To The Question Of Determination Of Raw Materials Mineralogical Composition

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Abstract - The possibility to use a new computer program "Mineral" to determine the quantitative content of rock-forming minerals of silicate raw materials is shown.
Quantitative mineralogical composition of raw materials is being determined by means of calculations with the use of initial data obtained through chemical, thermal and X-ray phase analyzes. Solution of the problem is carried out using a computer program written in the C # programming language and is executed on a PC running the Windows operating system. The algorithm for solving the problem of determining the amount of each mineral is to solve sequentially the corresponding system of linear equations. The program created is characterized by efficiency while carrying out calculations of substance of rock-forming minerals on the basis of experimental data obtained through instrumental analysis. The principle of feedback is implemented: the accuracy of the calculations depends on the initial data, and the negative result of the calculations indicates the shortcomings of the preliminary analysis of the chemical and qualitative mineralogical composition of the raw material samples. The effectiveness of the practical use of the created computer program is confirmed by determining the quantitative mineralogical composition of carbonate and clay raw materials of various deposits. The use of the new computer program is an additional factor in solving the problem of analysis and quantification of the mineralogical composition of raw materials. Definitions of that kind are necessary both for the qualification of grades of raw materials and for the optimization of mass compositions and technological parameters of production, including production of silicate building materials.

Keywords - Raw material, silicates, composition, mineral, analysis, calculation, software

I. INTRODUCTION

The technology of production of silicate materials is associated with the use of a large amount of raw materials both of natural and technogenic with different chemical and mineralogical compositions [1-3].

The mineralogical composition of raw materials is an important factor in the structure formation of dispersed systems and materials based on them in the technological processes of production and ensuring of the specified physical and technical as well as of operational characteristics of the final products [4-8]. At the same time, the qualitative composition of rock-forming minerals and their quantitative ratio in raw materials depend on the rheological, structural-mechanical and technological properties of water systems (such as sludge, slurries and plastic masses), drying properties, the degree of sintering and the peculiarities of phase transformations during firing.

Instrumental methods of analysis (such as microscopy as well as a thermal one or by means of X-ray) are mainly used to determine the qualitative mineralogical composition of raw materials and to compare the content of individual minerals in samples, in particular by comparing the intensity and area of characteristic endothermic effects and diffraction peaks [9,10]. However, for a sufficiently accurate classification of raw materials, it is necessary to quantify the content of each of the rock-forming minerals [11-14].

Development of a mathematical apparatus for processing the results of research as well as of computer technology made it possible to increase the efficiency and effectiveness of determining the quantitative content of rock-forming minerals [15,16]. However, the constant increase in the number of varieties of potential raw materials makes it expedient to improve the method of quantitative determination of a mineralogical composition using computer calculations and modern software [17,18]. The work presented is a step in this direction.

II. THE PURPOSE AND PRINCIPLE OF THE PROBLEM SOLUTION

The varieties of raw materials which are used in the chemical technology of silicates constitute a set of certain rock-forming minerals of known chemical composition. Determination of the quantitative content of rock-forming minerals of a raw material is possible by means of calculations using basic data regarding chemical and qualitative mineralogical compositions.

The essence of the task is as follows.

Known:

- chemical composition of a certain raw material;

- qualitative mineralogical composition of that raw material;
- chemical composition of rock-forming minerals;

To be determined:

- the quantitative content (a percentage one) of rock-forming minerals in that raw material.

The very first step in the study is to determine the chemical content of the raw mix studied. Evaluation of the quantity of free quartz is not necessary what differs this method from some other known methods of the research.

At the next step mineralogical contents of the mix is determined using X-ray, thermo- and micro-analysis.

Solution of the problem is executed by means of Mineral computer desktop application. The program is developed using programing language C# (C-Sharp). The application runs under any contemporary OS Windows.

Mathematically, the goal and solution algorithm are formulated in the following way/

Source information:

The matrix MH (m rows per n columns) of the chemical composition of minerals is given. The rows of the matrix contain minerals, and the columns contain the chemical compounds that make up these minerals.

The list of rock-forming minerals of the sample is determined

(p elements, p <= min (m, n)).

The vector of chemical composition of the sample of a raw material AH (n elements) is known.

The vector X of the percentage of rock-forming minerals in the test sample of a raw material is to be determined.

Suggested algorithm.

The problem is divided into a number of separate problems, in each of which a system of linear equations is being solved. The matrix of the system in each of these intermediate tasks is an extract of the matrix MH' p columns (p is the number of rock-forming minerals). Obviously, the number of such intermediate tasks equals to the number of combinations n through p.

The further solution is provided as follows:

- sequence of p numbers k_i ($i \in [1, p]$, $k_i \in [1, m]$) representing the numbers of rows in the matrix for certain rock-forming minerals is fixed;
- sequence of p different numbers l_i ($l_i \in [1, n]$, $i \in [1, p]$) is selected;
- matrix M with the elements M_{ij} ($i \in [1, p]$, $j \in [1, p]$) is formed of the elements of the basic matrix MH;
- vector A with the elements A_i ($i \in [1, p]$) is formed of the elements of the basic vector AH;
- system of linear equations MX = A with the matrix M and the vector of the right-hand side A is solved;
- vector X, presenting the result of the solution of this intermediate system, is stored.

The application and source information for calculations are located in the C:\Mineral folder. Application name – Mineral.exe. Source information is stored in the Components.csv file (Fig. 1**)** which can be created by any text editor or by using Excel.

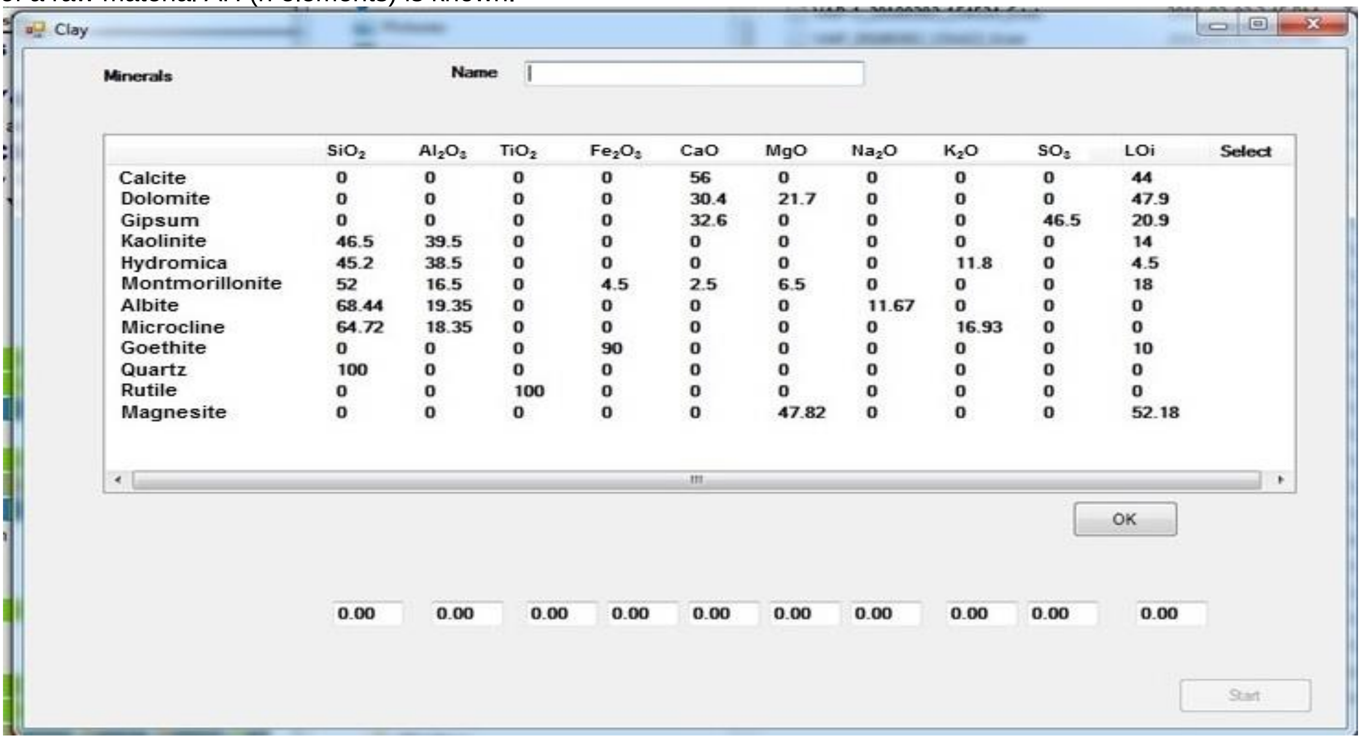

Figure 1. Initial view after the application is called

The input of the initial information for the calculation begins with the name of the sample (the Name window). The next step is to fill in the data regarding the qualitative mineralogical and chemical composition of the sample (Fig. 2, 3).

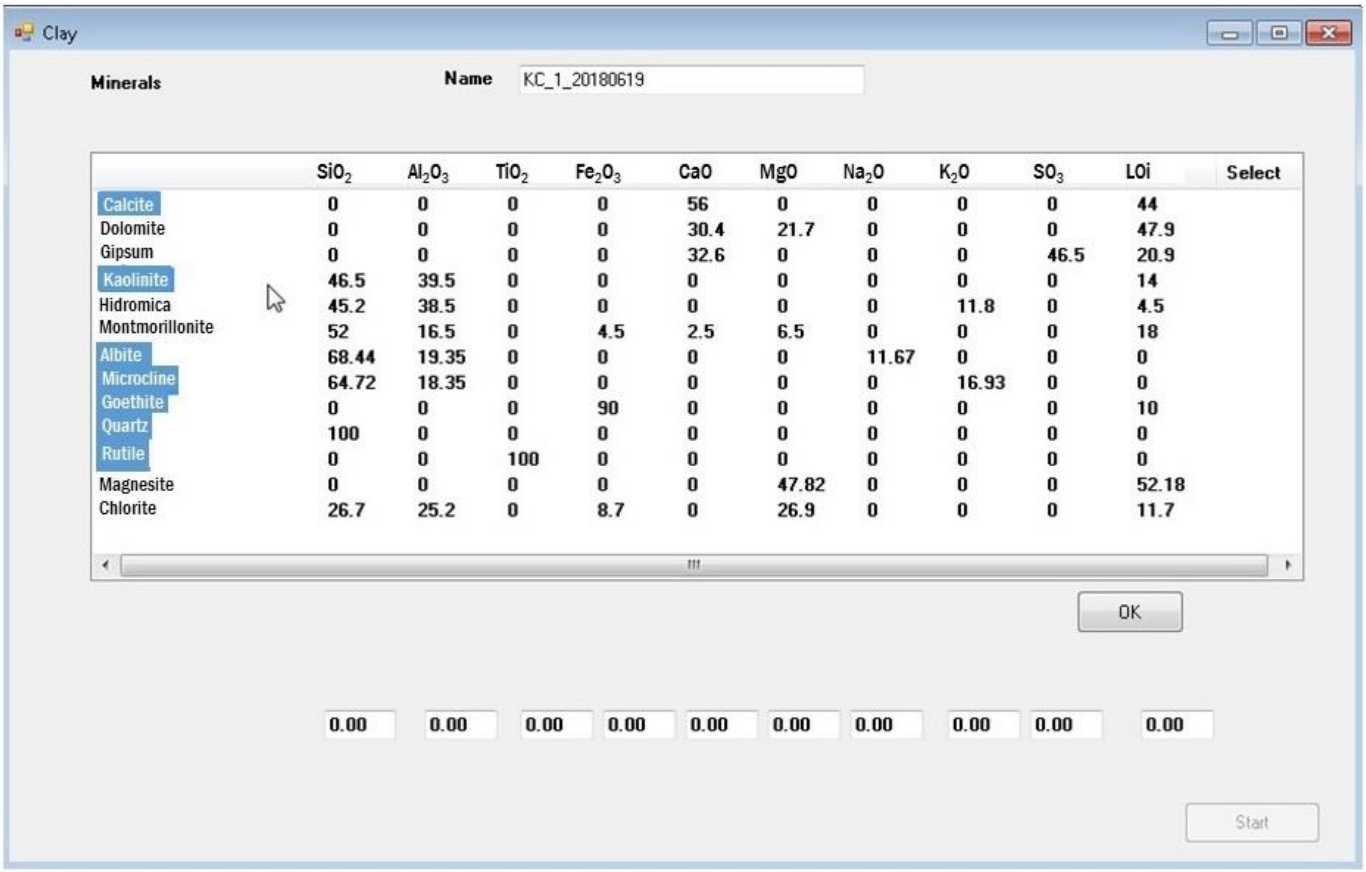

Figure 2. List of minerals of the mix included

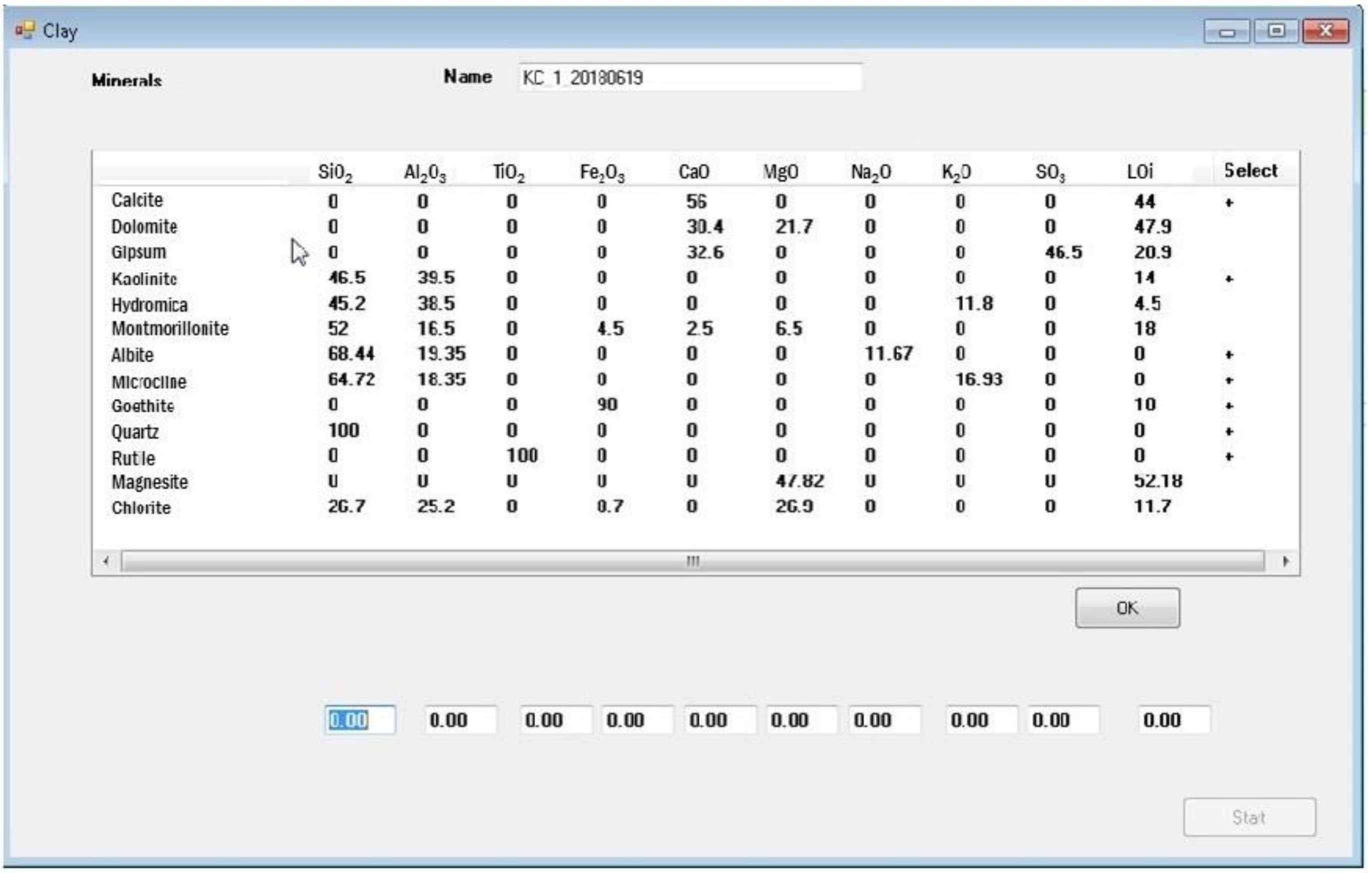

Figure 3. Source information is entered, the program is ready for calculation

Pressing the <Start> button initiates the calculation, one or more correct decisions are obtained, their average vector is calculated, the result is presented in the right column, and the successful completion message is displayed (Fig. 4)

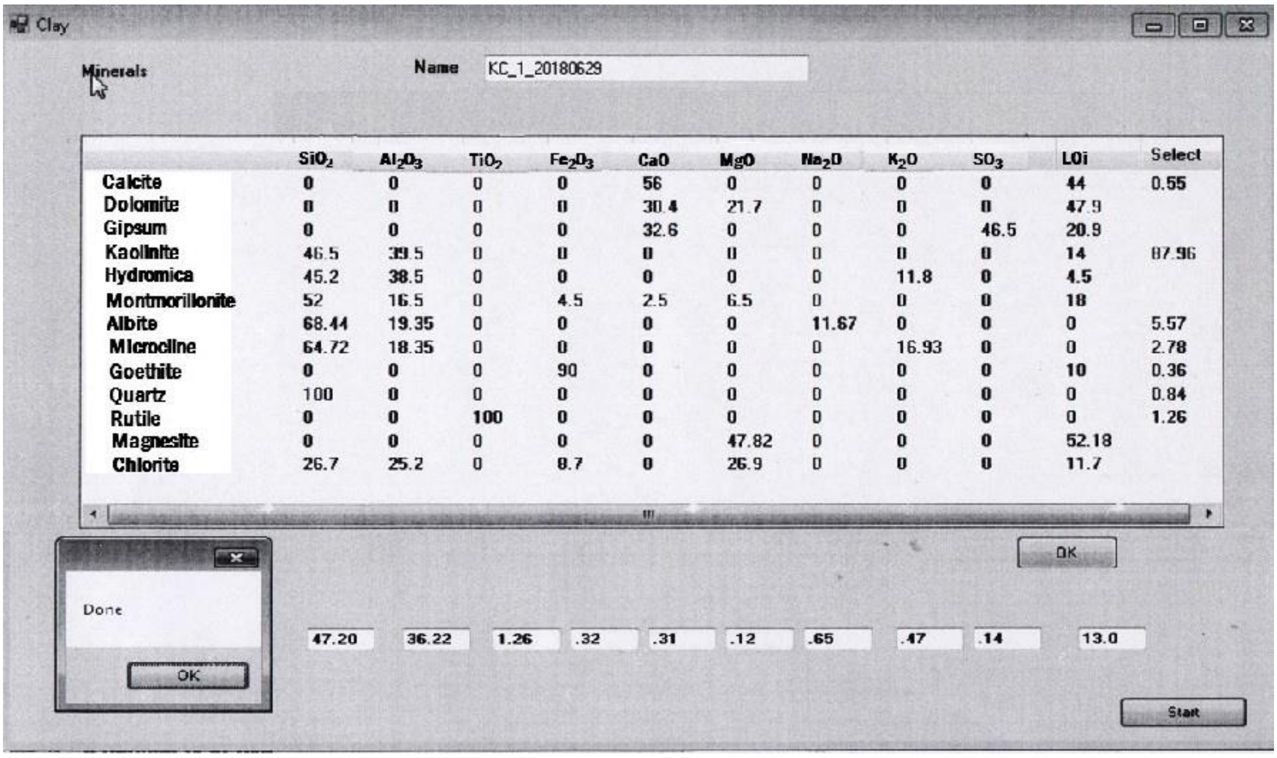

Figure 4. The program run is completed, the results are presented

III. EXAMPLES OF COMPUTER CALCULATION OF RAW MATERIALS COMPOSITION

As the confirmation of the Mineral application efficiency, the results of calculation of the mineralogical contents of variety of the raw materials from different quarries of Ukraine are presented below (tables 1,2).

Table I. Mineralogical composition of carbonate raw materials

Raw material	***Content of minerals, %***				
	Calcite	**Dolomite**	**Quartz**	**Kaolinite**	**Goethite**
chalk	97,62	1,15	0,48	0,63	0,14
limestone	93,02	2,40	3,06	0,15	1,17
shell deposit	81,30	13,46	1,84	3,19	0,54
mergel	73,33	3,13	10,01	14,30	1,90

It was determined that the precision of the results depends exclusively on the precision of the source data provided. With poor data either the result will not be obtained at all or it will be apparent that it does not correspond to source data.

Table 2. Mineralogical composition of clays

Raw material	***Content of minerals, %***								
	Kaolinite	**Hydromica**	**Montmorilonite**	**Quartz**	**Calcite**	**Feldspar**		**Goethite**	**Rubie**
						Albite	**Microcline**		
Clays krry-vinska	2,97	22,88	31,38	31,16	4,55	2,57	-	4,62	0,79
Vesko-Granitik	53,29	17,29	-	22,24	-	3,60	-	1,09	1,39
Kaolin KO-1	94,23	-	-	2,31	-	-	-	0,76	1,00
KS-1	85,19	3,98	-	2,03	-	5,57	-	0,36	1,26
KSSK	36,60	-	-	35,48	0,55	5,14	20,91	0,36	0,33

IV. CONCLUSION

The use of a new computer program is an additional factor in addressing the issue of analyzing and quantifying the mineralogical composition of raw materials. Those determinations are necessary both for the qualification of varieties of raw materials and for the optimization of the composition of masses and technological parameters of production, including silicate building materials.

The program developed is characterized by the efficiency of calculations of the content of rock-forming minerals. In doing so, the feedback principle is implemented: the accuracy of the calculations depends on the original data, and the negative result of the calculations indicates the disadvantages of preliminary analysis of the chemical and qualitative mineralogical composition of the raw material samples.

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