Development of mathematical descriptions of the processes of distillation of multicomponent solutions with an inert gas based on system analysis

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Abstract. In this article, a multi-stage interconnected hierarchical structure has been developed, taking into account the input and output parameters of each elementary process, based on a systematic analysis of the distillation process of multicomponent solutions. In the proposed method, the analysis of the process according to the hierarchical structure is carried out gradually from the lower, molecular level, to the upper level, taking into account the interrelation of elementary processes.

1. Introduction
As a multicomponent solution, consider cottonseed oil and the process of its distillation - deodorization. In the process of deodorization, according to technological requirements, cottonseed oil must be purified from several components, such as aldehydes and fatty acids, which give it a smell and taste. From the data obtained from literary sources, the boiling point above these components at atmospheric pressure is very high.

Under production conditions, there is no possibility of technical implementation of such temperature regimes. Proceeding from this, it is necessary to develop new energy-saving technological modes for carrying out the processes of distillation of multicomponent solutions, such as the process of deodorization of cottonseed oil.

2. Methods
The use of systems analysis methods based on the development of a multi-stage hierarchical structure, when solving the problem of studying the distillation process of a multicomponent solution, makes it possible to take into account the interests of related technological processes.

The possibility of conducting research on a unified methodology of system analysis is associated with the generality of the stages of the process and the forms of existence of the concentrated solution. This also provides an opportunity to present a single semantic aspect of the qualitative analysis of the structure of the physicochemical system of the cottonseed oil distillation process when applying the strategy of a systematic approach to its research and modeling.

3. Results and discussion
The investigated process of deodorization of cottonseed oil flowing in the technological apparatus—deodorizer can be conditionally divided into the following sub-processes: liquid injection; heating the
liquid in the heat exchanger; moving fluid through a pipeline; spraying liquid using spraying devices; heat and mass transfer processes in the spray zone; accumulation of finished oil in the lower part of the apparatus; pumping out oil by pumps.

The processes of pumping, moving, accumulating and pumping out can be considered as complete elements of the hierarchical structure of the deodorization process, which cannot be further divided.

When identifying the structure of the technological operator of heating the oil solution with ethyl alcohol, one can use the results given in [1], since the heat engineering parameters of the cottonseed oil solution with ethyl alcohol are close to those of the cottonseed oil micelle.

The process of distillation of a solution of cottonseed oil in a spray apparatus can be divided into the following apparatus-process units, fixed in the form of certain processes: the process of evaporation of the solution as a whole; for the process of formation of drops, for processes occurring in the liquid phase; for processes occurring in the vapor phase; the phenomenon of phase interaction, as well as processes associated with the supply and condensation of steam.

At the next stage of the system analysis of the technological process, it is required to partition the system into interrelated constituent elements, i.e. determination of the hierarchical structure of the risers of the processes under consideration, taking into account the hydrodynamic structure of flows of interacting counter phases.

To reveal the efficiency of using ethyl alcohol as a solvent for deodorization of a multicomponent mixture of cottonseed oil, the processes occurring in the ensembles of particles can be divided (see figure 1) into the following sub-processes: TMT processes occurring due to self-evaporation (BLOCK A, consisting of processes; occurring in the dispersed phase, this is a change in the concentration of the solution, a change in the amount of heat, a decrease in the temperature of the solution; and also occurring in a continuous phase: this is a change in the composition of the vapor phase, a change in heat, vapor movement, mass transfer and heat exchange between phases): TMO processes occurring during the spraying of the liquid phase I BLOCK B, which is hierarchically composed of processes; flowing in the dispersed phase: this is the formation of liquid droplets when spraying by means of spraying devices, the movement of liquid droplets in the vapor phase, the transfer of the distributed substance and heat in the liquid phase [2].

In this case, the processes occurring in a continuous medium can be divided into the following sub-processes: the movement of steam in the internal volume of the apparatus, the transfer of the distributed substance and heat in the vapor phase.

The next step in the hierarchy is the processes of heat and mass exchange interaction of phases. They add up to the processes of mass transfer between phases, heat transfer, changes in the state of aggregation of a substance under the influence of the vapor phase. Due to insignificance. the influence of the shape of liquid droplets on the overall technological process, the last factor at this hierarchical level can be neglected.

The processes occurring at the molecular level include the following phenomena: chemical reactions into which accompanying substances remaining in the oil after refining enter, changes in the fatty acid composition of the oil, oxidation of the oil with oxygen dissolved in the oil mixture or in water vapor, changes in the diffusion coefficients, thermal conductivity, etc.

From the above phenomena and effects, a multilevel hierarchical structure of the deodorization process by spraying pressed cottonseed oil is synthesized, consisting of five hierarchy levels.

The sixth level of the hierarchy can also be distinguished, which will be a set of processes that determine the coordinated operation of interconnected technological devices of the entire installation or the technological complex as a whole.

The analysis of the system is carried out starting from the lower hierarchical level. In this case, a solution of cottonseed oil is considered in the form of a multicomponent mixture, consisting of: a solvent, odorizing and unsaponifiable substances, free fatty acids and neutral oil. For the convenience of analyzing the deodorization process, the groups of substances listed above are represented by the following individual components with the corresponding physicochemical properties: ethyl alcohol, aldehyde, fatty acid (oleic).
Figure 1. Hierarchical structure of cottonseed oil deodorization process.
It should be noted that with a variation in the methods of deodorization of vegetable oil, the significance of various levels of the hierarchy is different and can vary significantly from complete degeneration to acceptance of a global character in terms of the degree of influence on the entire system as a whole.

When implementing a systematic approach to the study of deodorization of a multicomponent mixture of cottonseed oil, it is necessary to identify the scheme of interaction of counter flows in the apparatus, to assess the contribution of each hierarchy level to the solution processing process, i.e., it is necessary to reveal the general physical picture of the process under study [3, 4].

Then the formalization of the properties and phenomena of the corresponding levels of the hierarchy is carried out, the aggregate modeling of the process as a whole, the verification of the adequacy of the model to the real process and, if necessary, the adaptation of the model to the object.

The principle of block formation of the generalized mathematical model of the object as a whole, applied in the system analysis, makes the following sequence of working out its stages appropriate for the developed mathematical description of the process of deodorization of cottonseed oil:

- formalization of the properties of a multicomponent solution of cottonseed oil as an object of technological processing;
- formalization of the properties of distilled oil components;
- formalization of the properties of a thermal agent - water vapor;
- fixation of the real hydrodynamic situation in the vehicle in the form of a typical or combined model of the structure of interacting counter flows;
- drawing up balances of flows of matter and energy;
- investigation of the kinetics of the process during the distillation of several components from the composition of the initial solution;
- aggregation of a complete or generalized mathematical model of the subsequent process as a whole from local models for individual levels of the hierarchy;
- selection of a criterion for evaluating the effectiveness of the process, carried out in accordance with the purpose of modeling and optimization.

The result of a generalized system analysis of the process under study is the optimal process modes, deodorization methods and apparatus designs.

Processes at the first level of the hierarchy. The first step of the hierarchy includes the phenomena that take place at the molecular level. This is a change in the physicochemical properties of the processed oil, the effect of high temperatures on the fatty acid composition of black prepress, extraction, and refined cottonseed oil [5]. The effect on the fatty acid composition of black and refined cottonseed oil during its thermal processing, under the conditions of adding ethyl alcohol to it before deodorization, has been investigated. For these purposes, the method of gas-liquid chromatography was used, since the nutritional advantages and the main physicochemical properties of vegetable oils are due to their fatty acid composition. Below in table 1 shows the results of the analysis.

| Fatty acid | Cottonseed oil after deodorization | Black fore press | Refined press | Salad |
|------------|-----------------------------------|------------------|--------------|-------|
| C          | 0.17                              | 0.16             | 0.37         |       |
| C 14:0     | 0.98                              | 1.20             | 1.18         |       |
| C 16:0     | 25.90                             | 28.10            | 26.10        |       |
| C 16:1     | -                                 | 0.90             | 1.01         |       |
| C 18:0     | 2.86                              | 2.93             | 2.96         |       |
| C 18:1     | 20.42                             | 21.71            | 22.00        |       |
| C 18:2     | 49.41                             | 43.82            | 44.65        |       |
Processes at the second level of the hierarchy. These include the phenomenon of the transfer of a distributed substance in the liquid phase due to the molecules of highly volatile components; it occurs from the inner layers of the drop to the outer ones. At this stage of the hierarchy, the phenomenon of transfer of substances from the liquid phase to the vapor phase will proceed in two stages: the first - due to the self-evaporation of the liquid as a whole (BLOCK A), the second - multistage spraying of the liquid phase (BLOCK B).

This is due to the fact that during deodorization of a multicomponent mixture of cottonseed oil with added ethyl alcohol, the total partial pressure of volatile components increases sharply in relation to a given total pressure in the apparatus. The evaporation of highly volatile components begins due to an increase in pressure above the liquid phase. This process will continue until the limit value of the concentration of the components is reached. Naturally, the concentration of highly volatile components in the liquid phase also changes, that is, they pass into the vapor phase [5].

Processes at the third level of the hierarchy. This level of the hierarchy includes the processes occurring in the vapor and liquid phases, as well as the processes of their interaction.

Mathematical description of the equilibrium concentration of volatile components.

Obeying Raoult’s law for ideal gases, the partial vapor pressures of highly volatile components will be proportional to the vapor pressure of pure components at a given temperature [6,7]:

\[ P_j \cdot X_j = P_j \]

where \( P_j \) - is the partial pressure of the j-th highly volatile component, \( X_j \) - content of the j-th volatile component in oil, \( P_j \) - the vapor pressure of the j-th component in the pure state.

Using the reference data, you can write the following following empirical formula to determine the vapor pressure of the components at a certain interval of the process temperature:

\[ P_j = B_{0j} + B_{1j} \cdot t \]

where \( B_{0j}, B_{1j} \) - constant coefficients obtained as a result of processing reference data, \( t \) - volatile component temperature, °C. To determine the content of a highly volatile component, you can use the dependence, given in the work [8]. When distilling a multicomponent mixture, it has the following form:

\[ X_j = \frac{a_j}{M_j} \]

where \( M_1, M_2, M_3, M_4 \) - molecular weights of volatile components and cottonseed oil, kg / kmol; \( a_1, a_2, a_3 \) - concentration of volatile components in oil, %.

Substituting expression (2) into equation (1), we can obtain a system of equations describing the partial pressure of highly volatile components of a multicomponent mixture:

\[
\begin{align*}
P_1 &= (b_0 + b_1 \cdot t) \cdot \frac{a_1}{M_1 + \frac{a_2}{M_2} + \frac{a_3}{M_3} + \frac{1 - a_1 - a_2 - a_3}{M_4}} \\
P_2 &= (b_2 + b_3 \cdot t) \cdot \frac{a_2}{M_1 + \frac{a_2}{M_2} + \frac{a_3}{M_3} + \frac{1 - a_1 - a_2 - a_3}{M_4}} \\
P_3 &= (b_4 + b_5 \cdot t) \cdot \frac{a_3}{M_1 + \frac{a_2}{M_2} + \frac{a_3}{M_3} + \frac{1 - a_1 - a_2 - a_3}{M_4}}
\end{align*}
\]

After some mathematical transformations from the system of equations (4), we obtain the following system of equations:

\[
\begin{align*}
\frac{a_1}{M_1 - M_3} \left( \frac{M_1 - M_3}{M_1 - M_2} \cdot \frac{P_1}{(b_0 + b_1 \cdot t)} - \frac{1}{M_1} \right) + & \frac{a_2}{M_2 - M_3} \left( \frac{M_2 - M_3}{M_2 - M_4} \cdot \frac{P_1}{(b_0 + b_1 \cdot t)} - \frac{1}{M_2} \right) + \frac{a_3}{M_3 - M_4} \left( \frac{M_3 - M_4}{M_3 - M_2} \cdot \frac{P_1}{(b_0 + b_1 \cdot t)} - \frac{1}{M_3} \right) = \frac{1}{M_4} \cdot \frac{P_1}{(b_0 + b_1 \cdot t)} \\
\frac{a_1}{M_1 - M_3} \left( \frac{M_1 - M_3}{M_1 - M_2} \cdot \frac{P_2}{(b_2 + b_3 \cdot t)} - \frac{1}{M_1} \right) + & \frac{a_2}{M_2 - M_3} \left( \frac{M_2 - M_3}{M_2 - M_4} \cdot \frac{P_2}{(b_2 + b_3 \cdot t)} - \frac{1}{M_2} \right) + \frac{a_3}{M_3 - M_4} \left( \frac{M_3 - M_4}{M_3 - M_2} \cdot \frac{P_2}{(b_2 + b_3 \cdot t)} - \frac{1}{M_3} \right) = \frac{1}{M_4} \cdot \frac{P_2}{(b_2 + b_3 \cdot t)}
\end{align*}
\]
The solution of this system of equations by the Cramer method makes it possible to determine the values of the final concentrations of highly volatile components in oil depending on the temperature \( t \) in the apparatus and the partial pressures of the components.

\[
a_{kj}^* = \frac{\Delta a_j}{\Delta}
\]  

(6)

Or

\[
a_j^* = f(p_j^*, t)
\]  

(7)

Since during the distillation of multicomponent mixtures, the change in the concentration of one component depends on the content of the rest in it, i.e., on the partial pressure of the remaining components, which can be seen from the system of equations (5).

Mathematical description of the change in the amount of heat in the liquid phase.

When distilling solutions with an inert gas (sharp water vapor), concentration occurs due to the heat of the liquid. From the heat balance equation we can determine the temperature of the liquid phase.

\[
q_M = q_{M1} + q_{lkj}
\]  

(8)

Where \( q_M \) - the warmth that comes with oil; \( q_{M1} \) - heat leaving with oil; \( q_{lkj} \) - heat leaving with volatile components.

Expanded, the last expression looks like this:

\[
(G_M + \sum G_{lkj})C \times t_0 = G_M \times C \times t_1 + \sum G_{lkj} \times t
\]  

(9)

From here we can determine the temperature of the liquid phase. After some mathematical transformations, we have:

\[
t = t_0 - \frac{\sum G_{lkj} i}{G_M \times C}
\]  

(10)

Where \( G_{lkj} \) - consumption of volatile components, \( kg/s \); \( G_M \) - oil consumption, \( kg/s \); \( i \) - enthalpy of vapors of highly volatile components, \( kJ/kg \); \( C \) - heat capacity of oil, \( kJ/kg \).

The volatile components leaving the liquid phase carry away the heat. From the material balance for the liquid phase, you can determine their values by the expression:

\[
G_{lkj} = G_M \times (a_{hj} - a_{kj})
\]  

(11)

Then the complete mathematical model of the distillation process by self-evaporation in block A will have the following form:

\[
\begin{align*}
P_{lkj} &= f(a, l, k) \\
a_{kj}^* &= f(P_{lkj}, t) \\
G_{lkj} &= G_M(a_{hj} - a_{kj}) \\
T &= T - \frac{\sum G_{lkj} i}{G_M \times C}
\end{align*}
\]  

(12)

In the spray zone, the oil moves from top to bottom without undergoing longitudinal mixing, and therefore the hydrodynamic structure of oil flows along the block B of the hierarchy is close to the ideal displacement model [5].

To compile a mathematical description of the process of distillation of volatile components (fatty acids) from the composition of the oil sprayed by a conical disk atomizer, let us assume that the concentration process is instantaneous.

According to the authors, [3, 6], thermal and mass disturbances in a drop occur on its surface, while the intra-distribution of concentration and temperature occurs along the radius. The latter ranges from
50-150 microns. Here, the process time is negligible compared to the residence time of the product in this zone.

A mathematical description reflecting the change in the concentration of the treated medium during spray distillation is given in [10], taking into account the above assumption, it has the form:

\[ a_k = a_p \] (13)

Where \( a_k \) - concentration of volatile substances, \%; \( a_p \) - equilibrium concentration of volatile substances, \%; the expression is also valid for the elementary j - th zone.

\[ a_{kj} = a_{pj} \] (14)

Where \( a_{kj} \) - concentration of volatile components in the j - th zone \%; \( a_{pj} \) - equilibrium concentration of components in the j - th zone %.

When deodorizing a multicomponent mixture of cottonseed oil, the resulting vapor phase can be considered an ideal gas, since there is a large difference between the boiling points of volatile components and cottonseed oil. Therefore, in accordance with Dalton’s law, a certain number of molecules of each of the highly volatile components corresponds to its own partial pressure [1,2,4]

\[ \frac{N_j}{\sum N} = \frac{P_j}{P_{total}} \] (15)

Where \( N_j \) and \( \sum N \) respectively, the number of molecules of the j-th volatile component and the sum of the molecules of all volatile components and inert gas (live water vapor); \( P_j, P_{total} \) - respectively, the partial pressure of the j - th volatile component and the total pressure in the apparatus.

The number of molecules per unit time \( N_j \) - can be expressed by the ratio of the mass flow rate of highly volatile components \( G_j \) to their molar mass \( M_j \).

\[ N_j = \frac{G_j}{M_j} \] (16)

Then equation (15) can be described in the following form:

\[ \frac{P_j}{P_{total}} = \frac{\frac{G_j}{M_j}}{\sum_{i=1}^{n} \frac{G_i}{M_i}} \] (17)

From this we obtain an expression for calculating the partial pressures of highly volatile components in the vapor phase. In this case, the vapor phase is created by the molecules of three highly volatile components and live water vapor.

\[
\begin{align*}
P_1 &= \frac{\frac{G_1}{M_1}}{\frac{G_1}{M_1} + \frac{G_2}{M_2} + \frac{G_3}{M_3} + \frac{G_p}{M_p}} * P_{total} \\
P_2 &= \frac{\frac{G_2}{M_2}}{\frac{G_1}{M_1} + \frac{G_2}{M_2} + \frac{G_3}{M_3} + \frac{G_p}{M_p}} * P_{total} \\
P_3 &= \frac{\frac{G_3}{M_3}}{\frac{G_1}{M_1} + \frac{G_2}{M_2} + \frac{G_3}{M_3} + \frac{G_p}{M_p}} * P_{total}
\end{align*}
\] (18)

Where \( G_1, G_2, G_3 \) costs of volatile components, \( M_1, M_2, M_3 \) molecular weights of highly volatile components, \( G_p \) live steam consumption, \( M_p \) - molecular weight of water vapor.

Flow value \( G_j \) - th volatile component that has passed into the vapor phase from the liquid is determined by the expression:

\[ G_{kj} = G_M(a_{hj} - a_{kj}) \] (19)
Where \( G_M \) - initial oil consumption kg/s, \( a_{hj} \) - initial concentration of volatile components in oil %, \( a_{kj} \) - final concentration of volatile components in oil %, To calculate the concentration of volatile components \( a_{kj} \), we can use the system of equations (5).

Then the complete mathematical model of the spray deodorization process (according to the second block B of the hierarchy) will have the form of the following system of equations:

\[
\begin{align*}
    a_{kj} &= a_{kj}^* \\
    G_{tkj} &= G_M (a_{hj} - a_{kj}) \\
    P_{tkj} &= \frac{G_{tkj}}{\sum_{i=1}^{n} \frac{M_k}{M_i} \frac{a_{ij}}{a_{kj}}} P_{total} \\
    T &= T - \frac{\sum G_{tkj} \cdot t}{G_{total}}
\end{align*}
\]

(20)

Processes at the fourth level of the hierarchy. At this level of the hierarchy, the processes occurring in the individual elements of the installation are considered. In this case, we will consider only the heat-mass transfer process, during which volatiles are distilled off from the composition of the pressed cottonseed oil.

Mathematical description of the heat and mass transfer process of multicomponent distillation (deodorization). Along with other heat and mass transfer processes, deodorization also occurs under the action of driving forces. In this case, the driving force of the process is the difference between the actual and equilibrium concentrations.

To aggregate the mathematical descriptions of individual elements of the process of multicomponent distillation of pressed cottonseed oil, described by blocks A and B of hierarchy 2.1 - 2.20, into a system of equations, we obtain the following complete generalized mathematical model of the deodorization process of a multicomponent mixture of cottonseed oil, the hydrodynamic structure of flows of which is fixed by a typical model of ideal mixing:

\[
\begin{align*}
    P_j &= (b_{oj} + b_{1j} \cdot t) \frac{a_j}{\sum_{i=1}^{n} \frac{a_j}{M_i} + \sum_{i=1}^{n} \frac{a_j}{M_i}} \\
    a_{jp}^* &= f (p^*, t) \\
    a_{jk} &= a_{jp}^* \\
    G_{skj} &= G_M (a_{hj} - a_{kj}) \\
    P_j &= \frac{G_{skj}}{\sum_{i=1}^{n} \frac{M_k}{M_i} \frac{a_{ij}}{a_{kj}}} P_{total} \\
    T &= T - \frac{\sum G_{skj} \cdot t}{G_{total}}
\end{align*}
\]

(21)

4. Conclusion
A systematic analysis of the process currently used at factories for the production of vegetable oils shows that in order to carry it out with the lowest energy consumption in devices without stagnant zones, it is necessary to develop new designs that have an improved hydrodynamic structure of phase flows.

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