THEORETICAL ASPECTS OF THE PROCESS OF COAGULATION OF IMPURITIES IN DISPERSED FLOWS

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Abstract

The article presents theoretical calculations of the process of coagulation of impurities in dispersed flows. The change in the dispersed composition of impurities during coagulation is considered on the basis of the concept of anisotropy of the free path of particles and a special scale of class intervals of the histogram of their size distribution. The probabilities of class intervals are determined by the methods of Markov chain theory.

Key words: coagulation, impurities, dispersed flows, Markov chain theory.

Introduction

In dispersed flows, the suspension-carrying medium has a velocity field, which generates a second velocity field, where there is a new parameter – particle size δ (Khmelev, 2010; Harutyunyan et al., 2004). This parameter is included in the particle velocity distribution. Abbasi et al., 2016). This is a fundamental difference between the kinetics of gas molecules and the kinetics of impurity particles (Asgari, et al., 2017; Osadchuk et al., 2020). If in the kinetic theory of gases, the mean free path does not depend on the direction, then the probability of a particle colliding depends on the direction of its movement (Bird et al., 1974; Gurman, 1973; Mahmood-Fashandi et al., 2017).

This implies the advisability of introducing the concept of anisotropy of the free path of particles. In rotary machines, it is necessary to distinguish between the free paths in the radial and tangential directions, and in the case of plane-parallel motion - in the longitudinal and transverse directions. (Osadchuk et al., 2022). Therefore, in what follows, by the velocity of a particle we will understand one of its components (the one in the direction of which the largest number of collisions occurs). (Osadchuk et al., 2021; Osadchuk et al., 2023).

Results and Discussion

Let us denote $\vartheta(\delta)$ the speed of a particle with diameter δ. Here, by diameter we mean the diameter of the ball, which is equivalent in volume to the particle. At a distance of mean free path λ, an equivalent ball displaces a space having a volume:

$$B = \frac{\pi\delta^2}{4}\lambda$$

Since the volume of a sphere equivalent to a particle is equal to:

$$B = \frac{\pi\delta^3}{6},$$

then during the free run the ball occupied a fraction of the space displaced by it equal to:

$$C = \frac{B_0}{B} = \frac{2\delta}{3\lambda}$$

This fraction is a local model of volumetric concentration, from which the formula for the mean free path of particles follows:

$$\lambda = \frac{2\delta}{3c}, \qquad (1)$$

where c – is the volume concentration of particles in the dispersed flow.

In equality (1) all three quantities have average values. A more accurate formula (1) has the form:

$$\lambda = \frac{2m_3}{3cm_2},$$

where m_2, m_3 – are the initial moments of the particle diameter distribution:

$$m_2 = \int_0^\infty \delta^2 f(\delta) d\delta, \qquad m_3 = \int_0^\infty \delta^3 f(\delta) d\delta$$

$f(\delta)$ – probability density of particle size distribution.

For most impurities, $f(\delta)$ – is t prohebability density of the lognormal distribution law.

To determine the dependence of coagulation efficiency on time, we write down the free travel time:

$$t = \frac{\lambda}{\vartheta}, \qquad (2)$$

where is ϑ – the diffusion velocity equal to the standard deviation,

that is: $\vartheta = \sqrt{D_V}$,

where $$D_V = \frac{1}{\sigma(\delta_{\max} - \delta_{\min})} \iiint_\sigma d\sigma \int_{\delta_{\min}}^{\delta_{\max}} (\vartheta(\delta) - \bar{\vartheta})^2 d\delta,$$

$$\bar{\vartheta} = \frac{1}{\sigma(\delta_{\max} - \delta_{\min})} \iiint_\sigma d\sigma \int_{\delta_{\min}}^{\delta_{\max}} \vartheta(\delta) d\delta,$$

σ – volume of the working area,

δ_{max}, δ_{min} – boundaries of variation of particle diameters.

Taking the free travel time as a unit of discrete time, it is possible to construct matrices of transition probabilities of the Markov chain.

The coagulation of dispersed medium particles is determined by a non-stationary random process with a particle size distribution function for any moment in time. If the range of sizes x_0 π x π x_n is divided into n classes (x_{i-1} π x π x_i, i = 1; 2;….; n) then the state of the system consisting of these classes will be described by the vector:

$$\bar{p}(t) = (p_1(t), p_2(t), \ldots\ldots, p_i(t), \ldots\ldots, p_n(t)), \tag{3}$$

where $p_i(t)$ – is the probability of the particle size belonging to the i-th class at time t.

Thus, studies of particle coagulation can be reduced to the study of systems with a discrete number of states, using for this purpose the theory of Markov chains; a graphical interpretation of the state of the Markov chain is depicted by a histogram of the particle size distribution at time t. To obtain the vector p, it is necessary to determine the class boundaries so that the matrix of transition probabilities p_{ij} has the simplest form, that is, it has the largest possible number of zeros.

It is obvious that p_{ij} = 0 if i φ j. This property follows from the fact that when two particles are glued together, the new particle cannot have an equivalent size smaller than either of them. Let us show that with the relation:

$$\frac{x_k}{x_{k-1}} = \sqrt[3]{2}$$

the diagonal elements of the transition probability matrix are equal to zero. Indeed, if two minimal particles of the i-th class formed a new particle, then the new equivalent diameter δ_j is obtained from the equality:

$$\delta_j^3 = 2\delta_{i-1}^3$$

Where it follows:

$$\frac{\delta_j}{\delta_{i-1}} = \sqrt[3]{2}$$

Therefore, for any two particles δ' and δ'' and from the interval δ_{i-1} π δ π δ_i the following inequality holds:

$$(\delta')^3 + (\delta'')^3 \geq 2(\delta_{i-1})^3 = \delta_i^3$$

Then, under the condition p_{ii} = 0, the matrix of transition probabilities has the form

$$A = \begin{pmatrix} 0..p_{12}p_{13}\ldots\ldots p_{1i}\ldots\ldots p_{1,n-2}p_{1,n-1}p_{1n} \\ 0..0..p_{23}\ldots\ldots p_{2i}\ldots\ldots p_{2,n-2}p_{2,n-1}p_{2n} \\ ------------------ \\ ------------------ \\ 0..0..0\ldots\ldots 0\ldots 0\ldots\ldots p_{n-2,n-1}\ldots p_{n-2,n} \\ 00000\ldots\ldots 0\ldots 0\ldots\ldots 0\ldots\ldots\ldots p_{n-1,n} \\ 00000\ldots\ldots 0\ldots 0\ldots\ldots 0\ldots\ldots\ldots 1 \end{pmatrix}$$

The last row of matrix *A* gives the diagonal element p_{nn} = 1, if the number *n* in is assigned to the class interval x_{n-1} π *x* π ∞.

Let's calculate the transition probabilities of the first row of matrix *A*. To do this, write the class boundaries in ascending order.

$$x_0 \ \pi \ \sqrt[3]{2}x_0 \ \pi \ \sqrt[3]{4}x_0 \ \pi \ 2x \ \pi \ 2\sqrt[3]{2}x_0 \ \pi \ 2\sqrt[3]{4}x_0 \ \pi \ \ldots\sqrt[3]{2^i}x_0 \ \pi \ \ldots \ \pi \ \sqrt[3]{2^n}x_0 \ \pi \ \ldots$$

If particles of the first class combine, then they form particles in the interval

$$\sqrt[3]{2x_0^3} \ \pi \ x \ \pi \ \sqrt[3]{2(\sqrt[3]{2}x_0)^3}\,; \sqrt[3]{2}x_0 \ \pi \ x \ \pi \ \sqrt[3]{4}x_0$$

Similarly, we obtain the intervals of new particles formed as a result of the adhesion of particles of the first class with particles of other classes (Table 1).

Table 1. Intervals of new particles after coagulation involving particles of the first class

J	New particle interval	Interval length
1	$2^{\frac{1}{3}}x_0 \ \pi \ x \ \pi \ 2^{\frac{1}{3}}(1+2^0)^{\frac{1}{3}}x_0$	$\sqrt[3]{2}(\sqrt[3]{2}-1)x_0$
2	$(1+2)^{\frac{1}{3}}x_0 \ \pi \ x \ \pi \ (2(1+2))^{\frac{1}{3}}x_0$	$\sqrt[3]{3}(\sqrt[3]{2}-1)x_0$
3	$(1+2^2)^{\frac{1}{3}}x_0 \ \pi \ x \ \pi \ (2(1+2^2))^{\frac{1}{3}}x_0$	$\sqrt[3]{5}(\sqrt[3]{2}-1)x_0$
.	………………………………………	……………………
.	………………………………………	……………………
.	………………………………………	……………………
J	$(1+2^{j-1})^{\frac{1}{3}}x_0 \ \pi \ x \ \pi \ (2(1+2^{j-1}))^{\frac{1}{3}}x_0$	$\sqrt[3]{1+2^{j-1}}(\sqrt[3]{2}-1)x_0$
.	………………………………………………	…………………………
.	………………………………………………	…………………………
.	………………………………………………	…………………………
N	$(1+2^{n-1})^{\frac{1}{3}}x_0 \ \pi \ x \ \pi \ (2(1+2^{n-1}))^{\frac{1}{3}}x_0$	$\sqrt[3]{1+2^{n-1}}(\sqrt[3]{2}-1)x_0$

Let's denote:

S_{ij} – is the length of the interval obtained as a result of the intersection of the *i*-th class of the histogram with the *j*-th class of Table 1;

l_j – length of the *i*-th histogram class;

L_i – length of the *j*-th interval of table 1.

Each interval of Table 1 can be represented by a linear combination of histogram classes and obtain the equality:

$$\sum_{i=1}^{n} S_{ij} = L_j = (\sqrt[3]{2-1})\sqrt[3]{1+2^{j-1}}x_0$$

The left side of this equality can be transformed to the:

$$\sum_{i=1}^{n} S_{ij} = \sum_{i=1}^{n} \theta_{ij} l_i$$

Where θ_{ij} – is a coefficient whose values lie in the interval [0,1].

After substitution:

$$l_i = \sqrt[3]{2^{i-1}}(\sqrt[3]{2}-1)x_0$$

we find

$$(\sqrt[3]{2}-1)x_0 \sum_{i=1}^{n} \theta_{ij} \sqrt[3]{2^{i-1}} = (\sqrt[3]{2}-1)x_0 \sqrt[3]{1+2^{j-1}} \tag{4}$$

Now we can calculate the transition probability P_{ij}, which is equal to the geometric probability, that is, the ratio of the sum of segments with lengths S_{ij} to the sums of segments with lengths L.

$$P_{ij} = \frac{\sum_{j=1}^{n} S_{ij}}{\sum_{j=1}^{n} L_j}$$

After reductions taking into account (4) we obtain:

$$P_{ij} = \frac{\theta_{ij}}{\sum_{i=1}^{n} \sqrt[3]{1+2^{i-1}}} \tag{5}$$

All transition probabilities P_{ij} are calculated similarly. The concepts of event flux density a_{ij} of a given state system are defined by the relation:

$$a_{ij} = \frac{p_{ij}}{\bar{t}}$$

where is the $\bar{t}$ average free travel time of a dispersed phase particle. For known values of flux densities, calculating vector (3) reduces to solving the system of Kolmogorov equations with initial conditions:

$$P_1(0) = p_{01}; p_2(0) = p_{02}; \ldots; p_n(0) = p_{0n}; \sum_{i=1}^{n} p_{0i} = 1.$$

To calculate the coagulation process, we use (5) and obtain a matrix of transition probabilities:

$$A = \left\| p_{ij} \right\| = \begin{pmatrix} 0..0{,}165..0{,}168..0{,}145..0{,}135..0{,}131..0{,}129..0{,}127 \\ 0..0........0{,}199..0{,}180..0{,}165..0{,}157..0{,}150..0{,}150 \\ 0..0........0........0{,}231..0{,}210..0{,}194..0{,}181..0{,}183 \\ 0..0........0........0........0{,}276..0{,}252..0{,}249..0{,}221 \\ 0..0........0........0........0........0{,}347..0{,}317..0{,}339 \\ 0..0........0........0........0........0........0{,}462..0{,}538 \\ 0..0........0........0........0........0........0........1 \\ 0..0........0........0........0........0........0........1 \end{pmatrix}$$

In these calculations we will use the concentration of impurities c_0 and the mean free

$$l_0 = \frac{2m_3}{3c_0 m_2}$$

Where l_0 – is the average free path of impurity particles before it merges with another particle.

If the average speed of a particle ϑ_0 is equal to, then the travel time is equal to:

$$\tau_1 = \frac{l_0}{\vartheta_0} = \frac{2m_{31}}{3c_0 m_{21} \vartheta_0}$$

The second index of both moments shows the number of the calculation step of the program.

Let us consider in detail the process of changing the granulometric composition of impurity particles as a result of coagulation during the first interval τ_0. According to the theory of Markov chains, during the first step of changing the state of the system, its state vector will become equal to:

$$\overline{P_1} = (P_{01}, P_{02}, P_{03}, \ldots\ldots, P_{08}) * A$$

Here P_{0i} is the class probability of containing a particle in a i class.

$$\sum_{i=1}^{8} P_{0i} = 1$$

Table 2 shows a histogram of the initial particle size distribution. Let's write the histogram data in tabular form:

Table 2. Histogram of initial particle size distribution

N	Class	Probability P_i
1	$\delta_0 - \sqrt[3]{2}\delta_0$	0,02
2	$\sqrt[3]{2}\delta_0 - \sqrt[3]{4}\delta_0$	0,08
3	$\sqrt[3]{4}\delta_0 - 2\delta_0$	0,10
4	$2\delta_0 - 2\sqrt[3]{2}\delta_0$	0,33
5	$2\sqrt[3]{2}\delta_0 - 2\sqrt[3]{4}\delta_0$	0,29
6	$2\sqrt[3]{4}\delta_0 - 4\delta_0$	0,15
7	$4\delta_0 - 4\sqrt[3]{2}\delta_0$	0,02
8	$4\sqrt[3]{2}\delta_0 - \infty$	0,01

Let's write down the matrix – the row of the initial state vector

$$\overline{P_0} = (0{,}02;0{,}08;0{,}10;0{,}33;0{,}29;0{,}15;0{,}02;0{,}01) \quad (6)$$

Using a computer program, we calculate the vector $\overline{P_1}$ by multiplying the row matrix by the square matrix $\overline{P_0}$ of transition probabilities A. As a result of the calculation, a new distribution of larger particles is obtained:

$$\overline{P_1} = (0;0{,}033;0{,}019;0{,}04;0{,}128;0{,}199;0{,}254;0{,}302) \quad (7)$$

So, over time τ_1, the initial dispersed composition (6) due to coagulation processes changed due to the enlargement of particles (7).

First step: $P_1 = P_0 A$

$$\overline{P_1} = (0;0{,}033;0{,}019;0{,}041;0{,}129;0{,}198;0{,}255;0{,}302)$$

$$\Delta P_1 = 1 - 0975 = 0{,}025$$

Second step:

$$\overline{P_1} = (0;0;0{,}007;0{,}01;0{,}021;0{,}061;0{,}148;0{,}729)$$

$$\Delta P_1 = 1 - 097 = 0{,}03$$

The granulometric composition obtained over time is calculated in a similar way.

$$\tau_2 = \tau_1 + \frac{2m_{32}}{3c_0 m_{22}\vartheta_0}$$

After the *n* program steps, the dispersed composition will obey the formula

$$\overline{P_n} = \overline{P_0} * A^n$$

$$\begin{pmatrix} \overline{P_1} = \overline{P_0} * A \\ \overline{P_2} = \overline{P_1} * A = P_0 * A * A = P_0 * A^2 \\ \overline{P_3} = P_2 * A = (P_0 * A^2) * A = P_0 * A^3 \end{pmatrix}$$

The time during which the dispersed composition was formed $\overline{P_n}$ is equal to,

$$\tau_n = \frac{2}{3c_0 V} \sum_{k=1}^{n} \frac{m_{3k}}{m_{2k}}$$

At each step, the probability density $f_k(\delta)$, is calculated, from which both moments are calculated:

$$m_{2k} = \int_0^\infty \delta^2 f_k(\delta) d\delta$$

$$m_{3k} = \int_0^\infty \delta^3 f_k(\delta) d\delta$$

The probability density $f_k(\delta)$ is approximated by smoothing the distribution histogram P_k.

Figure 1 shows the initial particle size distribution.

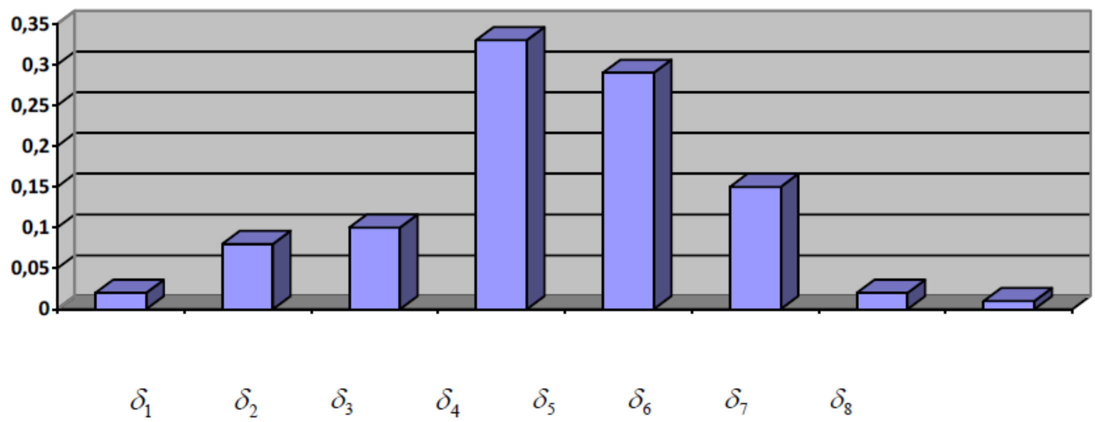

Figure 1. Initial particle size distribution

Following this technique, a table of transition probabilities of particles in class intervals as a result of adhesion after the first collision was calculated. The results presented were used to select the optimal residence time of oil in the working area of the machine.

Conclusion

Theoretical calculations of the process of coagulation of impurities in dispersed flows have been developed. Based on the theory of Markov chains, the probabilities of class intervals are determined.

The process of changing the granulometric composition of impurity particles as a result of coagulation over a certain time interval is considered.

The change in the dispersed composition of impurities during coagulation is considered on the basis of the concept of anisotropy of the free path of particles and a special scale of class intervals of the histogram of their size distribution.

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