MATHEMATICAL AND SOFTWARE SUPPORT OF CALCULATION AND OPTIMIZATION OF MULTICOMPONENT RAW MIXES

P. A. Trubaev † and P. V. Besedin

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Formalization of methods of calculation and optimization of multicomponent raw mixes in silicate production engineering is proposed. It allows one to proportion raw mixes with an unlimited number of components using any combinations of demands concerning the raw mixes being used and the product to be obtained and to take into account any number of additives and doping agents. The structure of the information support and an algorithm of calculation and optimization of multicomponent raw mixes are described.

Keywords: optimization, raw mixes, multicomponent mixes, silicate building materials.

INTRODUCTION

The efficiency of the process of obtaining building materials in calcining kilns is determined in many respects by the properties and structure of the raw material being processed. Building materials are mainly multicomponent silicate systems and are produced by calcination of raw mixes composed of natural materials and by-products mixed in required proportions. For example, the number of components of raw mixes can be equal to 3 ... 5 and more in cement making and to 15 ... 20 in glasswork. As the experience of leading enterprises shows, the choice of an optimum combination of raw-material components and properties of a raw mix makes it possible to decrease the fuel consumption for calcination and to purposefully control the quality of the product obtained [1]. The determination of an optimum composition of a raw mix is also necessary in developing energy-saving technologies that consist of using by-products such as ashes of power stations, metallurgical slags, and colliery wastes.

For modern working conditions, the information support tools of raw mix design must be universal, i.e., any constraints on the quantity and kind of raw-material components and on calculation and optimization methods must be absent. They must also allow for the tuning to the composition of the raw materials being used and production being produced, must use a broad spectrum of characteristics during calculation and optimization with the possibility of addition of new characteristics, and must optimize in accordance with arbitrarily specified requirements. Software products that are well known at the present time and are reviewed in [2] do not satisfy the above requirements. Their main drawback is the absence of universality. The existing methods of silicate raw mix design were created for special cases connected with specific production lines, and optimization methods were not practically used [3] up to quite a recent time in view of a small number of raw-material components used in producing building materials. For example, the majority of programs of cement raw mix design make it possible to calculate only two-, three-, and four-component raw mixes with fixed collections of characteristics such as the saturation coefficient, silica modulus, and alumina modulus or to optimize one or two criteria. In this case, optimization is realized by methods of minimization of multivariable functions but, as is shown in [2], these methods are inefficient in the context of multicomponent systems of cement technology. The methods of calculation of glass mixtures that are well known at the present time are not systematized, they are usually illustrated by particular examples, and some of such methods make it possible to calculate a glass mixture only approximately when impurities are present in raw materials. Thus, the present-day conditions, in
particular, the increase in the number of raw-material components, output of special products, use of man-caused raw materials and nontraditional fuel, and increase in the number of raw-material repartitions and stages of mixing require the further perfection of existing methods of calculation and optimization of multicomponent silicate raw mixes.

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A formalization of calculation of multicomponent mixes is considered in [4, 5], and an optimization method in simplex coordinates under constraints is investigated in [6]. The calculation of a composition of a multicomponent raw mix is a conditioned problem that has an unambiguous solution and consists of the determination of the contents of components \( x_i \), \( i = 1, \ldots, N \):

\[
M = \left[ k_0' + \sum_{j=1}^{N} k_j' S_j \right]^{-1}
\]

that implies the following linearized characteristic \( T_i (S) \):

\[
T_i (S) = \frac{1 - L_i}{1 - L_j} (k_0' - M_{\text{fix}} S_j) + \sum_{j=1}^{N} (k_j' - M_{\text{fix}} k_j') \frac{S_{ij}}{1 - L_i}.
\]

Here, \( k \) are coefficients, \( L_i \) and \( L_{\text{fix}} \) is the fraction of calcination loss (FCL) of the \( i \)th raw-material component and that of this component at the stage of processing for which its characteristic \( M \) is specified, \( L = (1 - \text{FCL})^{-1} \), \( M_{\text{fix}} \) is a given value of the characteristic \( M \) (a requirement imposed upon the entire raw mix or a product of calcination), and \( S_{ij} \) is the content of the \( j \)th item of the chemical composition in the \( i \)th component.

To calculate \( N \)-component raw mixes, the following formalized equation is proposed in [4]:

\[
\sum_{i=1}^{N-1} T(\vec{S}_{ij}) x_j = \left[ M_{\text{fix}} - \sum_{k=1}^{R} T(\vec{S}_{adk}) q_{adk} \right] \left[ 1 - \sum_{k=1}^{R} q_{adk} \right]^{-1} - T(\vec{S}_{Nj}),
\]

where \( \vec{S}_{ij} = \{ [L_i S_{ij} - L_N S_{nj}] \text{ for } i = 1, \ldots, N - 1 \} \wedge [L_N S_{nj}] \text{ for } i = 1 \} \), \( x_N = 1 - \sum_{i=1}^{N-1} x_i \), and \( R \) and \( q_{ad} \) are the quantity and fraction of total mass of additives and doping agents in the calcined product.

Equation (3) describes problems of calculation of raw mixes in cement making, glass making, and other industries and allows one to use an unlimited number of components in calculations and to take into account the addition of additives and doping agents that are usually by-products to a raw mix and into a kiln.

The optimization of multicomponent raw mixes of silicate building materials is a nonlinear programming problem in which nonlinear equality and inequality constraints specified for the characteristics \( M \) are imposed on the independent variables \( \{X\} \) whose optimum values are searched for to minimize (maximize) the optimality criterion \( K_{\text{opt}} = f_{\text{opt}} (\{X\}) \).

\[1\] In the technology of building materials, a chemical composition is understood to be a symbolic notation of the content of minerals and other chemical compounds in terms of oxides, for example, the composition of a cement raw mix or a clinker is denoted by the content of oxides CaO, SiO\(_2\), Al\(_2\)O\(_3\), Fe\(_2\)O\(_3\), MgO, etc.