Mathematical model of solid impurity coagulation processes in liquid suspensions based on random function convolution operation

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Abstract. Methodology of modeling and identification of mathematical model of process of coagulation of solid impurities in liquid suspensions on the basis of linear mathematical apparatus - convolution of random functions is presented. The non-linearity of the coagulation process is taken into account by the mathematical model of the second level, namely, the time dependence of the weighted random convolution function, which is a characteristic of the type of coagulation and physico-geometric parameters of technical systems for cleaning liquid media. This approach has proven itself in applied problems, provides a solution to the problems of calculating and optimizing cleaning systems for arbitrary initial distributions of the dispersed composition of particles, and is characterized by reduced time and resource costs.

1. Introduction
Process of coagulation of suspension particles in dispersed systems is called coagulation. An important factor in the process of coagulation are the physical mechanisms of convergence and adhesion of particles, which include free molecular (Brownian) motion, diffusion, motion under the influence of electric and magnetic forces or gravitational deposition, etc.

The mathematical theory of coagulation aims to describe the distribution of suspended particles by their size (or mass) as a function of time. The General stochastic coagulation theory is based on discrete and continuous nonlinear integro-differential equations (IMU) (1)-(2) M Smolukhovsky:

\[ \frac{dc_i}{dt} = \frac{1}{2} \sum_{j=1}^{i-1} K_{i,j} c_i c_j \sum_{j=1}^{\infty} K_{i,j} c_j ; \]  

\[ \frac{df(t, m)}{\partial t} = \frac{1}{2} \int_0^m K(m', m-m') f(m') f(m-m') dm' - \int_0^\infty K(m, m') f(m') dm', \]

expressing the concentration \( c_i(t) \) of \( i \)-dimensional particles or the function \( f(t, m) \) of the density distribution of the dispersed composition of the solid phase. In this case, the coagulation mechanisms define a symmetric function \( K(m_i, m_j) \), which is called the coagulation nucleus. The nucleus characterizes the probability (frequency) of collision of particles with masses \( m_i \) and \( m_j \), which is inversely proportional to their lifetime.
Due to the nonlinearity of the IMU of M Smolukhovsky, the problem in general has no solution, for each particular case of the distribution of initial particles, special mathematical studies, individual algorithms and limiting machine resources are required. For magnetic coagulation, the problem in this formulation was not solved [1].

Coagulation is an inseparable process in the technology of purification of aqueous process fluids (VTZH) from solid impurities and ferromagnetic impurities under the action of an external magnetic field. The account of coagulation processes is necessary at design and optimization of cleaners of VTZH from firm impurity. Otherwise, the calculated characteristics of the cleaning efficiency become negligible and do not correspond to the actual ones. However, the calculation of the characteristics of the efficiency of purification of aqueous liquids from solid impurities taking into account coagulation using M. Smolukhovsky equations becomes an insurmountably difficult task. These difficulties are multiplied in problems of optimization of technical means of purification of water technological liquids.

In this paper we consider a new approach of mathematical modeling of coagulation, which is useful in applied problems.

2. Mathematical model of coagulation processes

The kinetics of the coagulation process is based on the approximation of the binary Union of particles with mass \( m_i \) and mass \( m_j \), creating aggregates with mass \( m_k = m_i + m_j \).

If we take an ordered set consisting of \( N \) discrete particles with ordered masses \( m_i = M \cdot i \), where \( i = 1, 2, ..., N \); \( M \) is the sampling interval of the particle masses, then the number of binary aggregates with a fixed mass \( m_k = m_i + m_j \) will be determined by a random law of arrangement of pairs of particles relative to each other with numbers \( i \) and \( j \) and their physical mechanism rapprochement. Note that a fixed value \( m_k = m_i + m_j \) can be realized by several sets of numbers \( i \) and \( j \) (for example, for \( k = 7 \), \( i + j = (1+6); (2+5); (3+4) \)). The set of binary aggregates \( x_k \) with mass \( m_k \) form a discrete random variable \( X \). The probability of the adoption of a random value \( X \) of the mass value \( m_k \) is denoted by \( g^*(nM) \).

If the set consists of arbitrary particles with the distribution \( p_a[nM] \), then the disordered dispersed composition of the particles leads to the formation of an additional number of binary aggregates \( y_k \) of the same mass \( m_k = m_i + m_j \). In this case, the aggregate of an additional number of binary aggregates of mass \( m_k \) form a discrete random variable \( Y \).

The combination of the total number of aggregates \( z_k = x_k + y_k \) with mass \( m_k \) form a discrete random variable \( Z = X + Y \) with a probability of distribution \( p_c[nM] \).

The distribution of the starting particles is independent of coagulation processes. In the approximation of weakly concentrated suspensions, the initial distribution of particles will not affect the coagulation mechanism (in mechanical engineering and in the metallurgical industry, spent VTZH contain no more than 0.01 - 1% solid and ferromagnetic impurities). Therefore, the random variables \( X \) and \( Y \) are independent. Then, the distribution probability of dispersed composition during coagulation in accordance with the provisions of probability theory [2] can be expressed by the convolution \( \sum_{k=1}^{\infty} p_a[kM] g^*(n-kM) \) discrete distribution functions of independent random quantities. Given that there are no negative and zero masses of particles, the convolution formula takes the following form:

\[
p_c[nM] = \sum_{k=1}^{\infty} p_a[kM] g^*(n-kM) . \tag{3}
\]

Similarly, instead of the continuous M Smoluchowski equation as a mathematical model of the processes of coagulation we use the convolution formula for continuous random variables:
\[ f_c(m) = \int_0^m f_u(\eta) g(m - \eta) d\eta, \quad (4) \]

where \( f_c(m) \) – density function of the probability distribution of the dispersed phase by mass during coagulation; \( f'_c(m) \) – probability density function of the distribution of the initial dispersed phase by mass (before coagulation); \( g(m) \) – probability density function of the distribution of the initial dispersed phase by mass (before coagulation).

Convolution operator is a linear operator. In the theory of linear systems, the functions \( g^*[nM] \) and \( g(m) \) included in expressions (3) and (4), respectively, are called weighted functions and represent the responses of the system to normalized impulse actions - on a single sample or on generalized delta function respectively:

\[ \delta[k] = \begin{cases} 1, & k = 0; \\ 0, & k \neq 0; \end{cases} \]

\[ \delta(m) = \begin{cases} \infty, & m = 0; \\ 0, & m \neq 0 \end{cases} \quad (5) \]

The great advantage of the convolution model is the ability to determine the weight function \( g(m) \) (called model identification) from any particular test source distribution of solid particles [3]. For this purpose, solutions obtained on the basis of the equations of M Smoluchowski are suitable, since these equations have an analytical solution for some simple initial distributions of the solid phase [4]. Moreover, the resulting mathematical models will combine the advantages of both methods for describing coagulation processes.

In [5], a technique was developed for identifying the mathematical model of coagulation, which includes four stages: 1 - mathematical modeling of the binary particle fusion probability for a particular discrete initial distribution, the most convenient of which is the equiprobable distribution; 2 - synthesis of a discrete weight function of magnetic coagulation by the method of Z-transformations; 3 - transition to a continuous weight function based on the theorem on counts of V A Kotelnikov; 4 - modeling of the coagulation depth coefficient based on the physical approach based on the average approximation.

In [1], the law of mass conservation was confirmed \( \bar{m}N_v = C = \text{inv} \) during coagulation of the solid phase in a polydispersion medium, where \( \bar{m} \) is the average mass of the aggregates; \( N_v \) – average concentration of the number of impurity particles, \( m^3 \); \( C \) – average mass concentration of impurities, \( \text{kg/m}^3 \).

To characterize the coagulation depth, we introduce the coefficient \( \gamma_c \) of the coagulation depth, which we set as a criterion for the magnetic coagulation process

\[ \gamma_c = \frac{\bar{m}_c}{\bar{m}_u} = \frac{N_v}{N_v}, \quad (6) \]

where the index "c" corresponds to any moment of coagulation, the index "u" to the initial moment.

Further consideration will be carried out on the example of magnetic coagulation of ferroparticles in a uniform external magnetic field. The rigid anisotropy of the magnetic coagulation process, due to the forces longitudinal and transverse relative to the magnetic lines [1], requires taking into account the interaction of only neighboring pairs of particles located along the magnetic lines.

The continuous weight function of magnetic coagulation, defined in [2], has the following form:

\[ g(m) = \frac{2}{(N-1)M} \left[ \sum_{n=1}^{N/2} \frac{\sin \pi (2n - \frac{m}{M})}{\pi (2n - \frac{m}{M})} + \sum_{n=N+1}^{2N-1} \frac{(-1)^n \sin \pi (n - \frac{m}{M})}{\pi (n - \frac{m}{M})} \right], \quad (7) \]

where \( M \) - is the parameter of discretization of the mass of aggregates (a chain of ferromagnetic particles); \( N \) - is the number of samples in the segment \([0, m_m = MN]\); \( m_m \) - is the maximum mass of the unit.
Let us prove the statement (see Appendix) that, during magnetic coagulation, a change in the coefficient of coagulation depth $\gamma_c$ leads to a change in the discretization parameter of the mass of aggregates. Using the formula (A.6) we write:

$$M = \frac{2\bar{m}_u}{N-4} \left[ \frac{\pi \gamma_c (N-1)}{3.7N} + \frac{2}{N} - 1 \right].$$  \hfill (8)

Therefore, the statement is proved.

Expressing $M$ from (8) and substituting in (5), we obtain a mathematical model of the distribution of the dispersed composition of the aggregates of the ferromagnetic suspension during magnetic coagulation, depending on the coefficient of magnetic coagulation depth $\gamma_c$. The value of $N$ is set from the contradictory requirement between the accuracy of the description and the time required to obtain the result.

3. Discussion

Figure 1 shows in graphical form the results of a numerical experiment using the mathematical model (4), (7), (8). The logarithmically normal law of probability density distribution is used as the distribution of the initial particles:

$$f(m) = \frac{\bar{m}_u e^{-4.5s^2}}{3\sqrt{2\pi}m^2} \exp \left\{ -\frac{[\ln(m/\bar{m}_u)]^2}{18s^2} \right\}, \quad s = \ln \left( \frac{\sigma^2}{\bar{m}_u^2} + 1 \right),$$  \hfill (9)

where $\sigma$ - is the variance. From figure 1 it follows that with an increase in the value of $\gamma_c$ the distribution of aggregates by mass is shifted towards increasing mass.

In [6] an example of mathematical modeling of the averaged coefficient of coagulation depth $\bar{\gamma}_c$ for gravitational purifiers of VTZH from impurities is given as the ratio of the average time $T_m$ of the dispersed system stay in the coagulation zone to the average time $\tau_{\nu}$ of the binary union, where the index "$\nu=1, 2, 3, \ldots$ " in the average statistical approximation indicates the number of the act of binary fusion of particles and aggregates in the suspension.

As a result, complete models of the processes of formation and distribution of the dispersed composition of solid impurities during coagulation are obtained, ready for use in practical problems of designing and optimizing effective and economically available purification systems, for example, for cleaning aqueous process liquids from solid impurities.

4. Conclusion

A methodology for modeling and identifying a mathematical model of the process of coagulation of solid impurities in liquid suspensions based on a linear mathematical apparatus, a convolution of random functions, is presented.
The non-linearity of the coagulation process is taken into account by the mathematical model of the second level, namely, the time dependence of the random weight function of the convolution, which is a characteristic of the type of coagulation and physic-geometric parameters of technical systems for cleaning liquid media.

The two-level coagulation model has proven itself in applied problems, it provides solutions to the problems of calculating and optimizing purification systems for arbitrary initial distributions of the dispersed composition of particles and is characterized by reduced time and resource costs.

5. Application
Substituting (7) into (4), we compute:

\[
f_c(m) = \frac{2}{(N-1)M} \int_0^m f_u(\xi) \left[ \sum_{n=1}^{N/2} \frac{\sin \pi \left( 2n - \frac{m-\xi}{M} \right)}{\pi \left( 2n - \frac{m-\xi}{M} \right)} + \sum_{n=N+1}^{2N-1} \frac{(-1)^n \sin \pi \left( n - \frac{m-\xi}{M} \right)}{\pi \left( n - \frac{m-\xi}{M} \right)} \right] d\xi =
\]

\[
= \frac{2}{\pi (N-1)M} \left[ \sum_{n=1}^{N/2} \int_{y_1}^{y_2} f_u \left( \frac{M y}{\pi} - 2nM + m \right) \frac{\sin y}{y} dy + \sum_{n=N+1}^{2N-1} \int_{z_1}^{z_2} f_u \left( \frac{M z}{\pi} - nM + m \right) \frac{\sin z}{z} dz \right];
\]

\[
y = \pi \left( 2n - \frac{m-\xi}{M} \right); \quad z = \pi \left( n - \frac{m-\xi}{M} \right); \quad y_1 = \pi \left( 2n - \frac{m}{M} \right);
\]

\[
z_1 = \pi \left( n - \frac{m}{M} \right); \quad z_2 = \pi n; \quad y_2 = 2\pi n.
\]

The function \( \sin x / x \equiv 0 \) for \( |x| \geq \pi \); therefore, the upper limits of the integrals (10) can be limited to \( y_2 = z_2 = \pi \). The lower limit of integration is \( y_1 = -\pi \) provided that \( m \geq m_{b1} = (2n + 1)M \); the limit \( z_1 = -\pi \) under the condition \( m \geq m_{b2} = (2n + 1)M \). Given the separation of the lower limit of integration

\[
\int_{-\pi}^{\pi} f_u \left( \frac{M y}{\pi} - 2nM + m \right) \frac{\sin y}{y} dy \equiv f_u(m - 2nM) \int_{-\pi}^{\pi} \frac{\sin y}{y} dy \equiv (m - 2nM) \text{Si}(\pi).
\]

In the integral (11), the integrand varies from \( f_u(-M - 2nM + m) \) to \( f_u(M - 2nM + m) \). With a small value of \( M \), the function changes insignificantly; therefore, the average value of this function is chosen. Similarly, we have:

\[
\int_{-\pi}^{\pi} f_u \left( \frac{M z}{\pi} - nM + m \right) \frac{\sin z}{z} dz \equiv 2f_u(m - nM) \text{Si}(\pi).
\]

At \( 0 \leq m \leq m_{b1} = (2n+1)M \); \( 0 \leq m \leq m_{b2} = (n+1)M \) and correspondingly

\[
f_u \left( \frac{M y}{\pi} - 2nM + m_{b1} \right) = f_u \left( \frac{M y}{\pi} - M \right); \quad f_u \left( \frac{M z}{\pi} - nM + m_{b2} \right) = f_u \left( \frac{M z}{\pi} - M \right)
\]

and within the range of variation of the integration variables \( -\pi < y, z \leq \pi \), we obtain negative values \( \pi^1 M y - 2nM + m \leq 0; \quad \pi^1 M z - nM + m \leq 0 \). Then, within these limits, \( f_u \left( \pi^1 M y - 2nM + m \right) = f_u \left( \pi^1 M z - nM + m \right) = 0 \). As you can see, the values of the integrals (11), (12) are the values of the same integrals in the entire range of variation of the integration limits \( (y_1, y_2) \) and \( (z_1, z_2) \), respectively. After substituting (11) and (12) in (10) we obtain

\[
f_c(m) = \frac{4 \text{Si}(\pi)}{\pi (N-1)} \left[ \sum_{n=1}^{N/2} f_u(m - 2nM) + \sum_{n=N+1}^{2N-1} (-1)^n f_u(m - nM) \right].
\]
We calculate the average mass value of the aggregates and the initial polydisperse particles 
\[ m_c = \int_0^\infty m f_c(m) dm, \quad m_u = \int_0^\infty m f_u(m) dm, \]
have:
\[ m_c = 4Si(\pi) \pi (N-1) \sum_{n=1}^{N/2} \int_{-2nM}^{\infty} (\eta + 2nM) f_u(\eta) d\eta + 4Si(\pi) \pi (N-1) \sum_{n=N+1}^{2N-1} (-1)^n \int_{-nM}^{\infty} (\epsilon + nM) f_u(\epsilon) d\epsilon = \]
\[ = 4Si(\pi) \pi (N-1) \sum_{n=1}^{N/2} (m_u + 2nM) + \sum_{n=N+1}^{2N-1} (-1)^n (m_u + nM) \]
\[ = \frac{3.7N}{\pi(N-1)} \left[ m_u \left( 1 - \frac{2}{N} \right) + M \left( \frac{N}{2} - 2 \right) \right], \]
(14)

where \( \eta = m - 2nM, \epsilon = m - nM. \)

When calculating the integrals in (13), we took into account the condition \( f_u(\eta) = 0 \) for \( \eta \leq 0 \) and \( \pi Si(\pi) = 1.85. \)

Expressing \( M \) from (14) and substituting into the expression \( M = m_m N^{-1} \) and taking into account (15) we obtain the dependence of the maximum mass value \( m_m \) on \( \gamma_c: \)
\[ m_m = MN = \frac{2N m_u}{N-4} \left[ \frac{\pi N(N-1)}{3.7N} + \frac{2}{N-1} \right]. \]
(15)

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