

# STUDY OF THE EQUILIBRIUM CONCENTRATION OF VOLATILE SUBSTANCES IN THE DEODORIZATION OF COTTON OIL WITH THE HELP OF A COMPUTER MODEL

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**Abstract.** A model of the process of periodic deodorization of cottonseed oil made in Matlab. Technological, technical, ecological, economic and other phenomena studied by modern science in many cases cannot be fully and accurately realized as expected by traditional theoretical methods.

**Keywords:** *deodorization, thermodynamics, coefficient, deodorizer, partial pressure, Raoult's law, structural analysis, mathematical modeling, computer modeling, liquid phase, vapor phase.*

**Introduction:** Technological, technical, ecological, economic and other phenomena studied by modern science in many cases cannot be fully and accurately realized as expected by traditional theoretical methods. Experimenting in the original facility can be time-consuming, expensive, and sometimes simply impossible. A mistake made in experimenting with the original is very expensive. Therefore, mathematical modeling is an inevitable component of scientific and technical progress.

When modeling the deodorization process, the following restrictions are accepted: no condensation of steam is observed in the column; the value of heat and mass transfer coefficients is unchanged; the temperature of the liquid phase does not change; the shape of the steam bubbles rising from the oil layer does not change.

In order to thoroughly analyze, calculate and optimize the process of separation of light volatile components in cottonseed oil, the process will need to be systematically analyzed, mathematically modeled, computer modeled and many computer experiments should be carried out.

Style. Mass transfer is usually a reversible process. At the same time, the direction of the substance transition is determined by the substance concentrations and equilibrium conditions in the phases. To model the processes of matter and heat exchange, it is first necessary to know their final state, that is, the state of equilibrium to which each system strives. For this reason, the analysis of mass transfer processes begins with the fundamental theory of thermodynamics, which determines the state of a system with a large number of particles in equilibrium. According to the second law of thermodynamics, the entropy of the system increases during spontaneous processes. In an isolated system, the entropy  $S$  reaches its maximum value, so  $dC = 0$ . In addition to this condition, the equilibrium conditions for constructing a mathematical model are assumed to be zero, with the total differential of the state parameters determining the properties of the substance:

$$dP = 0; dT = 0; d\mu_i = 0, \quad (1.)$$

where  $P$  is pressure,  $T$  is temperature,  $\mu_i$  is the chemical potential of component  $i$  in the mixture.

The first equation characterizes the mechanical equilibrium, the second equation characterizes the thermal equilibrium, and the third equation characterizes the diffusion

equilibrium, that is, the exchange of substances does not occur. In the process of exchange of substances, the state of equilibrium is also written using the concentration of substances:  $dC_i = 0$ , where  $C_i$  is the concentration of component  $i$ .

In the process of separation of light volatile components in oil, the state of interphase equilibrium can be generally expressed as follows:

$$x^* = f(t, p, y). \quad (1.1)$$

$$y^* = f(t, p, x). \quad (1.2)$$

Below we will consider the method of using mathematical expressions that allow to analytically find the state of equilibrium and calculate it with high accuracy.

According to Raoult's law, when its vapor is in equilibrium with an ideal liquid mixture, the partial pressure of any component in the vapor is equal to the product of the vapor pressure of that component in the pure state and its concentration in the liquid:

$$p_i = x_i P_i. \quad (1.3)$$

For natural mixtures different from ideal mixtures, fugacity  $g$  also affects:

$$p_i = x_i P_i \gamma_i. \quad (1.4)$$

It is known that, according to the laws of thermodynamics, there is a certain relationship between vapor pressure and temperature. Nernst expressed this relationship through the following formula:

$$\ln p = -\frac{\lambda_0}{RT} + 1,75 \ln T - \frac{\varepsilon}{R} T + C', \quad (1.5)$$

where  $p$  is the vapor pressure of a given fatty acid at temperature  $T$  (oK);  $\lambda_0$  is the molecular heat of vaporization of a substance at absolute zero temperature;  $R$  is the gas constant, 1.985 cal/degree (1.985•4.1868 J/degree);  $\varepsilon$  is the difference between the heat capacities of the substance in its liquid and vapor states.

The above equation can be rewritten as follows:

$$\lg P = -\frac{\lambda_0}{4,571T} + 1,75 \lg T - \frac{\varepsilon}{4,571} T + C \quad (1.6)$$

Using the values of  $\lambda_0$ ,  $\varepsilon$  and  $C$ , it is possible to calculate the vapor pressure of fatty acids over a wide range of temperatures. The values of these constants for some fatty acids are as follows

Calculation coefficients of vapor pressures of fatty acids

Fatty acids	Carbon number	$\lambda_0$	E	C
Caprin	10	22920	0.0334	11.318
Laurin	12	23590	0.0349	11.408
Myristin	14	24960	0.0334	11.493
Palmitin	16	26050	0.0326	11.568
Stearin	18	27280	0.0317	11.636

The values of these constants are  $\lambda_0 = 23590$ ,  $\varepsilon = 0.0349$  and  $C = 11.408$  for lauric fatty acid with 12 carbon atoms per molecule. And for palmitic fatty acid,  $\lambda^0 = 26050$ ,  $\varepsilon = 0.0326$  and  $C = 11.568$ .

Using the formula and tabular values given above, it is possible to calculate the values of the parameters of liquid and vapor interphase equilibrium states of the mixture components entering the system with sufficient accuracy for modeling.

Using the formula 1.3 1.4, if the pressure value in the device and the concentration of the light volatile component in the mixture of fatty acids in one of the two phases are given, the corresponding equilibrium concentration in the second phase can be determined.

The ratio of partial pressures gives the relative volatility a:

$$\alpha_{ij} = \frac{p_i}{p_j} \quad (1.7)$$

The value of relative volatility changes with temperature. Until now, calculations have taken the average value of and performed calculations without changing this value:

$$\alpha_{\text{ypm.}} = \sqrt{\alpha_1 \alpha_2} \quad (1.8)$$

If the relative volatility value and the concentration of the substance in one of the phases are known, the corresponding equilibrium concentration in the other phase can be calculated:

$$Y = \frac{\alpha X}{1 - (\alpha + 1)X} \quad (1.9)$$

Below is a method for calculating the interphase equilibrium concentrations of fatty acids with the number of carbon atoms in the molecule from C 10 to C 18 using a computer.

The following equation is used to calculate the equilibrium concentration of the light volatile component in fatty acid mixtures at a certain pressure and temperature:

where X is the equilibrium concentration of the light volatile component in the liquid phase; P - total pressure;  $p_1$  is the partial pressure of the light volatile component vapor;  $p_2$  is the partial pressure of the heavy volatile component vapor.

The following formula is used to calculate the equilibrium concentration in the vapor phase:

$$X = \frac{P - p_2}{p_1 - p_2}, \quad (2.1)$$

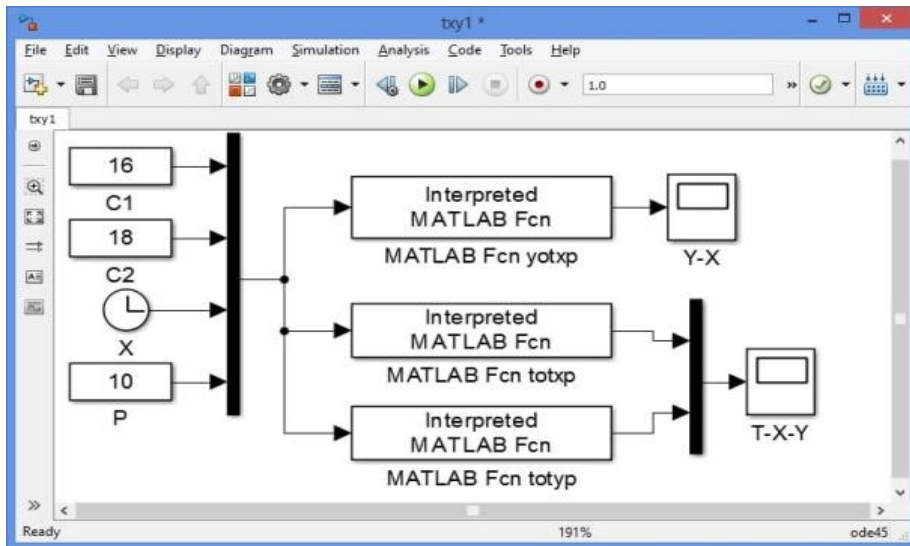
It is convenient to represent the equilibrium concentrations of liquid and vapor interphases of two-component mixtures at a given pressure and temperature on a t-x-y diagram. If the pressure is known and the concentration of the light volatile component in the fatty acid mixture in one of the two phases is given, the corresponding equilibrium concentration in the second phase can be calculated.

Result. Using the programs compiled in the MATLAB Simulink package, it is possible to quickly, accurately and easily perform calculations on mixtures of fatty acids, build appropriate graphs, and create Simulink dynamic models.

$$Y = \frac{p_1 X}{P}$$

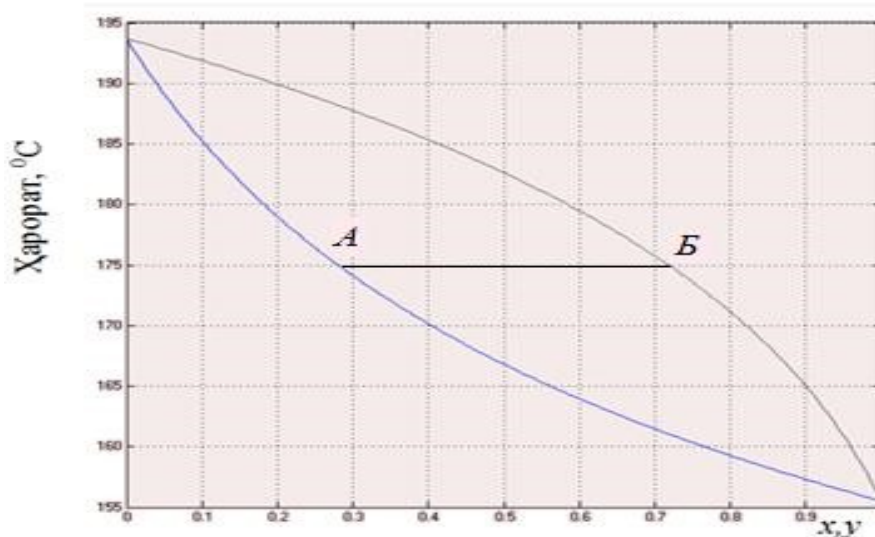
During the research of the process of periodic deodorization of cottonseed oil, a number of issues of technological importance were considered to determine the equilibrium states of various fatty acids. Computer models were built to investigate these issues. The image of the model built in Matlab to determine the equilibrium state of this process is shown in the figure below.

View of the computer model constructed using the Matlab package to determine the equilibrium state of the cottonseed oil deodorization process



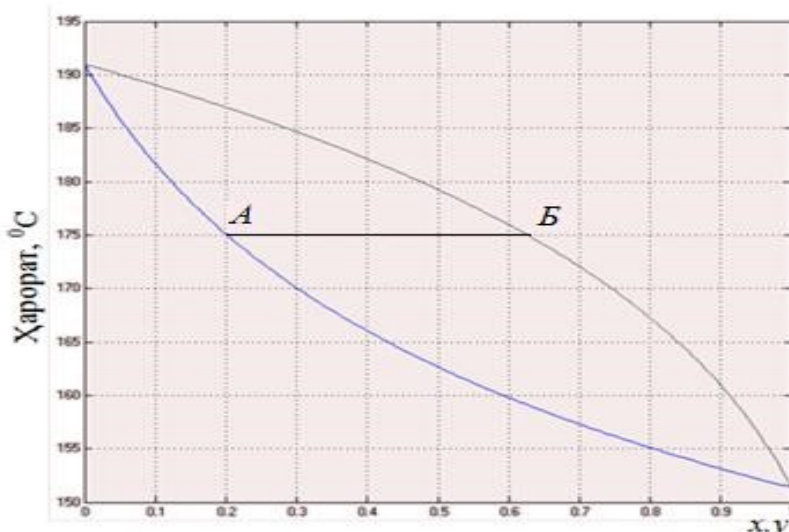
With the help of this computer model, t-x-y diagrams representing the equilibrium concentrations of C12÷C16 fatty acid mixtures in the deodorizer at different values of working pressure and temperature will be constructed.

In the process of deodorizing cottonseed oil, the equilibrium concentrations of C12÷C16 fatty acid mixtures are 6÷25 mm of the working pressure in the device. sim. above was determined within the limits of equal values. In this case, the determined values of the pressure of the saturated vapors of the components are put into the equations, and the total pressure in the deodorizer is initially 5 mm. sim. above, then 10 mm. sim. above A t-x-u diagram representing the equilibrium concentrations of the fatty acid mixture at different temperatures was constructed.



C12-C16 fatty acid mixture at different temperatures and  $R = 5$  mm.sim.above. t-x-u diagram representing equilibrium concentrations at pressure

Discussion. As can be seen from the diagrams, the liquid and vapor have the same temperature in the equilibrium state, that is, all the state points corresponding to the equilibrium state of the liquid and vapor phase lie on one horizontal straight line in the diagram. Point A in the diagrams represents the composition of the light volatile component in the liquid phase, and point V represents their composition in the vapor phase in equilibrium with the liquid. (2) C12-C16 fatty acid mixture at different temperatures and  $R = 10$  mm.sim.ust. t-x-u diagram representing equilibrium concentrations at pressure



Conclusion. It can be seen that during the process, as the temperature of the mixture increases and the operating pressure in the deodorizer decreases, the share of the light volatile component in the vapor phase increases. For example, the pressure in the apparatus according to current technology is  $R = 5$  mm. sim. above and when the temperature is  $175$  °C, the relative amount of fatty acids in the vapor phase is 0.73, and their amount in the liquid phase is 0.29. Pressure in the device  $R = 10$  mm.sim.above. and when the temperature is  $175$  °C (the temperature does not change), the amount of fatty acids in the vapor phase is 0.2, and the amount in the liquid phase is 0.64.

To increase the amount of fatty acids in the vapor phase, it is necessary to further reduce the pressure in the apparatus, which in turn leads to an increase in production costs. For this situation, it was recommended to use floating nozzles in order to increase the contact surface between the vapor and liquid phase.

When superheated open water vapor is passed through a layer of oil heated to a high temperature in a hermetic apparatus under vacuum, a strong boiling state occurs in the apparatus. Water vapor easily relieves the residual pressure in the apparatus. In such conditions, aromatic substances, despite the very small elasticity of their vapors, begin to evaporate and form a mixture with water vapor and are removed from the apparatus.

Open water vapor also plays another important role in the deodorization process. When water vapor is introduced into the oil layer in the form of small bubbles, it forms a vapor-oil suspension with a very large contact surface. In this case, the oil must travel a very short distance to mix with water vapor. In this case, the resistance of the deodorization process is reduced, so the speed of its passage accelerates.

Since the concentration of the vapor of aromatic substances is small and their elasticity is very low, they can evaporate from one place, fall into the oil layer in another place of the working chamber, condense again and dissolve in it. For this reason, in modern deodorizing equipment working in continuous mode, it is envisaged to process oil in a relatively thin layer (up to 30÷50 cm). The height of the oil layer is 1.8÷2.0 meters in periodically operating devices, which naturally causes the duration of the process to be extended.

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