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CONSTRUCTION OF A MATHEMATICAL MODEL OF THE FILM ABSORBER FOR SULFATING TWO-COMPONENT MIXTURES OF ORGANIC SUBSTANCES

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The processes that occur in film absorbers during the sulfation of two-component mixtures of organic substances are quite complex and require mathematical modeling. This paper reports the construction of a mathematical model that makes it possible to adequately describe the process of sulfation involving gaseous sulfur trioxide in the production of surfactants. Based on the model, it became possible to investigate this process for higher alcohols of fractions C_{12}–C_{14} and monoethanolamides of higher fatty acids of coconut oil.

The data are given on the comparison of mathematical modeling results based on the mathematical model built with known experimental data and results of alternative mathematical modeling for different ratios of the length of the reaction pipe to its diameter (l/d). It is shown that the error in comparing the experimental data was 4.8–9.6 % at l/d=29; 1.1–8.7 % at l/d=70; 3.9–12.3 % at l/d=144. The error in comparing known results of alternative mathematical modeling was, respectively, 6.3–7.2 %, 0.1–6.5 %, 0–1.0 %. These results were obtained for the molar ratio in the range of 1.0–1.15 and the SO_3 concentration in the stream of 4.0–6.0 %.

Such findings suggest that the established dependences of the basic parameters for the sulfation process are adequate in terms of the absorber length and its radial direction. Therefore, the mathematical model built does hold within the considered ranges of input variables. Consequently, it could be used in the theoretical study of the process of sulfation of two-component mixtures of organic substances by gaseous sulfur trioxide in a film absorber with a downward flow of phases. The results obtained could be used in practice, in particular in the manufacture of high-quality products for the cosmetic industry

Keywords: mathematical model, process of sulfation, film absorber, surfactant, two-component mixture

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1. Introduction

Film absorbers are widely used in various industries, mainly in those processes that require effective heat transfer [1]. An integral condition for the successful implementation of these processes in the industry is the design of appropriate reaction equipment whose calculation methods cover the issues related to chemical kinetics, hydrodynamics, heat and mass transfer.

There are data reported in several studies into the area of a falling flow of liquid films [2, 3], which make it possible to determine the characteristics of the current as an important mechanism of processes in the system. The characteristic of the film flow is significantly different from the characteristics of a continuous flow. This is mainly due to a moving free surface where waves usually appear at relatively low airflow speeds. Thus, surface tension and gravity play a dominant role. Another reason is due to the geometry of the falling film, its small thickness, and a large interphase surface. There are limited data on hydrodynamic and mass-exchange behavior when there are significant temperature gradients in the film of the liquid. This occurs, for example, in the process of sulfation of organic substances with gaseous sulfur trioxide where the reaction is exothermic.

The sulfation process involves the interaction of SO_3 with the organic oxygen atom with the formation of C-O-S bonds and a sulfate group. Although sulfation processes are used in the industry to obtain various products, their main application is the production of anionic surfactants [4]. To obtain shampoos, foam products, the higher alcohols of

C_{12}–C_{14} fraction are used. To increase the foaming ability, mixtures of the higher alcohols of C_{12}–C_{14} fraction and monoethanolamides of higher fatty acids of coconut oil are sulfated [5].

As one can see, processes in film absorbers when sulfating two-component mixtures of organic substances directly form the quality of the products received, which are widely used. However, they are complex enough and require deeper research. Given this, mathematical modeling of such processes is a relevant task.

2. Literature review and problem statement

The review of works [6, 7] allows us to state that gaseous sulfur trioxide has recently acquired great importance as a sulfating agent. However, it is important to note that the interaction of two-phase flows in the processes of film sulfation of organic matter with sulfur trioxide is determined by complex chemical and physical phenomena. These phenomena directly affect the formation of quality indicators of finished products through the interconnected mechanisms of occurring processes [8]. However, it is worth noting that no results from analyzing the interaction of the gas phase with the fluid film, which could make it possible to quantify the transportation of reagents to the interphase surface, were revealed. However, this is especially important for systems in which resistance to the transfer process is concentrated in the gas phase.

Technological implementation of such processes is possible with various structural execution of reactors with the downward movement of phases, in particular in crevice-type devices. Products obtained in such devices are of high quality but these devices are inferior to tubular ones due to the simplicity of the latter's designs. In this case, the organic matter flows down the inner wall of the tube while the gaseous sulfur trioxide is fed in the center of the tube [9]. A striking example of such reactors is those made by the company "Balestra" (Italy), in which organic matter and SO_3 are fed in parallel through the reactor pipes. As a result of the reaction, the product exits the bottom of the reactor into the separator, the heat of the reaction released in this process is removed by cooling water. The implementation of such processes achieves the degree of sulfation of higher alcohols at the level of 97–99 %. That allows us to assert that such equipment and technological design is promising under modern conditions in the industry. However, for its effective implementation, there must be a working model of the process, which would make it possible to determine rational or optimal technological parameters. This would make it possible, in particular, to determine control processes according to the selected priority criteria for the effectiveness of the functioning of a given chemical and technological system.

Mathematical modeling of film absorbers in the production of surfactants is given considerable attention [10–19]. Thus, the authors of [10] suggested that the reaction takes place only on the surface of the gas-liquid interphase. Gilliland-Sherwood empirical equation was used to calculate the mass transfer coefficient. The heat exchange coefficient between the gas flow and the interphase boundary was calculated according to the Nusselt equation. The coefficient of heat transfer to the hard wall was assessed with the help of the Davis and David correlation. Taking into consideration these coefficients and accounting for the linear profile of temperature in the film of the liquid, they derived dependences of the quality indicators of products on temperature conditions along the length of the absorber. An alternative model was proposed in work [11] where the hydrodynamics of the film were given and the thickness of the film and speed profiles in the radial direction were determined. However, the basic equations used for calculating mass transfer and heat transfer coefficients were borrowed from the Johnson and Kraines model.

Paper [12] reports approximately 40 experimental data on the sulfation of dodecylbenzene with gaseous SO_3 using a laboratory absorber with a falling film. The mathematical model for calculating the degree of sulfation of dodecylbenzene by the length of the absorber depending on the main technological parameters of the process is also given: the temperature of the liquid phase, the molar ratio of reagents, the SO_3 concentration in the gas-air flow, the length of the absorber. The main disadvantage of this model is the use of numerical corrective coefficients in the equations of heat and mass transfer.

Paper [13] reports the results of the construction of a mathematical model, as well as comparative data obtained from the model with a data set [12]. The mathematical model built is suitable for both laminar and turbulent films, and takes into consideration the effects of the wave motion of the film using the parameter of turbulent diffusion. The authors showed sufficient convergence of the model with the experimental data given in [12]. The additional effect of surface tension, as well as the physical properties of the liquid phase depending on the thickness of the film, were determined in [14]. However, the use of equations for calculating mass and heat transfer coefficients is not sufficiently substantiated.

A mathematical model of the process of sulfation of tridecyl benzene in a film absorber is described in paper [15]. It has made it possible to derive the dependences of quality indicators of products on the basic technological parameters and determine the parametric sensitivity of the absorber depending on the main disturbing influences. However, the authors also used the equation for calculating the mass transfer coefficient proposed in [6]; therefore, the reported results require additional analysis.

Works [16, 17] proposed a model that is suitable for laminar and turbulent films and takes into consideration the effects of wave formation of the film flow using the whirlwind diffusion parameter. The effects of interphase resistance at the boundaries of the gas-liquid interface and the resistance of heat and mass transfer in the gas phase were taken into consideration. The model accounts for the application of the physical properties of the liquid depending on the temperature and provides conversion profiles, the fluid temperature in the axial direction, and the thickness of the liquid film by the length of the absorber. A model for the sulfation of methyl esters of fatty acids, based on the mathematical model reported in [16], was proposed in [18]. However, unlike [16], the results of wider studies are presented. In particular, the following features of this model should be noted. Input variables are the length and diameter of the absorber, the flow rate of the liquid phase, the molar ratio of the reagents, the content of sulfur trioxide in the gas-air flow, the temperature of the process. The mathematical model makes it possible to calculate the profiles of interphase temperature, the density of a liquid film, the viscosity of a liquid, longitudinal conversion profiles.

Work [19] defines regularities in the process of sulfation of mixtures of organic substances, based on which the dependences of the degree of sulfation and color of pastes on the main technological parameters of the process were established. One of the features of the obtained results, important for the construction of a mathematical model of sulfation of mixtures of organic substances, is determining, by the authors of the cited work, the patterns of changes in the physical and chemical parameters of the reaction mass during the process of sulfation. However, the result reported in the work demonstrated an insufficiently high degree of sulfation (η<95 %), which is associated with the use of a volumetric reactor.

As the above analysis reveals, a significant number of experimental studies and studies involving mathematical modeling have been carried out. However, the issue related to building adequate mathematical models of film absorbers for the sulfation of two-component mixtures of organic substances with gaseous sulfur trioxide remains open. Given that this task is practically important, for example, in the production of surfactants for cosmetic drugs, appropriate theoretical studies are advisable.

3. The aim and objectives of the study

The purpose of this research is to construct a mathematical model of the sulfation process involving two-component mixtures of organic substances based on the higher alcohols of C_{12}–C_{14} fraction and monoethanolamides of higher fatty acids of coconut oil with gaseous sulfur trioxide in a film absorber with a downward flow of phases. This would make it possible to choose the parameters of the process that ensure the production of high-quality products for the cosmetic industry.

To accomplish the aim, the following tasks have been set:

– to determine the structure and parameters for the model of a film absorber for sulfating two-component mixtures of organic substances with gaseous sulfur trioxide in the production of surfactants;

– to study the regularities of the process of sulfation of two-component mixtures of organic substances in a film absorber.

4. The study materials and methods

To build a mathematical model of the film absorber, we used data given in [6–15] and the study results reported in [5]. The mathematical model accepted the following assumptions:

– there are no heat losses to the environment;

– the liquid film is symmetrical with respect to the absorber axis;

– the liquid does not evaporate; the gas does not condense;

– the input and output end effects are not taken into consideration;

– there is no drip carry of liquid.

The base of organic matter is a mixture of the highest alcohol of C_{12}–C_{14} fraction with an average molecular weight of 188 g/mol and monoethanolamide of higher fatty acids of coconut oil with an average molecular weight of 280 g/mol. The mixture of these substances is sulfated with gaseous sulfur trioxide diluted with drained air.

The film absorber was a reaction pipe with a diameter of 0.037 m and a length of 5.5 m, which consists of two sections for cooling: the upper section is 1/3 of the length of the absorber, the lower section is 2/3 of the length of the absorber. The main method of research into the process of sulfation is the method of mathematical modeling.

The initial data to build a model:

– the temperature of the liquid phase at the input to the absorber is 313 K;

– the gas-air flow temperature at the input to the absorber is 30 K;

– the cooling water temperature in the upper and lower sections is 293 K;

– the linear density of irrigation is $0.63\cdot10^{-4}$ m^2/s;

– the gas-air flow rate is 0.02 m^3/s;

– the molar ratio of reagents is 1.08:1.0;

– the concentration of sulfur trioxide in the gas-air flow is 3.7 % by volume.

5. Results of studying the process of sulfation using the mathematical model of film absorber

5. 1. Determining the structure and parameters of the film absorber model

The mathematical model is represented by the following equations:

$$V_z \frac{\partial C_A}{\partial z} = \frac{\partial}{\partial y}\left[\left(D_A + D_T\right)\frac{\partial C_A}{\partial y}\right] - r, \tag{1}$$

$$V_z = \frac{\rho_L \cdot g}{\mu_L}\left(\delta \cdot y - \frac{y^2}{2}\right) + \frac{\tau_{bnd} \cdot y}{\mu_L}, \tag{2}$$

$$\delta = \sqrt{\frac{G}{\delta / 3\mu_L + \tau_{bnd} / 2\mu_L}}, \tag{3}$$

$$\tau_{bnd} = f \cdot \rho_L \cdot V_G^2, \tag{4}$$

$$f = \frac{86}{\mathrm{Re}_G}, \tag{5}$$

$$W_G \frac{dN_B}{P \cdot dz} = -K_G \cdot P_B \cdot A_G, \tag{6}$$

$$K_G = B \cdot P\mathrm{r}_D^{-0.704} \cdot \left(\frac{\tau_{bnd}}{\rho_G}\right)^{0.5}, \tag{7}$$

$$V_z \cdot \rho_L \cdot C_L \cdot F \frac{\partial T_L}{\partial z} = -\frac{\partial}{\partial y}\left(-\lambda_L \frac{\partial T_L}{\partial y}\right) + H_R \cdot r \cdot F, \tag{8}$$

$$\rho_L = 852 + 2.0 \cdot \eta - 0.68 \cdot \left(T_L - 273\right), \tag{9}$$

$$\mu_L = 0.158 \cdot \exp\left\{-0.5 \cdot \begin{bmatrix} 0.00013 \cdot \left(T_L - 273\right)^2 + \\ +0.00078 \cdot \left(78 - \eta\right)^2 \end{bmatrix}\right\},$$

$$0<\eta<73\%, \tag{10}$$

$$\mu_L=0.0011\left[\begin{array}{l}595.6-11.34\cdot\eta+0.07\cdot\eta^2+\\+0.1\cdot\left(T_L-273\right)-0.01\cdot\left(T_L-273\right)^2\end{array}\right],$$

$$\eta>73\%, \tag{11}$$

$$K_{TG}=K_G\cdot C_G\cdot\rho_G\left(\frac{\mathrm{Pr}_D}{\mathrm{Pr}_T}\right)^{0.67}, \tag{12}$$

$$K_{TC}=\frac{1}{\frac{1}{\alpha_1}+\frac{\delta_W}{\lambda_W}+\frac{1}{\alpha_2}}, \tag{13}$$

$$\alpha_1=0.34\cdot\frac{\lambda_L}{d}\cdot\left(\frac{\rho_L}{\rho_G}\right)^{0.28}\cdot\left(\frac{d\cdot G_{bnd}}{\mu_L}\right)^{0.87}\cdot\mathrm{Pr}_T^{0.4}, \tag{14}$$

$$\alpha_2=0.021\cdot\frac{\lambda_X}{d_{eqv}}\cdot\left(\frac{V_X\cdot d_{eqv}\cdot\rho_X}{\mu_X}\right)^{0.8}\left(\frac{c_X\cdot\mu_X}{\lambda_X}\right)^{0.4}. \tag{15}$$

Boundary conditions:
– at $y=0$

$$\frac{\partial C_A}{\partial y}=0, \tag{16}$$

$$\lambda_L\frac{\partial T_L}{\partial y}=K_{TC}\left(T_L^{y=0}-T_C\right), \tag{17}$$

– at $y=\delta$,

$$\frac{\partial C_A}{\partial y}=0, \tag{18}$$

$$\lambda_L\frac{\partial T_L}{\partial y}=K_{TG}\left(T_G-T_L^{y=\delta}\right), \tag{19}$$

where C_A is the molar concentration of the initial organic matter in the liquid phase, mol/m^3; V_z is the fluid phase velocity, m/s; r is the reaction speed, mol/(m^2·s); z – axal coordinate, m; D_A is the molecular diffusion coefficient in a liquid phase, m^2/s; D_T is the coefficient of turbulent diffusion in the liquid phase, m^2/s; y is the radial coordinate; ρ_λ is the density of the liquid phase, kg/m^3; g is the acceleration of free fall, m^2/s; δ is the thickness of the liquid phase film, m; τ is the tangent tension on the surface of the gas-liquid interphase, Pa; μ_l is the dynamic viscosity of the liquid phase, Pa·s; G is the linear density of irrigation, m^2/s; V_G is the gas-air flow rate, m/s; f is the friction coefficient; Re_G is the Reynolds criterion for the gas-air flow; P is the total pressure of the gas-air flow, Pa; P_B is the current partial sulfur trioxide pressure in the gas-air flow, Pa; N_B is the ratio of the SO_3 partial pressure to the total pressure of the gas-air flow; W_G is the ratio of the molar flow rate of sulfur trioxide per unit of perimeter length of the reaction pipe, mol/ (m·s); A_G is the corrective coefficient; K_G is the mass transfer coefficient, m/s; B is a constant coefficient; ρ_G is the density of the gas-air flow, kg/m^3; Pr_D is the Prandtl's diffusion criterion; T_l is the liquid phase temperature, K; C_l is the specific heat capacity of the liquid phase, J/(kg·K); F is the heat exchange area, m^2; λ_p is the coefficient of thermal conductivity of the liquid phase, W/(m^2·K); H_R is the thermal reaction effect, J/mol; η is the degree of sulfation, %; K_{TG} is the heat transfer coefficient from the liquid phase to the gas-air flow, W/(m^2·K); Pr_T is the Prandtl's thermal criterion; K_{TC} is the heat transfer coefficient from the liquid phase to a cooling water flow, W/(m^2·K); α_1 is the heat transfer coefficient from the liquid phase to the wall of the reaction pipe, W/(m^2·K); α_2 is the heat transfer coefficient from the reaction pipe wall to the cooling water flow, W/(m^2·K); δ_W is the thickness of the wall of the reaction pipe, m; λ_W is the specific thermal conductivity of the wall, W/(m·K); d is the diameter of reaction pipe, m; G_{GR} is the mass flow rate of the gas-liquid flow, kg/s; λ_C is the specific thermal conductivity of cooling water, W/(m·K); d_{eqv} is the equivalent diameter, m; V_C is the flow rate of cooling water, m/s; ρ_C is the density of cooling water, kg/m^3; μ_C is the dynamic viscosity of cooling water, Pa·s; C_C is the specific heat capacity of cooling water, J/(kg·K).

For our study on the mathematical model, a program was developed to calculate the process of sulfation of two-component mixtures of organic substances in a film absorber using the MATLAB software package (USA).

The adequacy of the mathematical model was tested by comparing our results with experimental data [12] and the results from alternative mathematical modeling [13]. At the same time, the conditions under which experimental research and mathematical modeling were carried out in [12, 13] were repeated.

Table 1

Results of experimental studies [12] and results from mathematical modeling [13] with the comparison of results from the constructed mathematical model

The ratio of the length of the reaction pipe to its diameter, *l/d*	Molar ratio	SO_3 flow concentration, %	Experimental data [8]: degree of sulfation, %	Mathematical modeling results [9]		Results of the mathematical modeling using the mathematical model built		
				Sulfation degree, %	Error, %	Sulfation degree, %	Error, % (comparing to [8])	Error, % (comparing to [9])
29	1.0	4.0	74.9	66.8	10.8	71.3	4.8	7.0
29	1.0	6.0	76.0	67.9	10.6	72.2	5.0	6.3
29	1.1	4.0	83.7	70.8	15.4	75.6	9.6	6.9
29	1.1	6.0	81.0	70.8	12.6	75.9	6.3	7.2
70	1.0	4.0	87.3	89.0	2.0	89.1	2.1	0.1
70	1.0	6.0	83.9	87.9	5.0	91.2	8.7	3.8
70	1.05	4.0	89.7	91.0	1.4	92.3	2.9	1.4
70	1.05	6.0	87.6	88.7	1.0	93.0	6.2	5.5
70	1.1	4.0	90.3	92.2	2.0	93.7	3.7	1.6
70	1.1	6.0	87.9	88.9	1.0	94.0	7.0	5.8
70	1.15	4.0	93.5	92.9	0.6	94.5	1.1	1.7
70	1.15	6.0	92.0	89.0	3.0	94.8	3.0	6.5
144	1.0	4.0	84.6	94.8	12	95.0	12.2	0.2
144	1.0	6.0	85.2	95.7	12.3	95.7	12.3	0
144	1.1	4.0	93.0	97.1	4.4	96.5	3.9	0.5
144	1.1	6.0	91.4	96.2	5.3	97.2	6.3	1.0

In other words, it can be argued that the constructed mathematical model could be used when mathematically modeling the process of sulfation of two-component mixtures of organic substances with gaseous sulfur trioxide in a film absorber with a downward flow of phases with reliable results. The system of equations is calculated numerically using the method of finite differences.

5. 2. Determining the regularity of the process of sulfation of two-component mixtures of organic substances in the film absorber

Fig. 1 shows data on changes in the interphase temperature, the gas-air flow temperature, and cooling water temperature by the absorber length.

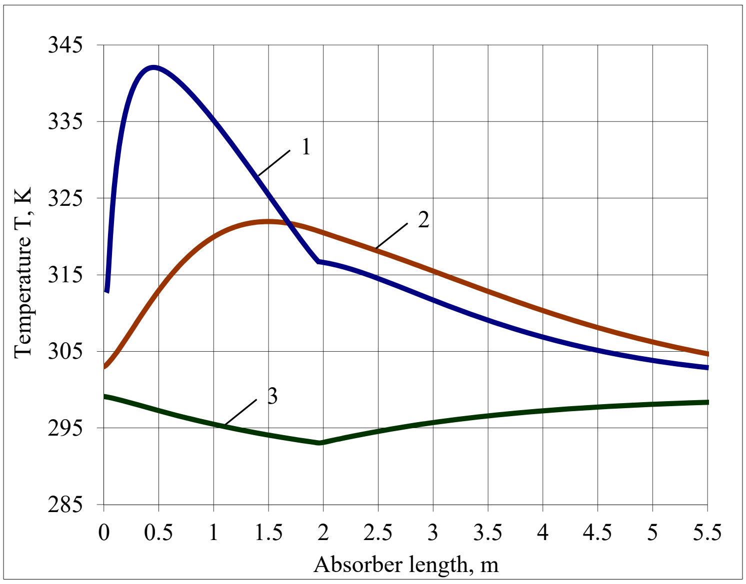

Fig. 1. Patterns of change in temperature along the length of the absorber: 1 – change in the interphase temperature, 2 – change in the temperature of the gas-air flow, 3 – change in the temperature of the cooling water

Fig. 2 shows data on changes in the temperature of the liquid phase in the radial direction (above the peak of the interphase temperature).

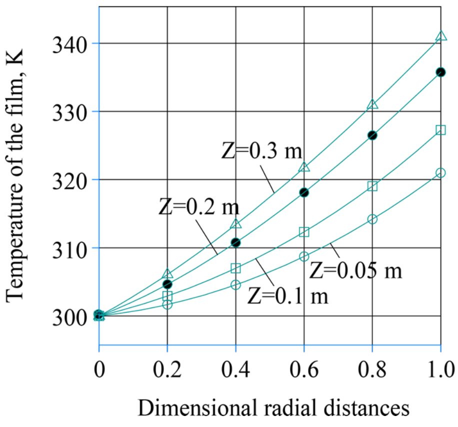

Fig. 2. Change in the temperature of the liquid phase in the radial direction (above the peak of the interphase temperature)

Fig. 3 shows data on changes in the temperature of the liquid phase in the radial direction (in the lower section of the absorber).

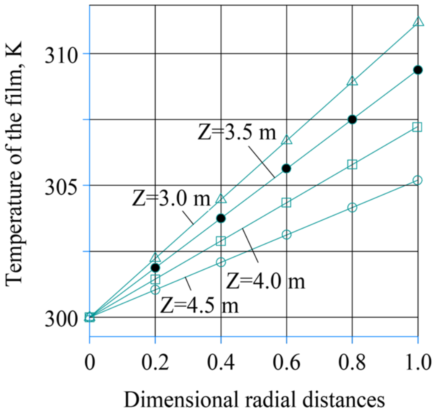

Fig. 3. Change in the temperature of the liquid phase in the radial direction (in the lower section of the absorber)

Fig. 4 shows data on the change in the degree of sulfation by the length of the absorber.

Fig. 5 shows data on the change in the thickness of the film of the liquid phase by the length of the absorber.

Fig. 6 shows data on changes in the dynamic viscosity of the liquid phase and data on changes in the heat transfer coefficient from the liquid phase to the stream of cooling water by the length of the absorber.

Fig. 1–3 make it possible to estimate the temperature profiles in the absorber; Fig. 4–6 define the parameters of the technological process as a function of the length of the absorber.

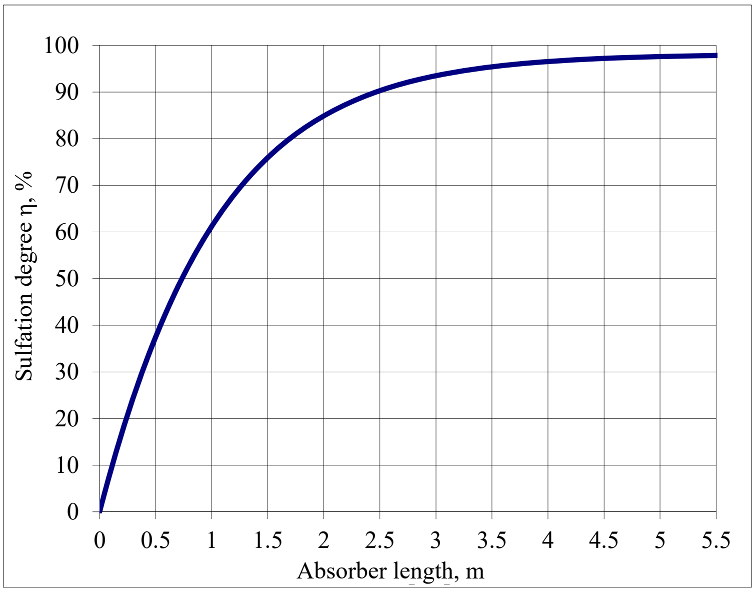

Fig. 4. Change in the degree of sulfation of a two-component mixture of organic substances by the length of the absorber

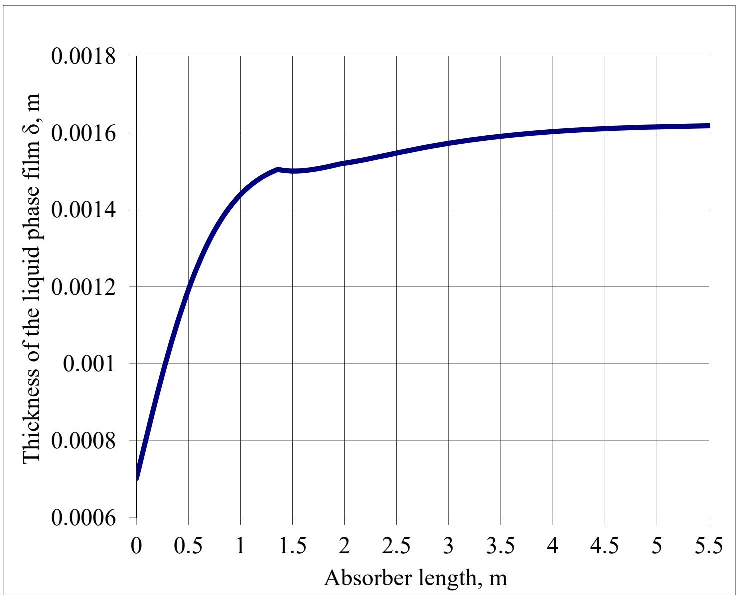

Fig. 5. Change in the thickness of the liquid phase film by the length of the absorber

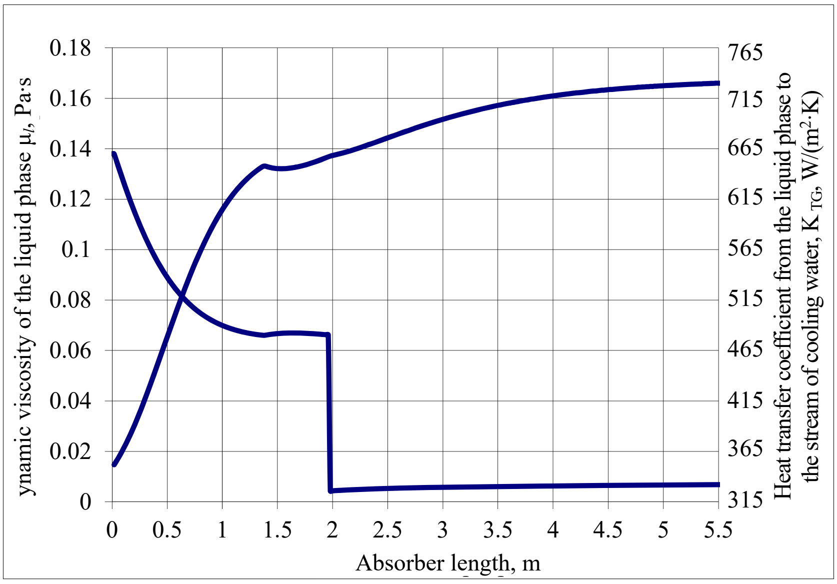

Fig. 6. Change in the dynamic viscosity of the liquid phase and data on changes in the heat transfer coefficient from the liquid phase to the stream of cooling water by the length of the absorber

6. Discussion of results of building a mathematical model of the process of sulfation of two-component mixtures of organic substances

Our mathematical model (1) to (15) can be compared to the model reported in [19] in terms of equations for calculating the density of the liquid phase and the dynamic viscosity of the liquid phase, due to the use of a two-component mixture of organic substances. It should be noted that the presented model includes more modern equations for calculating the mass transfer coefficient, a new equation for calculating the friction coefficient, and, accordingly, the equation for calculating the tangent stress on the gas-liquid surface. Table 1 demonstrates the error in mathematical modeling when using the mathematical model built, when compared with experimental data [8], is equal at 4 points to 8.7÷12.3 %, and mostly 1–7 %; when compared with the results of mathematical modeling [9], the error is no more than 7.2 %.

Fig. 1 shows that the interphase temperature accepts a fairly high maximum (343 K) at 1/12 of the length of the absorber, and then the temperature decreases. A sharp increase in temperature drives the progress of an exothermic reaction with the release of 167.5 kJ/mol of heat. In this case, part of the heat is transmitted to the gas-air flow, and the second part – the flow of cooling water. As the length of the absorber changes, the amount of heat released decreases sharply while the temperature decreases.

Fig. 1 also illustrates that the temperature of the gas-air flow in the upper section of the absorber rises, and then decreases to the end of the absorber. The increase in temperature is caused by the transfer of heat from the liquid phase where there is a significant temperature difference.

Fig. 1 shows that in the upper section when supplying cooling water with an anti-current, the temperature drops, and in the lower section gradually rises, which is due to the nature of the change in the temperature of the liquid phase. When compared to [19], Fig. 1 depicts a change in the interphase temperature by the length of the absorber, which more accurately characterizes the process of mass exchange and the process of chemical absorption at the gas-liquid border. The temperature of the gas-air flow and the flow of cooling water are also changed: the maximum temperature of the gas-air flow decreases to 307 K, at the end of the absorber – to 304 K. The maximum temperature of the cooling water is maintained within the following limits: the upper section, 298 K, the lower section, 300 K.

Fig. 2 demonstrates that the change in the temperature of the liquid phase along the thickness of the film at a slight distance from the top of the absorber is nonlinear. As the distance increases, the nature of the temperature change is almost linear.

Fig. 3 shows that in the lower section of the absorber, the change in the temperature of the liquid phase along the thickness of the film is almost linear. In comparison with [19] the data of Fig. 2, 3 in this paper are not given.

Fig. 4 illustrates that the degree of sulfation increases sharply at the top of the absorber, and then there is a slight increase in the degree of sulfation along the length of the absorber. This is due to the fact that at the top of the absorber there is a high concentration of SO_3 in the gas-air flow, and then it decreases while the increase in the degree of sulfation slows down. When compared to [19], the nature of the degree of change in the degree of sulfation by the length of the absorber is also different, for example, at the length of the absorber of 1 m, the degree of sulfation reaches 62 % versus 54 % reported in [19].

Fig. 5 shows that of significant interest is the change in the thickness of the film by the length of the absorber. In the upper section of the absorber, the thickness of the film begins to increase, which is associated with a sharp increase in the viscosity of the liquid phase. As the length of the absorber increases, the viscosity of the liquid phase slows down and then the thickness of the film almost does not change. The thickness of the film increases from 0.0007 m to 0.00162 m, versus work [19], in which the changes are from 0.0006 m to 0.0014 m.

Fig. 6 demonstrates that the nature of change in the dynamic viscosity of the reaction mass can be compared with the thickness of the film by the length of the absorber. The dynamic viscosity value varies from 0.018 Pa·s, versus [19], where the changes are from 0.012 Pa·s to 0.135 Pa·s.

Fig. 6 illustrates that the heat transfer coefficient from the liquid phase to the cooling water flow to the upper part of the absorber falls, and, in the lower section, it increases slightly. A sharp difference of 1/3 of the absorber length is associated with a decrease in the cooling water flow rate in the lower section of the absorber. The value of the heat transfer coefficient from the liquid phase to the cooling water flow in the upper section decreases from 665 W/m^2·K to 480 W/m^2·K, versus [19] where the decrease occurs from 630 W/m^2·K to 465 W/m^2·K. In the lower section, the data are almost identical.

The limitations of this study are related to the ranges of input data within which the theoretical results obtained are adequate to the actual process. In particular, the results have been obtained for the molar ratio in the range of 1.0–1.15 and the SO_3 concentration in the flow of 4.0–6.0 %, and the ratio of the length of the reaction pipe to its diameter (*l/d*) is in the range of 29–144. Expanding the scope of research and determining the impact of other technological factors of the process may outline directions to advance this work.

7. Conclusions

1. We have proposed a structure of the mathematical model of a film absorber for sulfating two-component mixtures of organic substances with gaseous sulfur trioxide, represented by a system of equations. They include, in particular, the differential equation in the particular derivatives of the molar concentration of the initial organic matter in the liquid phase as a function of reactor geometry. The peculiarity of this representation of the process in terms of the structure of the model and the parameters included in its description is:

– more modern equations for calculating the mass transfer coefficient;

– a new equation for calculating the friction coefficient;

– an equation for calculating the tangent stress at the gas-liquid surface.

This provides the possibility to model the process of sulfation of two-component mixtures of organic substances with gaseous sulfur trioxide in a film absorber with a downward flow of phases with reliable results.

2. The results of the mathematical modeling using the mathematical model built were compared with known experimental data and the results from alternative mathematical modeling. It is shown that the error of comparison with experimental data as a function of the ratio of the length of the reaction pipe to its diameter (*l/d*) was 4.8–9.6 % at *l/d*=29, 1.1–8.7 % at *l/d*=70, 3.9–12.3 % at *l/d*=144. The error of comparison with known results from alternative mathematical modeling was, respectively, 6.3–7.2 %, 0.1–6.5 %, 0–1.0 %. This gives reason to assert that the constructed mathematical model is feasible and the process modeling results obtained when using it are reliable.

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