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THE OPTIMIZATION ALGORITHM OF SEPARATION PROCESS IN ION CHROMATOGRAPHY

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ABSTRACT
In the article were elaborated evaluation and optimization of separation processes of the mixtures of complex composition by ion chromatography using a semi-empirical approach based on the use of the size and thermodynamic parameters of the group contribution of the systems “sorbent-sorbate” and “ion exchanger-ionate” (model LIQUAC). The developed algorithm allows to optimize the separation process of complex mixtures of electrolytes in ion chromatography.

KEYWORDS: Chromatography, algorithm, optimization, electrolyte, separation, model LIQUAC, cation exchanger KU2, anion exchanger Amberlet, eluent.

INTRODUCTION
Ion chromatography as a method of separation and analysis is widely used in various fields of science and technology, especially in the analysis of aqueous solutions of electrolytes [1]. Development of new and improvement of existing methods of optimization of separation in the chromatographic column is actual in terms of expanding the use of ion chromatography to solve a variety of problems.
The aim of the work is to develop an algorithm to optimize the separation process in ion chromatography based on the parameters of the model LIQUAC.

MATERIALS AND METHODS
Electrolytes solutions, cation exchanger KU2, anion exchanger Amberlet, eluent, ion chromatograph with conductometric detector.
Theory. It is known that the parameters determining the equilibrium between ion exchanger and ionate is an activity coefficient of electrolytes (ions) separated. Of the existing methods for calculation the preference is given to the method, based on the use of energetic parameters of interaction and size parameters of structure-group contributions of ion exchangers and components separated (models LIQUAC [2,3], UNIFAC [4,5], and others.). The essence of the latter is the use of Culon, the induction dispersion interactions for calculating the activity coefficient of electrolytes [2]:

$$G^E = G^E_{LR} + G^E_{MR} + G^E_{SR},$$

where $G^E_{LR} -$ isobaric-isothermal potential of the Culon interaction; $G^E_{MR} -$ isobaric-isothermal potential of induction interaction; $G^E_{SR} -$ isobaric-isothermal potential of dispersion interaction.

Then at T, P and $n_i \neq n_j$

$$ln\gamma_i = \frac{1}{RT}\left(\frac{\partial G^E_m}{\partial n_i}\right)_t = \frac{1}{RT}\left(\frac{\partial G^E_{LR,m}}{\partial n_i}\right)_t + \frac{1}{RT}\left(\frac{\partial G^E_{MR,m}}{\partial n_i}\right)_t + \frac{1}{RT}\left(\frac{\partial G^E_{SR,m}}{\partial n_i}\right)_t.$$

And, accordingly, the value of the activity coefficients for a group k in a solvent s:

$$\ln\gamma_k^{MR} = \sum_{ion} B_{k,ion}(I)m_{ion} - \frac{M_k\sum_k\sum_i v_k^{(i)}x'_i}{M}\sum_k\sum_{ion}\left[B_{k,ion}(I) + IB_{k,ion}(I)\right]x'_k\,m_{ion} - M_k\sum_c\sum_a\left[B_{c,a}(I) + IB_{c,a}(I)\right]m_c m_a$$

for ions:

$$\ln \gamma_j^{MR} = \frac{1}{M}\sum_k B_{j,k}(I)x'_k + \frac{z_j^2}{2M}\sum_k\sum_j B'_{k,ion}x'_k m_{ion} + \sum_c B_{c,a}(I)m_c + \frac{z_a^2}{2}\sum_c\sum_a B'_{c,a}(I)m_c m_a;$$

for solvent s: $ln\gamma_j^{MR} = \sum_k v_k^{(s)} ln y_k^{MR}$,

where x'_{k-} the mole fraction of the solvent group k, $M_k -$ the molar mass of the solvent group k, $M -$ the molar mass of a mixed solvent, $v_k -$ the number of group k in a solvent s, $B'_{i,j} = \frac{dB_{i,j}(I)}{dl}$.

The results and discussion. Based on the above mentioned approach, we have proposed an algorithm to optimize the separation process in ion chromatography (Fig.). The algorithm includes fulfillment of the following works:

1. Selection of the eluent for the separation of a particular mixture of ions in this ion exchanger.
2. Testing satisfaction of separation on all pairs of ions separated by the calculation of separation criteria ($R_S \geq 0{,}70$).
3. Finding the optimum length of the column and the optimal composition of the eluent.
4. Preparation of complete chromatogram of separated components of the mixture.

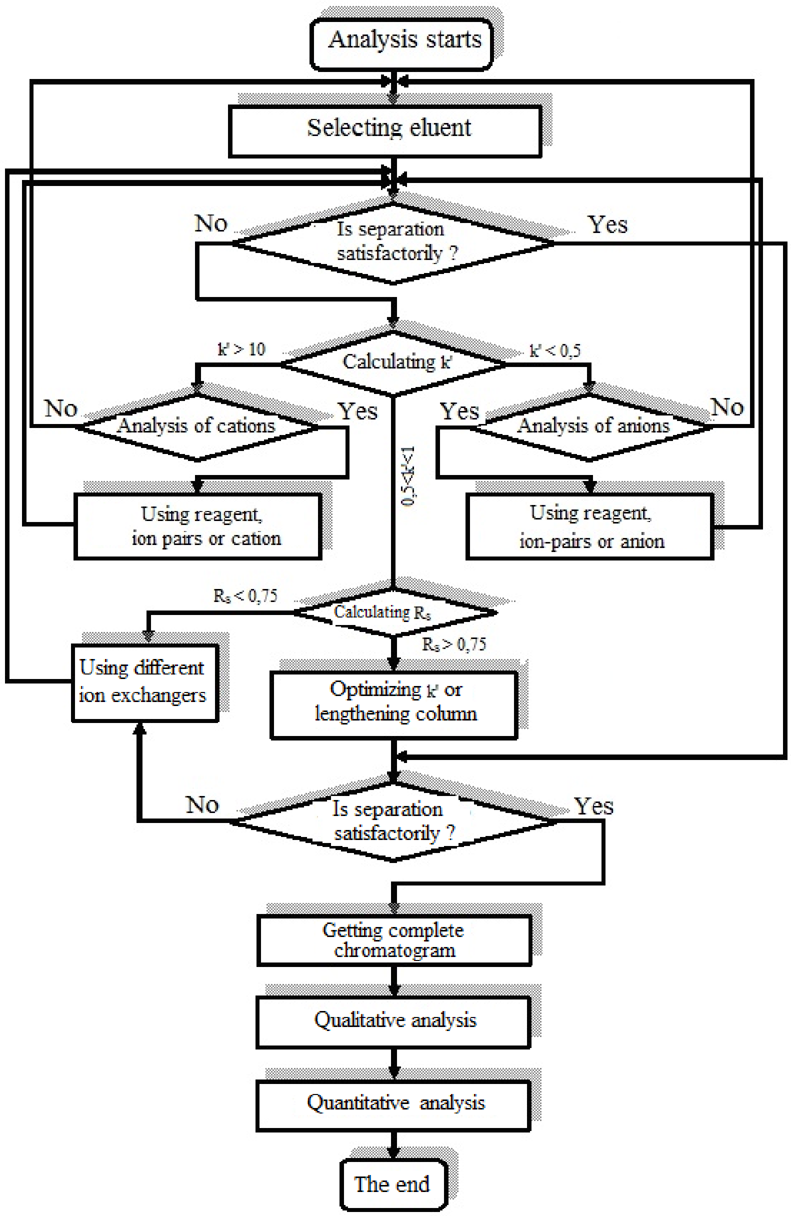

Fig. The optimization algorithm of separation process in ion chromatography

Testing of the optimization algorithm of separation process in ion chromatography was performed on an example of separation of model mixtures of cations and anions, as well as in the analysis of natural and waste waters, mixtures of amino acids, and others. The relative error in the selection of optimal separation conditions in $R_S \geq 0{,}70$ makes from 3 to 6%.

CONCLUSION

Thus, the evaluation and optimization of separation processes the mixtures of complex composition by ion chromatography using a semi-empirical approach based on the use of the size and thermodynamic parameters of the group contributions of the systems “sorbent-sorbate” and “ion exchanger-ionate” is perspective and have the advantage compared with the empirical methods . The developed algorithm allows to optimize separation process in ion chromatography.

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