 10^{-6}$ mol·l$^{-1}$.

| Components of the mixture | Number of the mixture component (j) | $\bar{x}^1$ | $\bar{x}^2$ | $\bar{x}^3$ |
|---------------------------|------------------------------------|------------|------------|------------|
| C$_{60}$                  | 1                                  | –          | –          | 8.43       |
| I                         | 2                                  | -1.13      | 6.82       | 3.11       |
The implementation of the 3rd stage was carried out on the aggregate data on all model mixtures at the same time. All components of the vector $\tau$ were assumed equal to 0.01. As a result, the maximum permissible approximation error was calculated $\xi^* = 0.3183$. (Note that the condition number of the matrix generated on a set of parameter values $\gamma_{ij}$ and $\delta_j$, $i, j=1,5$ based on the results obtained solutions of (7), is equal to 112.3. It is in 2.45 times smaller than the condition number of the matrix $A$.)

As a result of the 4th stage were calculated maximum permissible estimates $\gamma_{ij}^{\text{min}}, \gamma_{ij}^{\text{max}}, \delta_i^{\text{min}}, \delta_i^{\text{max}}, i, j=1,5$ (Table 3).

**Table 3. Maximum permissible estimates for the parameters $\gamma_{ij}$ and $\delta_i$.**

| $i$ | minimum value (min) / maximum value (max) | $\gamma_{11}$ | $\gamma_{12}$ | $\gamma_{13}$ | $\gamma_{14}$ | $\gamma_{15}$ | $\delta_1$ |
|-----|----------------------------------------|--------------|--------------|--------------|--------------|--------------|------------|
| 1   | min                                    | 0.968        | 1.318        | 1.318        | 1.318        | 1.172        | 0.995      |
|     | max                                    | 1.017        | 1.318        | 1.318        | 1.318        | 1.172        | 0.995      |
| 2   | min                                    | 0.906        | 0.895        | 1.284        | 1.298        | 1.302        | 0.995      |
|     | max                                    | 1.081        | 0.965        | 1.318        | 1.318        | 1.318        | 1.000      |
| 3   | min                                    | 0.998        | 0.744        | 1.113        | 1.197        | 1.214        | 0.995      |
|     | max                                    | 1.113        | 1.002        | 1.318        | 1.318        | 1.318        | 1.005      |
| 4   | min                                    | 0.832        | 0.682        | 0.682        | 0.682        | 0.682        | 0.995      |
|     | max                                    | 1.318        | 1.318        | 1.318        | 1.318        | 1.318        | 1.005      |

Maximum permissible estimates allowed to determine the uncertainty intervals for each of the parameters and generate of the 5th stage a set of uncertainty $\Lambda$ (8). The numerical implementation of the 6th stage on the set $\Lambda$ made it possible to determine the minimum of the condition number $(\text{cond}(A')=56.2)$ and the values of the parameters $\gamma_{ij}$ and $\delta_i$ at which it is achieved (Table 4). For comparison, we note that the condition numbers of the matrices $A'$ formed for each corner point of the set $\Lambda$ ranged from 106.8 to 2185.2.

**Table 4. Parameters $\gamma_{ij}$ and $\delta_i$ providing the minimum value of the condition number.**

| $i$ | $\gamma_{11}$ | $\gamma_{12}$ | $\gamma_{13}$ | $\gamma_{14}$ | $\gamma_{15}$ | $\delta_1$ |
|-----|--------------|--------------|--------------|--------------|--------------|------------|
| 1   | 1.017        | 1.318        | 1.318        | 1.318        | 1.172        | 0.995      |
| 2   | 1.107        | 1.318        | 1.227        | 1.318        | 1.150        | 0.995      |
| 3   | 0.906        | 0.894        | 1.318        | 1.318        | 1.302        | 0.995      |
| 4   | 0.998        | 0.744        | 1.318        | 1.318        | 1.214        | 0.995      |
| 5   | 0.832        | 1.192        | 1.318        | 1.318        | 0.682        | 0.995      |
The obtained parameters (Table 4) were used to adjust the matrix of coefficients of the Vierordt equation system:

\[
A' = \begin{bmatrix}
54937 & 40605 & 47197 & 37573 & 36207 \\
34200 & 30058 & 34715 & 36782 & 33133 \\
17764 & 18767 & 28740 & 24389 & 20904 \\
50400 & 18141 & 23242 & 19867 & 14324 \\
50543 & 28790 & 20237 & 17138 & 7975 \\
\end{bmatrix}.
\]

Average relative deviations of the results of matrix multiplication \(A'\) by concentration vectors of model mixtures (i.e., vectors \(A'\mathbf{x}^1\), \(A'\mathbf{x}^2\), \(A'\mathbf{x}^3\)) differ from the experimental optical densities \(B^1\), \(B^2\), \(B^3\) by 1.4%, 2.4%, and 3.7%, respectively. Similar estimates when comparing vectors \(A\mathbf{x}^1\), \(A\mathbf{x}^2\), \(A\mathbf{x}^3\) with vectors \(B^1\), \(B^2\), \(B^3\) amounted to 17.9%, 19.7% and 13.3%, respectively. Thus, the results obtained indicate the feasibility of using the matrix \(A'\) in the analysis of mixtures whose composition is identical to the model ones.

5. Application of the results
As noted above, the main purpose of the system of equations of Vierordt is to establish the quantitative composition of mixtures. Determination of unknown concentrations of the components of mixtures based on the system \(A'\) is a logical reverse problem to address:

\[
\mathbf{x} = (A'^{-1}) B.
\] (9)

However, such an approach does not guarantee adequate results. So, according to formula (9), the calculated values of the concentrations of the components of the model mixtures (Table 5) cannot be considered satisfactory due to the fact that they differ significantly from the actual ones (Table 1), including due to a contradiction with the physical meaning of these quantities (the concentration value of the last component of the third model mixture is negative).

**Table 5.** Calculated values of the concentrations of model mixtures, \(\cdot 10^{-6}\) mol·l⁻¹.

| Number of the mixture component, \(j\) | According to the formula (9) | According to the model (11) |
|---|---|---|
| 1 | \(\mathbf{x}^1\) | \(\mathbf{x}^2\) | \(\mathbf{x}^3\) |
| 2 | 10.30 | 2.04 | 7.34 |
| 3 | 7.93 | 14.20 | 12.10 |
| 4 | 9.09 | 12.00 | 13.10 |
| 5 | 2.56 | 7.67 | -4.43 |

Obviously, the unsatisfactory results obtained are explained by the high sensitivity of linear systems to the errors of their parameters. This makes it expedient to use modeling methods for the direct calculation of the desired concentrations. In the most general case, to determine the component-specific concentrations in a multi-component solvent mixture the following model is proposed:

\[
\xi \rightarrow \min_{\mathbf{x} \in \mathbb{X}} \left| A'\mathbf{x} - B \right| \leq \xi, \quad \mathbf{x} \geq 0, \quad \mathbf{x} \geq 0,
\] (10)
wherein $X$ is set, formed with all the conditions for concentration values. Note that the type of model (10) was developed in the context of paper [5].

Based on the information on available model mixtures, namely, assuming that the first and third model mixtures are equimolar, and for all model mixtures, the total concentrations ($S^1$, $S^2$, $S^3$) are known, the determination of which is carried out with an error not exceeding 1% model to calculate the concentration will take the form:

$$
\xi \to \min , \\
|A\bar{x}^k - B^k| \leq \xi ,
$$

$$
0.99 \cdot S^k \leq \sum_{j=1}^{J^1} \chi^k_j \leq 1.01 \cdot S^k , \ j = 1, 4 , \ (11)
$$

$$
0.98 \cdot \frac{\sum_{j=1}^{J^2} \chi^k_j}{5} \leq \chi_j^3 \leq 1.02 \cdot \frac{\sum_{j=1}^{J^2} \chi^k_j}{5} , \ j = 1, 5 ,
$$

$$
\bar{x}^k \geq 0 , \ k = 1, 2, 3 , \ J^1 = J^2 = 4 , \ J^3 = 5 .
$$

The equilibrium condition for the first and third model mixtures was formalized as a requirement according to which each component of these mixtures should not differ by more than 2% from the average concentration value.

According to the results of the numerical implementation of model (10), adequate concentrations were obtained (Table 5), the average relative deviation of which from the actual (Table 1) was 14.03% (the optimal value $\xi$ was 0.073). Note that the application of model (10) without taking into account the adjustment of matrix $A$ is equivalent to the fact that instead of the condition $|A\bar{x}^k - B^k| \leq \xi$ the following condition $|A\bar{x}^k - B^k| \leq \xi$ is used. It also allows you to calculate the concentration values, but for them the average error in relation to the actual data is 55.88%. Analogous selective calculations by model (11), carried out using matrices $A'$ formed for the corner points of the set $\mathcal{X}$, also showed a worse agreement of the results compared with those obtained for the matrix with the minimum value of the condition number.

6. Conclusion

A method for solving the problems of a parametric database, which reduces to systems of linear algebraic equations has been developed. The method is based on minimizing the condition number of the coefficient matrix and develops an approach that involves the use of maximum permissible estimates of the desired parameters. The numerical implementation of the developed approach to solving the problem of parametric identification of the Vierordt equations confirmed the feasibility of determining exactly the coefficient matrix with the minimum condition number. According to the presented results, in this case, the best accuracy of the description of experimental data is ensured, the a priori inaccuracy of which, due to the high sensitivity of linear problems to variations in the values of the model parameters, does not allow an adequate solution using classical linear algebra methods. Within the framework of the presented approach, it is possible to determine the parameters of the Vierordt equations taking into account all available information, thereby improving the qualitative characteristics of the resulting solution.

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