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MATHEMATICAL MODEL OF THE FLOW STRUCTURE IN THE PULSATION CRYSTALLIZER

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The paper presents a mathematical model of a pulsation crystallizer, which includes heat and hydraulic calculations. Heat calculation is reduced to determining the refrigerant flow rate (cooled solvent and filtrate of the second stage) for each section of the unit. The minimum volume of the section based on the experimentally determined preliminary sectional temperature profile and cooling rate of the raw material flow, the specified flow rate of raw material and refrigerant, as well as their initial temperature [1]. The calculation is carried out bearing in mind the correction of the preadopted number of crystallizer sections. Heat calculation of the crystallizer is carried out after determining the technological parameters of the dewaxing process. Moreover, the thermal calculation carried out according to the described method is preliminary, because it does not take into account the reverse flow in the apparatus during pulsation. As a result, the hydraulic calculation determines: volume, frequency of pulsating flow, necessary mass of liquid, nozzle size, speed of crude mixture in the nozzles, pulsation frequency and the ratio of pulse and purge exhaust.

Introduction

The process of production of base oils and paraffins is a sequence of mass - exchange processes of removal of hydrocarbon groups and compounds, the presence of which in the oil is undesirable (resin - asphaltene compounds, polycyclic aromatic hydrocarbons with low viscosity index, solid paraffin hydrocarbons) [2]. The most important stage is the extraction of solid hydrocarbons (paraffin and ceresin), which can also serve as commercial products after proper purification.

The technology of dewaxing and de-oilification of gatches carried out on standard installations, but this process has not changed for the past 30–40 years. The long-term industrial operation of these facilities has revealed a number of deficiencies of the technology and equipment used.

Only catalytic dewaxing can compete with classical dewaxing based on crystallization followed by filtration. However, it has worked well only for synthetic oils but their production has not yet reached the desired level of development in our country.

Crystallization equipment (regenerative and evaporative scrubber crystallizers) used in refining and degassing processes and the corresponding technology for the production of paraffin suspensions contributes to the formation of a highly dispersed crystalline structure of the emitting solid phase. The filtration characteristics of such suspensions are determined by the deparaffinized oil reduced product slate and the increased oil content of paraffins and ceresines. Thus, the need to increase the ratio of solvent to the raw material in order to achieve the desired targets leads to the increase of the energy cost for its regeneration.

Application of vacuum filters during dewaxing and de - oiling does not allow intensification of this stage of these processes. The quality and speed of liquid phase separation are fully determined by the filtration characteristics of the suspension, which depends on the previous stage of the crystallization. The attempts to modernize this equipment, to optimize the filtration mode and new filtering materials did not lead to a significant increase in the selection of dewaxed oil and improve the quality of paraffins (ceresins). Besides, the currently used crystallization and filtering equipment is complex in design so as quite expensive to operate, maintain and repair.

The development of crystallization equipment with reduced refrigerant consumption and a simple design, which would allow to form easily extractable crystals in suspension, should be considered as a promising direction [3-5]. It was logical to avoid the use of complex scraper rolls and focus on vertical vessels.

For example, some of the first columns, in the working space of which there are sieve plates of dip type (without overflow pipes). Additional energy is given to moving liquid flows due to the use of pulsation devices or air mixing [6]. It is important to determine what effect is achieved in comparison with a tray-pulsation column of similar design, but without the use of additional energy when assessing the effectiveness of using one or another method of intensifying the interaction process in tray-pulsation column [7]. Therefore, it is necessary to consider the phenomena of hydrodynamics and mass exchange in a column with sieve plates of dip type. Should be mentioned that value of forces of inertia crushing liquid drops is determined mainly by difference of specific weights of liquids [8].

The modern technology of production of pure substances without highly solidifying components is mainly based on such type of apparatuses as pulsation crystallization columns. Since the demand for pure substances is increasing so as the demand for the pulsation column apparatuses. However, there is a fairly widespread prejudice against columns based on some doubts about the efficiency of industrial-scale apparatus. The reason is the difference between hydrodynamics of large-diameter columns and hydrodynamics of laboratory installations. This only raises the interest to modeling processes in pulsation apparatuses with the help of computational software. It can be defined as the main reliable tool of numerical analysis.

The pulsation crystallizer is a gas-liquid column, the mathematical model of which is based on balance equations.

The heat calculation of the mixing crystallizer is determined by refrigerant flow rate (cooled solvent and filtrate of the second stage) for each section of the unit and the minimum volume of the section based on the experimentally determined preliminary sectional temperature profile and cooling rate of the raw material flow, the given flow rate of raw materials and refrigerant, as well as their initial temperature [1].

The calculation is carried out in terms of the correcting of the pre-adopted number of crystallizer sections, if necessary.

Experiment

The specific heat capacity of a raw mixture is a function of two variables: concentration of raw material in solution and temperature. The nature of this dependence is the same for all wax-bearing crude, but the specific values depend on the content of paraffins in the raw material, its distillation volume and use of solvent. So, the necessary set of data for calculating the heat capacity of the crude mixture is determined experimentally in each case.

The diagram of the crystallizer section with the principal flow identifications is shown in Fig. 1. The heat balance of section *i* is recorded as

$$G_{i-1} \cdot C(x,T)_{x=xi-1} \cdot T_{i-1} + G_{x,i} \cdot C_x \cdot T_x = G_i \cdot C(x,T)_{x=xi} \cdot T_i, \tag{1}$$

where $G_{i-1}G_i$ is the crude mixture flow at the input and output of the *i* section, kg/s;

$C(x,T)_{x=xi-1}$, $C(x,T)_{x=xi}$ is the specific heat capacity of the crude mixture at the input and output of the*i* section at the respective raw material concentration and temperature, J/(kg·°C);

T_{i-1},T_i is the section *i* input and output temperature, °C;

$G_{x,i}$ - flow rate of the refrigerant (solvent or filtrate of the second stage for section *i*, kg/s;

C_x - heat capacity of the refrigerant, J/(kg·°C);

T_x - the temperature of refrigerant, °C.

The concentrations of crude oil in the mixture at the input and output of the *i* section are equal:

$$x_{i-1} = G_c/(G_c + \sum_{j=1}^{j=i-1} G_{x,j}), \quad \begin{pmatrix} i = 1, 2, 3, \dots, M \\ j = 1, 2, 3, \dots, i \end{pmatrix} \tag{2}$$

$$x_i = G_c/(G_c + \sum_{j=1}^{j=i} G_{x,j}), \tag{3}$$

G_c is the raw material flow rate, kg/s;

M is the number of sections in the crystallizer.

The heat capacity of the crude mixture at different temperatures and concentrations is represented as a two-dimensional array. The sectional flow rate of the solvent is determined by follows: the concentrationx_i, the corresponding value of heat capacity is determined from the specified array by interpolation using equation (3) as a preliminary accepted value of the refrigerant $G_{x,j}$ flow rate; the values $G_{x,j}$ are substituted into equation (1). The further calculation is carried out by the method of successive approximations until the specified divergence between the left and right parts of equation (1) is reached.

$$G_i = G_{j-1} + G_{x,j}\ \ C(x,T)_{x=xi}. \tag{4}$$

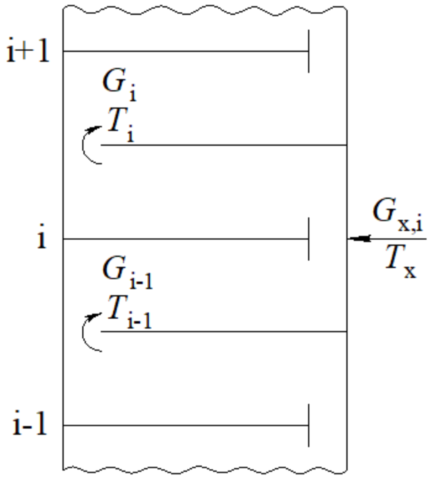

Fig. 1 Diagram of the pulsation displacement crystallizer section with defining of the main flows

The heat calculation of the crystallizer is carried out after determining the technological parameters of the dewaxing process. Thus, the heat calculation carried out according to the described method is preliminary, because it does not take into account the reverse flow in the apparatus during pulsation. The flow of crude mixture in the sections G_i is assumed unidirectional. Correction of the temperature profile in the crystallizer, taking into account the effect of reciprocating motion caused by pulsation of the medium in the apparatus, is carried out after a hydraulic calculation, as a result of which the volume and frequency of the pulsating flow are determined. In the process of hydraulic calculation, the necessary mass of the fluid making oscillating motions in the pulsation chamber, the nozzle size and the speed of the crude mixture in the nozzles are also determined based on the given raw material flow rate and the calculated sectional solvent flow rate, pulsation frequency and the ratio of pulse and purge exhaust.

The speed of the mixture in the nozzles and the productivity of the pulsation system should provide the required intensity of mixing in the crystallizer sections.

A diagram of the apparatus for hydraulic calculation with the designation of the corresponding flows is shown in Fig. 2.

In order to create a reciprocating motion in the nozzles, the mass of the raw mixture, emitting at a pulse from the M section, must be such that the oscillation scale at the top of the apparatus corresponds to the sum of the suspension masses emitted through the drain of the crystallizer, equal to the total input of raw material and solvent into the column over the full cycle of pulsation $t_и + t_в$ ($t_и$, $t_в$ pulse and purge exhaust respectively)

$$(G_c + \sum_{i=1}^{M} G_{x,i})(t_и + t_в), \tag{5}$$

and some minimum value $G_{в,\min}$ (кг), greater than the specified mass of the solvent entering the M section during the purge exhaust time $G_{x,i=M} \cdot t_в$. These two conditions provide that during the pulse time there is an output from the crystallizer of the amount of suspension corresponding to the capacity of the apparatus for a full pulsation cycle. But during the purge exhaust period there is a backflow of liquid in the upper nozzle, a specified number of times greater than the mass of solvent (the largest of all sections) coming into this nozzle. The second condition is chosen taking into account the fact that the mass of the fluid flowing through the nozzles grows downward from section to section, and the amount of solvent supplied to these sections decreases (this will be shown in the results of the heat calculation below).

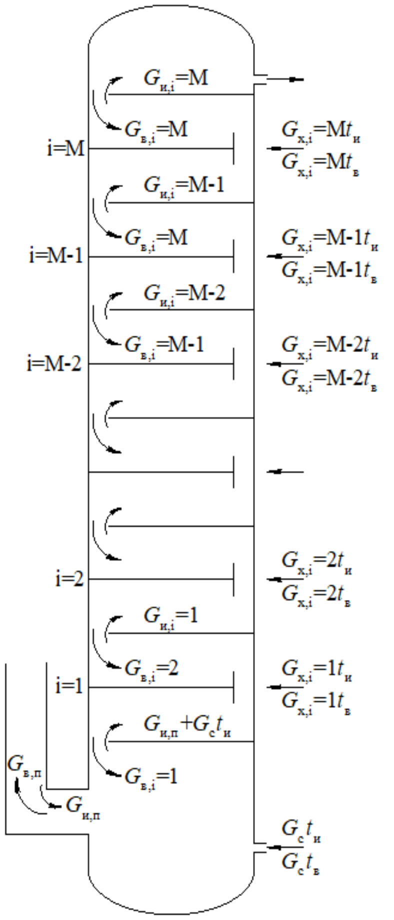

Fig. 2. Flow diagram in the pulsation mixing crystallizer for hydraulic calculation (symbols in the text)

Thus

$$G_{в,\min} = k \cdot G_{x,i=M} \cdot t_в, \tag{6}$$

will obtain

$$G_{и,i=M} \cdot G_{в,\min} + (G_c + \sum_{i=1}^{M} G_{x,i})(t_и + t_в), \tag{7}$$

$G_{и,i=M}$ is the mass of the slurry coming out at the pulse from the M section, kg.

This way the necessary mass of liquid displaced from the pulsation chamber at the impulse, satisfying the above conditions (taking into account that the mass of the slurry flowing through the nozzles grows from bottom to top from section to section), kg, is equal to

$$G_{и,п} = G_{и,i=M} - \left(G_c + \sum_{i=1}^{M} G_{x,i}\right) t_и. \tag{8}$$

Corresponding volume of liquid, making oscillations in the pulsation chamber, м^3:

$$V_{и,п} = G_{и,п}/\rho, \tag{9}$$

ρ is the average density of the crude mixture in the apparatus, kg/м^3.

The mass of the slurry flowing through the nozzles in the i section, kg, is equal to

$$G_{и,i} = G_{и,п} + \left(G_c + \textstyle\sum_{j=1}^{i} G_{x,j}\right)t_и. \tag{10}$$

At the purge exhaust, the mass of the slurry flowing through the nozzles in the section *i* is equal to

$$G_{в,i} = G_{в,\min} + \textstyle\sum_{j=M}^{i} G_{x,j} \cdot t_в. \tag{11}$$

Mass of liquid entering the pulsation chamber during the purge exhaust, kg:

$$G_{в,п} = G_{в,i=1} + G_c \cdot t_в. \tag{12}$$

Implementation of condition $G_{и,п}$=$G_{в,п}$ is a confirmation of the fairness of the calculations. As the greatest mass of the mixture flowing in the nozzle falls on the *M* section at the momentum, the cross-sectional area of the nozzle is calculated by the formula

$$F_c = G_{и,i=M}/(t_и \cdot \rho \cdot W_{\max}), \tag{13}$$

F_c is the nozzle areaм^2;
$W_{\max}$ - limit top speed flow velocity in the nozzles, m/s.

Then the radius of the nozzle, m, is

$$R_c = 0{,}5(F_c/0{,}39). \tag{14}$$

The speed of the crude mixture in the *i* nozzle at impulse and purge exhaust is

$$W_{и,i} = G_{и,i}/(F_c \cdot \rho \cdot t_и). \tag{15}$$

$$W_{в,i} = G_{в,i}/(F_c \cdot \rho \cdot t_в). \tag{16}$$

The pulsation mixer should provide the specified mixing intensity. In the case of sectioned apparatus, the intensity of mixing, c, can be assessed by the fluid flow rate in the nozzle and the ratio of the section volume to the capacity of the pulsation mixer:

$$I = V_0/(V_{и,п} \cdot f), \tag{17}$$

where *f* is the frequency of pulsation (level fluctuations in the pulsation chamber), 1/s;
V_0 - the volume of the apparatus section, м^3.

If the condition of a given mixing intensity is not met, the volume $V_{и,п}$ is corrected with subsequent calculation by formulas (6)–(16). The values of pulsation frequency *f* and the ratio of pulse and purge exhaust $t_и$ $t_в$ are taken according to the recommendations for pulsating mixing in column apparatuses. The value of *k* (in formula (6)), the maximum speed of the mixture in the nozzles $W_{\max}$ and the mixing intensity criterion *I* are determined experimentally.

Flow rates in the section are taken according to the heat calculations. The hydraulic calculation includes the calculation of the pulsation system of the crystallizer. The scheme for calculating the pulsation system is shown in Fig. 3. To ensure the required mode of fluid oscillation in the system (pulsation chamber, connecting pipeline, crystallizer), the difference of levels in the apparatus and the pulsation chamber must ensure the movement of the crude mixture during the purge exhaust time $t_в$. The corresponding equations are the sources of the formula for determining the magnitude of the level difference:

$$Н_{ст} = \sum_{i=1}^{M} {G_{B,i}}^2/(2gM\rho^2 {t_в}^2)\,[1/(\mu_н \cdot \omega_н)^2 + 1/(\mu_n \cdot \omega_n)^2] + W^2/(2g)\,(1 + \lambda\ L/d + \sum \varphi), \tag{18}$$

where μ_n и $\mu_н$ is the nozzle and overflow flow coefficient;

ω_n и $\omega_н$ - is the nozzle and overflow area, respectively, $м^2$;

W - velocity of liquid movement (during purge exhaust) in the pipeline connecting the pulsation chamber with the crystallizer, m/s;

g - gravity acceleration, m^2/c;

λ is the friction coefficient;

L - length of the pipeline from the pulsation chamber to the crystallizer, m;

d - pipeline diameter, m;

$\sum \varphi$ - the sum of the coefficients of local resistances in the pipeline.

The other designations are given earlier. That is, the loss of head when moving the mixture from the crystallizer to the pulsation chamber during the purge exhaust is the sum of the loss of head for flow through the nozzles and "holes in the flat wall" - overflows in the baffles and the loss of head in the pipeline connecting the pulsation chamber with the crystallizer.

It should be noted that the liquid pressure in the crystallizer and the pressure in the purge exhaust line are taken equal to atmospheric. The pressure of inert gas to move the crude mixture upwards through the crystallizer (during the pulse) should not be less than the pressure of the liquid column due to the level difference in the body and the pulsation chamber and the loss of head to overcome the hydraulic resistances of the system.

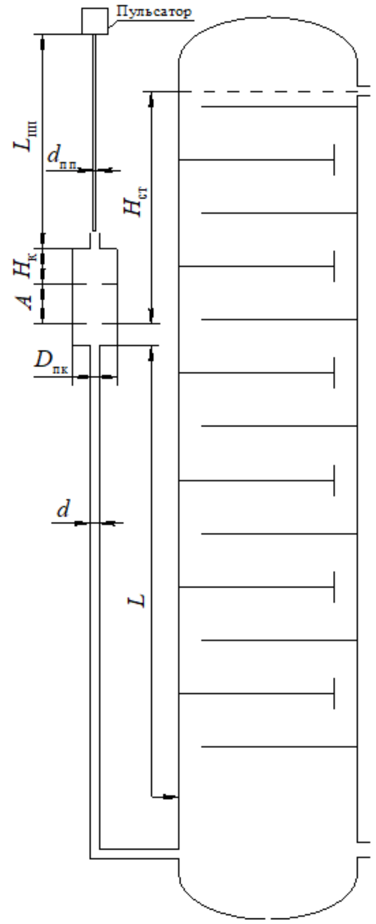

Fig. 3. Diagram of the pulsation mixing crystallizer to calculate the pulsation system

The pressure for overcome the resistance of the pipeline and the body is calculated by analogy with the determination of this value during the purge exhaust:

$$P_r = \rho \cdot g\,\{\sum_{i=1}^{M} {G_{и,i}}^2/(2 \cdot g \cdot M \cdot \rho^2 \cdot t_и^2)\,[1/(\mu_н \cdot \omega_н)^2 + 1/(\mu_n \cdot \omega_n)^2] + W^2/(2g)\,(1 + \lambda L/d + \sum \varphi), \tag{19}$$

This way, the pulse pressure must be at least

$$P_и = P_r + \rho g \cdot H_{ст}. \tag{20}$$

The total gas flow rate (kg/h) for the pulsation will be determined by the formula

$$Q_п = 3600\rho_н \cdot f\left[V_{п.тр}(P_{\max}/100 - 1) + V_{имп} \cdot P_{\max}/100\right], \tag{21}$$

$\rho_н$ is the gas density under normal conditions, kg/м^3 (for inert gas of the dewaxing and deoilizing plants, including mostly nitrogen and carbon dioxide, the calculated density is 1.4 kg/м^3);

$V_{п.тр}$ - volume of the pulsation path, м^3;

$V_{имп}$ - pulse volume in the pulsation chamber, м^3;

$P_{\max}$ - absolute pulsation pressure, kPa.

$P_{\max}$ can be found as the sum of atmospheric pressure (in kPa) and the pressure $P_и$, determined by the formula (20):

$$P_{\max} = P_а + P_и. \tag{22}$$

The volume of the pulse is equal (see Fig. 2):

$$V_{имп} = 0{,}785 \cdot A \cdot D_{пк}^2 , \tag{23}$$

where A is an amplitude of vibrations of the media in the pulsation chamber, m;

$D_{пк}$ - diameter of the pulsation chamber, m.

The volume of the pulsation tube can be defined as the sum of the volume of the pulsation pipe (the tube that connects the pulsator to the pulsation chamber) and the free volume of the pulsation chamber that is not filled with liquid:

$$V_{п.тр} = 0{,}785\ (L_{пп} \cdot d_{пп}^2 + H_н \cdot D_{пк}^2), \tag{24}$$

$L_{пп}$,$d_{пп}$ are length and diameter of the pulse line, m;

$H_н$ - height of the unfilled part of the pulsation chamber, m.

Thus, the calculation of the pulsation system, which is the part of the hydraulic calculation, is performed to determine the inert gas pressure required to implement the pulsation and the installation height of the pulsation chamber (in relation to the level of the slurry in the crystallizer).

Based on the consumed amount of inert gas $Q_п$, the gas pressure per pulsation $P_и$ and the pulsation frequency f, the pulsator parameters are calculated. To assess the energy consumption for pulsation, the specific energy consumption for gas compression and the calculated power for injection are determined.

The specific energy consumption for isentropic compression [4], J/kg, is

$$L_{ад} = k/\ (k\text{-}1) \cdot R \cdot T_1 \left[\left(\frac{P_2}{P_1} \right)^{\frac{k-1}{k}} - 1 \right], \tag{25}$$

$k = C_p/C_v$, for nitrogen $k = 1{,}4$;

R is the universal gas constant, for nitrogen $R = 297$ J/(kg·K);

T_1 - gas temperature, K;

P_2, P_1 is the absolute pressure at the compressor output and input, respectively, kPa.

Then the calculated power for gas injection, kW:

$$N = Q_п \cdot L_{ад} /\ (3600 \cdot 1000 \cdot \eta), \tag{26}$$

where η is the compressor efficiency.

As described above, after the hydraulic calculation, the temperature profile in the crystallizer is refined, taking into account the media pulsation in the crystallizer. The temperature in the section *i* is determined according to its heat balance equation for certain period *t* (the equation is obtained after some simplifications):

$$T_i = (G_{B.i+1} \cdot T_{i+1} \cdot f + G_{и.i-1} \cdot T_{i-1} \cdot f + G_{x.i} \cdot T_{x.i}) / \left[f \left(G_{и.i} + G_{B.i} \right) \right], \tag{27}$$

$T_{x.i}$ is the temperature of the refrigerant supplied to this section.

The other designations are given above and in Figs. 2 and 3. For the first section *i*=1 the temperature is determined by the formula

$$T_{i=1} = \left(G_c T_c + G_{в,п} T_{i=2} f \right) / \left(G_{и,п} \cdot f \right), \tag{28}$$

where T_c is the temperature of the raw material.

The calculation is carried out from section *i*=*M*, where the temperature does not depend on the flow pulsation and is determined only by the final quantity of refrigerant and its temperature, to section *i* =1. Using the method of successive approximations, the temperature calculation from section to section is repeated until the difference between successively determined temperature values in the 1st section is reduced to a specified value.

According to the given methods of heat and hydraulic calculation of the crystallizer, based on the developed mathematical models of the corresponding processes, the optimum sizes of sections of the apparatus and their number, the modes of refrigerant supply to the unit and pulsation, providing a given rate of cooling of raw material flow and intensity of mixing in the sections are determined.

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