Calculating the process of mixing fine-dispersed particles

E V Semenov, A A Slavyanski, I A Nikitin, M V Klokonos

K.G. Razumovsky Moscow State University of Technologies and Management (The First Cossack University), 73, Zemlyanoy Val, Moscow, 109004, Russia

E-mail: m.klokonos@mgutm.ru

Abstract. Mixing is one of the most common processes in food processing, chemical and other industries. This process is carried out in order to accelerate the flow of reactions, to ensure the uniform distribution of solid or liquid particles in the gas or liquid. When mixing, particles of bulk material move chaotically relative to each other in the working volume of the mixing device under the influence of internal and external forces. Due to the complexity of this process, most often the calculated dependencies are based on generalizing experimental data criteria modeling results that have a limited scope of use. Under conditions of significant uncertainty in the kinetics of the processed product in the work, a mathematical description of the mixing process is carried out using the scientific information approach and the entropy method based on this approach. Using this method, the calculation of the kinetics of the process is justified and analytical dependences are proposed for calculating the mixing efficiency of fine powder. On the basis of a meaningful analysis of the data of a numerical experiment, a check is made for the adequacy of the calculation results to the physical meaning of the phenomenon under study.

1. Introduction

In technological processes of food and related industries, many types of raw materials are used in the form of powders. For this purpose, mixing devices (MD) are used, among which the most common are mechanical MD, with rotational movement of the blade: slow-speed (rotation speed \( n < 1 \text{ min}^{-1} \)), high-speed, with (rotation speed \( n > 1 \text{ min}^{-1} \)). Moreover, in most cases, to calculate the mixing process, dependencies based on the results of criteria-based modeling generalizing experimental data are used, which limits the scope of their application.

2. The purpose of the study

Since the kinetics of powder mixing is characterized by significant uncertainty, an entropy method based on an informational scientific approach is used to carry out physical and mathematical modeling of the process [1-10].

3. The object of the study

In accordance with the provisions of this method, the quantitative analysis of the problem considers an elementary volume with a sufficiently large number of fine particles inside the cavity \( x > 0 \) bounded by the PU blades as a half-space (figure 1). In this case, under the conditions of diffusion transfer, the plane \( x = 0 \) simulating the PU blade is taken as the absorbing wall.
If we assume that this wall is in contact with an infinitely large cluster of monodisperse particles with the same counting concentration of \( n_0 \ (1/\text{m}^3) \), then under these conditions, the initial (1) and boundary (2) conditions must be met for the concentration of \( n(x,t) \) particles

\[
\begin{align*}
    n(x,0) &= n_0, \text{ for } x > 0, \\
    n(0,t) &= 0, \text{ for } t > 0.
\end{align*}
\]  

It is necessary, based on the provisions of statistical mechanics, to quantify the process of particle mixing.

![Figure 1](image)

**Figure 1.** The scheme for calculating the distribution of the calculated concentration of particles in the cavity between the blades of the mixing device

4. Materials and methods

4.1. Physics and mathematical simulation of the mixing process based on the entropy method

Assuming that the elemental volume contains a sufficient amount of particles to be considered macroscopic volume, then the density \( \varphi(x) \) of the counting distribution of particles can be introduced by dependence

\[ \varphi(x) = \frac{dn}{n_0 dx}, \]

and the probability that a given volume contains a relative amount of \( n(x) \) of this distribution is

\[ p(x) = \int \varphi(x) \ dx = \frac{n(X < x)}{n_0}, \quad X \in [0,x]. \]  

At the same time, as usual, the probability of \( p(x) \) should satisfy the rationing condition

\[ \int_0^\infty p(x) \ dx = 1, \]  

In addition, under the assumption that the mixing of the powder is characterized by the size of the module of the average deviation of \( x^* \) particles, the dispersion of \( x^* \) is also known.

As a result, according to the provisions of the entropy method, the ratio \( [4] \) is taken as the initial information for (3)

\[ \int_0^\infty p(x) \ x^2 \ dx = x^2, \]  

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In turn, following Janes’ formalism, which characterizes the uncertainty of the distribution of particle concentrations in elementary volume, information entropy is chosen in the form of

$$H = - \int_{0}^{\infty} p(x) \ln p(x) dx,$$

(6)

In the future, according to the principle of maximum entropy, to find a given probability (3) $p(x)$ expression (6) is maximized taking into account the limitations (1), (2), (4), (5), as a task for a conditional extreme, which result in

$$n/n_0 = 2/\sqrt{\pi} \int_{0}^{\infty} \exp (-\xi^2) d\xi = \exp(\lambda x),$$

(7)

where

$$\lambda = 1/(\sigma \sqrt{2}),$$

(8)

$\sigma$ – average quadratic deviation (AQD), $\text{erf}(\lambda x)$ – Integrated probabilities [12].

If in real-world conditions the blade of the MD together with the particles moves in convective transfer progressively with a constant speed $U$, then, in relative motion, replacing the coordinate $x$ by $(x - Ut)$, the ratio (7) is converted into formula

$$n/n_0 = \text{erf}[\lambda (x - Ut)],$$

(9)

where $t$ is time.

Since the subject of the study is the kinetics of the accumulation of fine particulate matter, it is to find the magnitude $x^2$ Einstein’s formula can be used

$$x^2 = 2Dt, D = kTB^2,$$

where $D$ is diffusion ratio, $T$ is temperature, $k$ is Boltzman’s constant, $B$ is mobility [15].

Therefore, the equation (9) is converted to the species

$$n/n_0 = \text{erf}[(x - Ut)/(4Dt)^{1/2}].$$

(10)

where, by analogy with (8) it is accepted $(4Dt)^{1/2} = (\sigma \sqrt{2})$.

As you can see, we have received an informational interpretation of the solution of the problem, namely, the ratio (10) characterizes the counting distribution of particles near the plane modeling the blade of the MD, which is moving progressively at the speed of $U$.

Considering that according to (10) the gradient of concentration on the wall $x = 0$ is calculated according to the formula

$$q(t) = D \frac{\partial n}{\partial x} \bigg|_{x=0} = \frac{D}{\sqrt{\pi t}} \exp[-U^2t/(4D)], 1/(m^2s),$$

the number of particles deposited over time $(t, t + dt)$ per unit wall area is

$$dN(t) = q(t) dt = n_0 \sqrt{D/(\pi t)} \exp[-U^2t/(4D)] dt, 1/m^2,$$

and over a period of time $t$

$$N'(t) = n_0 \sqrt{\frac{D}{\pi}} \int_{0}^{t} t^{-1/2} \exp[-U^2t/(4D)] dt, 1/m^2,$$

(11)

or if this amount is attributed to the volume $1^2 \times l, (l = Ut)$ of settled particles

$$N'(t)/(n_0 l) = J(t),$$

where $N'(t)$ is determined by (11),

\[3\]
\[ J(t, D, U) = \frac{D}{\sqrt{\pi t}} \int_0^t t^{-1/2} \exp\left[-\frac{U^2 t}{(4D)}\right] dt, \]  

(12)

If the physical and mathematical model of the mixing process is based on an analysis of the behavior of two test contiguous sphere layers \( R \leq r \leq \xi \) particles, then near the wall \( x = 0 \) there is a dependence (figure 2) [13]

\[ \xi(R, t, D, U, \varepsilon) = R \cdot [J(t, D, U) \cdot \varepsilon]^{-1/3} \]  

(13)

**Figure 2.** Scheme to calculate the mixing process

where \( R \) is radius of the ball, \( r \) is radial coordinate, \( \xi \) is half the distance between the centres of the balls, with \( c = (1 - \varepsilon), \varepsilon \) - porosity, \( J(t) \) is defined by (12), \( 0 < c < 1 \).

In order to detect the mixing of two adjacent particles in the powder an implicit equation is allowed

\[ \xi(R, t, D, U, \varepsilon) - \Delta x = 0, \]

relatively \( U \), as a process management parameter.

It is allowed that if \( \xi \Delta \leq x \), then the mixing of adjacent particles takes place, otherwise - there is no mixing.

Calculations of the powder mixing process were carried out on the basis of dependencies (12), (13).

4.2 A numerical experiment

As an object of quantitative analysis of the process of mixing powdered substance, sets of particles with radius \( 0.5 \times 10^{-6} \) and \( 10^{-6} \) m were chosen, which is close to, for example, the area of variability of diamond powder variance [18].

5. Discussion of the results

Consistency of the graphed figure 3 results of calculating the physical meaning of the phenomenon under study derives from a comparative analysis of the position of the curves in this figure.
Figure 3. Dependences of the speed $U$ of convective particle transfer at different porosity $\varepsilon$ of the powder and the radius $R$ of the particle on the time $t$ of the mixing process ($R = 0.5 \times 10^{-6}$ m, $D = 2.74 \times 10^{-11}$ m$^2$/s, $\Delta x = 5.9 \times 10^{-6}$ m: 1 – $\varepsilon = 50$; 2 – $\varepsilon = 75$%; $R = 10^{-6}$ m, $D = 1.27 \times 10^{-11}$ m$^2$/s, $\Delta x = 4.02 \times 10^{-6}$ m: 3 – $\varepsilon = 50$; 4 – $\varepsilon = 0.75$%)

For example, bearing in mind that diffusion transfer, and therefore mixing, in smaller particles, compared to large particles, is more intense, this transfer proceeds with a higher portable speed $U$ (curve 1 above the curve 3 on figure 3). As a result, the mixing processing period for smaller particles is completed faster than for larger particles.

Overall, as can be seen from the data fig. 3, the process of diffusion mixing of finely dispersed particles proceeds quite quickly under conditions of relatively low, not exceeding 1-2 sm/s, portable speed.

6. Conclusion

On the basis of the study, the prerequisites were created to use the obtained dependencies based on the diffusion model for calculating the mixing process of fine particles. The numerical effect on the efficiency of the process of mixing this substance of weight concentration, size and speed of convective particle transfer has been revealed.

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References

[1] Braginsky L H, Begachev V I and Barabash V I 1984 Stirring in Liquid Environments Leningrad: Chemistry 336
[2] Pischikov G B 1997 To the theory of mixing microorganisms in diffusion-type devices Storage and processing of agricultural raw materials 2 20-22
[3] Fangs M V and Alushkina T V 2019 Simulation of fluid flowing and mixing in columns of mass-exchange machines with mounds Chemical and oil and gas engineering 10 3-7
[4] Jaynes E T 1963 Information Theory and Statistical Mechanics New York, Benjamin: Statistical Physics 181
[5] Tribus M 1970 Thermostatics and thermodynamics M: Energy 504
[6] Wilson A J 1978 Entropy methods of modeling complex systems M: Science 248
[7] Mikomov V P 1981 Entropy modeling techniques in chemical technology M.: MIHM 159
[8] Kafarov V V 1985 Cybernetics techniques in chemistry and chemical technology M.: Chemistry 468
[9] Bajkova A T 1992 The generalization of maximum entropy method for reconstruction of complex functions Astronomical and Astrophysical Transactions 1 (4) 313-320
[10] Jaynes E T 1996 principle of maximum entropy, in maximum-entropy and bayesian methods in applied statistics Cambridge University Press: Cambridge 26
[11] Golitsyn G A 1997 Information and creativity M.: The Russian world 304
[12] Rudoy J G 2003 Generalized information entropy and non-canonical distribution in equilibrium statistical mechanics Theoretical and mathematical physics 135 (1) 3–54
[13] Schennach S M 2005 Bayesian Exponentially Tilted Empirical Likelihood Biometrika 92 (1) 31-46
[14] Semenov E V, Karamzin V A and Novikova G D 2002 Methods of calculations of hydromechanical processes in the food industry M.: MSUPP 492
[15] Bronstein I N and Semendayev K A 1986 Mathematics handbook for engineers and students in the tues M.: Science 544
[16] Babakin B S, Voronin M I, Semenov E V, Belozero G A and Babakin S B 2018 Quantitative analysis of the cooling process of the refrigeration vehicle using frozen developed surfaces Chemical and oil and gas engineering 54 (4) 16-18
[17] Semenov E V, Slavianskii A A, Karamzin V A and Karamzin A V 2019 Implementation of the process of centrifugal particle fractionaing Chemical and oil and gas engineering 2 22-25