Features of optimization synthesis of equipment for feeding nanodispersed materials

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Abstract. For the first time, in the analysis of the behavior of a nanodispersed material (i.e., its outflow and batching from the hopper unit, as well as movement and mixing), a conventional approach was used to calculate the hardware and technological design of its functionalization. Besides, the features of the behavior of the nanodispersed layer and single nanoparticles as applied to the feeding process from the hopper under vibrations, its movement along the guide blade and the pouring of the flow into the receiving tank were considered, dependencies were formulated, and recommendations were given for designing the hopper assembly used to process the nanodispersed materials. The results were tested and showed high convergence in practical implementation.

1. Introduction

Today, nanotechnologies are smoothly moving from the category of basic and theoretical research, laboratory and demonstration samples to the category of pilot and mass production, which implies stable product quality - whether it be carbon nanomaterials (CNMs) directly, or equipment for their production or processing. At the same time, not the CNMs themselves, but the hardware and technological design of the production process comes out on top, providing guaranteed characteristics of the resulting construction or functional nanomaterial. Medicine and pharmacology, powder metallurgy, as well as sorbent, polymer and construction material production, represent just a small list of areas where knowledge of the physical-mechanical characteristics of nanodispersed materials (NDMs), consisting of a continuous gas or liquid medium and dispersed nanoparticles, and the features of process equipment under their application, considering scaling and the actual production conditions, is in demand [1,2].

A large number of works are devoted to studying the characteristics of NDMs. The authors mark a complete analogy in the properties of these materials and particulate bulk materials (including powders and industrial dusts) [3,4]. So, for example, the influence of the electrostatic properties of nanosized materials on the processing process was considered in the paper [6]. The general physical-mechanical characteristics of single nanoparticles and the laws of their movement were discussed in [10], and in [5], the hygroscopicity and density of the nanomaterials as applied to transistors and microelectronics were determined. However, only certain NDMs characteristics are considered in relation to laboratory research, and not all their parameters, as well as operating conditions and equipment calculation, are taken into account, i.e. there are no works devoted to the practical use of NDMs [5-11].
Thus, the goal of this work is to apply classical approaches to the calculation and design of technological equipment for the nanoindustry, as the most dynamically developing area of innovative materials and technologies.

2. Modeling NDMs in calculations of typical equipment

The authors of the present work examined the design of a feeding unit device for a nanodispersed system consisting of a bunker, a vibration bottom and an inclined blade, and carried out an optimization synthesis to combine single units, each of which provides a specific state of the nanoparticle layer. The following stages of the NDMs state were taken as assumptions: in the bunker - the layer is fixed (nanoparticles are in constant contact with each other); on the vibration bottom – the nanoparticles are in the vibro-fluidized bed (chaotic nanoparticle motion); on the inclined blade – the nanoparticles are in the rolling layer (ordered layered motion); the detachment from the blade edge and the nanoparticle fall in the fan represent a free single-particle motion (up to the logjam).

Let us consider in more detail the stages of the nanodispersed system motion on the example of the above-mentioned bunker device (figure 1).

![Figure 1](image1.png)

Figure 1. A pattern of the NDM motion at the outflow from the bunker device. 1 – NDM; 2 – bunker; 3 – vibration bottom; 4 – lead blade.

![Figure 2](image2.png)

Figure 2. A diagram of forces acting on the nanoparticle when applying vibration.

At the first stage of feeding, the NDM 1 flows out of the bunker 2 onto the lead blade 4 along the vibration bottom 3, which, in our case, is used to equalize the flow rate and destroy arching.

Let us consider the vibration bottom as a plate (figure 2) oscillating with frequency $\omega$ and amplitude $A$ in the direction forming angle $\beta$ with the vertical axis [12,13]. The nanoparticle of mass $m$ is acted upon by the gravitation force $P=mg$, the friction force $F_F$ along the plate surface, the normal surface reaction $N$, and the inertia force $I$. The nanoparticle motion relative to the vibration bottom is described by the following equations:

$$m\ddot{x} = mA\omega^2 \cos \beta \sin \omega \tau - mg \sin \alpha - F_F$$  

$$m\ddot{y} = mA\omega^2 \sin \beta \sin \omega \tau - mg \cos \alpha + N$$

If the NDM is fed onto the vibration bottom, but does not come off from it, then the acceleration of the material relative to this surface is equal to $\ddot{y} = 0$. Then, from equation (2), it follows:

$$N = mg \cos \alpha - mA\omega^2 \sin \beta \sin \omega \tau$$

Numerous studies [13–16] have shown that during the vibration exposure, the properties of the nanodispersed system layer change significantly with the onset of the detachment of nanoparticles from each other and from the vibrating surface, on which they are located. Prior to the beginning of the separation, the NDM is liquefied on the vibrating surface.
After the onset of the detachment, with an increase in the intensity of oscillations, arbitrary motion of the NDM begins, the layer “boils up”, i.e. its porosity increases. The material nanoparticles are detached from the vibration bottom, when the normal reaction is \( N=0 \). Then, according to equation (3), we get the following:

\[
A_{\omega c} \omega^2_c = \frac{g}{\sin \omega \tau} \cdot \frac{\cos \alpha}{\sin \beta}
\] (4)

where \( \omega_c \) is the critical frequency. From equation (4), it can be seen that the minimum critical vibration acceleration of the vibration bottom, at which the nanoparticle separation occurs, will be at \( \sin(\omega \tau) = \pm 1 \). At these moments, the relative critical vibration acceleration is equal to:

\[
\frac{A_{\omega c} \omega^2_c \sin \beta}{g \cos \alpha} = \pm 1
\] (5)

As can be seen, for the nanodispersed system exposed to vibration, the transition of the layer to vibration liquefaction depends not on the nanoparticle mass, but on the vibration acceleration \( (A \omega) \) of the bottom. This makes it possible to control the vibration liquefaction and, accordingly, the porosity in the boundary layer of the material by adjusting the amplitude and frequency of the vibrator.

Thus, regarding the NDM mass effect, neglected when considering the motion of a nanoparticle along the vibration bottom, it is necessary to maintain a number of boundary conditions (assumptions):

1. The NDM is not detached from the vibrating surface (subject to the condition \( N>0 \));
2. The controlled liquefaction of the nanoparticle boundary layer occurs;
3. The destruction of arching occurs in the flow bulk;
4. The porosity remains constant in the NDM bulk, since its increase (nanoparticle liquefaction in the boundary layer along the vibration bottom) is compensated by compaction above the underlying layer due to vibration.

From the above, it is clear that the vibration will affect the flow indirectly, i.e. it will only “equalize” the flow rate, making the flow stable. Then, the nanoparticle rate \( v \) can be determined as follows:

\[
v = \lambda \cdot \sqrt{3.2 g R}
\] (6)

where \( R \) is the hydraulic radius of the hole (slit) of the outflow \( R=F/L \); \( g \) is the gravitational acceleration; \( \lambda \) is the outflow coefficient; \( L \) is the perimeter of the hole (slit). The rectangular area \( F \) is expressed as follows:

\[
F = (A - a')(B - a')
\] (7)

where \( A \) and \( B \) are the rectangle sides; \( a' = kd \); \( d \) is the particle diameter; \( k=1.25-1.70 \) (coefficient).

Considering equation (7), \( R \) can be defined as follows:

\[
R = \frac{A - a'}{2(A + B - 2a')}
\] (8)

At the second stage of the motion, the NDM comes from the vibration bottom to the lead blade. The equation expressing equilibrium for the NDM moving at angle \( \alpha \) to the horizon:

\[
\ddot{x}m + f_{Tp}mg \cos \alpha - mg \sin \alpha = 0
\] (9)

where \( \ddot{x} \) is the acceleration of the nanoparticle motion, which is determined as follows:

\[
\ddot{x} = f_{Tp}mg \cos \alpha - mg \sin \alpha
\] (10)

Consistently integrating equation (10), we obtain the expression for determining the rate of the NDM motion and the distance it has traveled:
under the following boundary conditions:

\[ \dot{x} = v_0, \tau = 0, \Rightarrow c_1 = v_0 \quad (12) \]

\[ \dot{x} = v_0 + g(\sin \alpha - f \cos \alpha)\tau \quad (13) \]

Next, we write the equation of the distance traveled along the guide blade by integrating equation (13):

\[ x = v_0\tau + \frac{1}{2} g(\sin \alpha - f \cos \alpha)\tau^2 + c_2 \quad (14) \]

where \( c_2 = 0 \) is the integration constant under the initial conditions; \( \tau = 0; x = 0 \).

Thus, equation (14) takes the following form:

\[ x = v_0\tau + \frac{1}{2} g(\sin \alpha - f \cos \alpha)\tau^2 \quad (15) \]

Being in the rolling layer on the lead blade, the NDM increases the porosity. The degree of loosening can be characterized by the loosening coefficient \( K \). It is an important parameter which determines the ratio of elemental volumes of the NDM in the bunker and in the flow moving along the lead blade. To obtain this value, it is necessary to find the average flow rate \( \dot{x}_{av} \):

\[ \dot{x}_{av} = \frac{\int_0^L \dot{x} \partial Q}{\int_0^L \partial Q} \quad (16) \]

where \( \dot{x} \) is the function of the nanoparticle rate in the flow depending on the distance traveled; \( \partial Q \) is the material amount on the lead blade. The NDM volume on the lead blade \( V_{lb} \) can be determined by the following formula:

\[ V_{lb} = L \int_S dS \quad (17) \]

where \( L \) is the length of the lead blade; \( S \) is the integration area, \( i.e. \) the surface area of the lead blade. Analyzing equation (16) for the average rate and simplifying it, we can write the following:

\[ \dot{x}_{av} = v'_{av} = \frac{L_{av}}{\tau_{av}} \quad (18) \]

where \( L_{av} \) is the average distance traveled by the \( i^{th} \) nanoparticle along the blade; \( \tau_{av} \) is the average time spent by the \( i^{th} \) nanoparticle for traveling. Whence it follows that the loosening coefficient for the NDM flow moving along the blade is equal to:

\[ K = \frac{v'_{av} \cdot h_L}{S_r} \quad (19) \]

where \( h_L \) is the thickness of the flow at the edge of on the edge of falling off the blade; \( S \tau \) is the area of the nanodispersed layer overlooking the falling-off line during traveling the length by the nanoparticles.

At the third stage of the NDM motion, free falling off the lead blade occurs. To analyze this motion, it is necessary to introduce the following assumptions confirmed in some papers [4,7,9]:

\[ \dot{x} = (g \sin \alpha - f_{Tp} \cos \alpha)\tau + c_1 \quad (11) \]
1. The nanoparticles fall off the blade as a flow consisting of a series of sublayers, with a thickness of each one determined by the average nanoparticle size.

2. At the time of the detachment from the blade, the nanoparticles of the same sublayer have the similar rate.

3. At the time of the detachment, the nanoparticle rate increases along the flow thickness, as the distance from the falling-off edge increases.

As a consequence of these assumptions, it follows that after the detachment from the blade, the nanoparticles do not collide with each other, so the “single-particle” approach can be employed to study the motion [17].

The motion of the nanoparticle in free fall after the detachment from the lead blade can be considered as a body motion in a gravitational field at some initial rate. The equation of the trajectory of the $i$th nanoparticle can be written as follows:

$$
\begin{align*}
\alpha \tau \cos \alpha & = -h_i \sin \alpha - v_i \tau \cos \alpha \\
\alpha \tau \sin \alpha & = h_i \cos \alpha - v_i \tau \sin \alpha - \frac{g \tau^2}{2}
\end{align*}
$$

where $x$ and $y$ are the current coordinates of the moving nanoparticle; $h_i$ is the distance between the nanoparticle and the falling-off edge of the lead blade at the time of the detachment, in the direction normal to the particle rate vector; $\alpha$ is the angle between the rate vector $v_i$ and the horizon; $\tau$ is the current time from the moment of particle detachment from the lead blade.

As noted before, the nanodispersed layer moving along the lead blade has a section close to rectangular. For a particle located at the lower boundary of the layer, $h_i = 0$ and $v_i = v_L$. The lower boundary of the nanoparticle incidence fan can be described by the following equations:

$$
\begin{align*}
\alpha \tau \cos \alpha & = 0 \\
\alpha \tau \sin \alpha & = h_i \cos \alpha - v_i \tau \sin \alpha - \frac{g \tau^2}{2}
\end{align*}
$$

For a particle moving along the upper boundary of the layer, $h_i = h$ and $v_i = v_U$. The upper boundary of the fan can be described by the following equations:

$$
\begin{align*}
\alpha \tau \cos \alpha & = -h_i \sin \alpha - v_i \tau \cos \alpha \\
\alpha \tau \sin \alpha & = h_i \cos \alpha - v_i \tau \sin \alpha - \frac{g \tau^2}{2}
\end{align*}
$$

The fan surface $S$ of the NDM falling off the lead blade is expressed as follows:

$$
S = (L_U + L_L)L_W
$$

where $L_U$ is the length of the upper boundary of the fan from the falling-off edge of the lead blade up to the open surface of the logjam; $L_L$ is the length of the lower boundary of the fan; $L_W$ is the width of the blade.

The lengths $L_U$ and $L_L$ can be found from equations (22)-(25) through curvilinear integrals in the following form:

$$
L_{(U,L)} = \int_L f(x; y) dL
$$

The integral expressed by equation (27) can be transformed into an ordinary integral by substituting into the integrand:

$$
x = x(\tau); \ y = y(\tau) dL = \sqrt{[\dot{x}(\tau)]^2 + [\dot{y}(\tau)]^2} d\tau
$$
after which you can take the integral in the measurement interval $\tau$, which corresponds to the integration line.

The time of falling off the lead blade for the nanoparticles $\tau_f$ is determined from the moment of their detachment from the blade up to the moment of contact with the open surface of the logjam. To define the numerical value of $\tau_f$, it is required to combine the solution of the equation of the trajectory of the nanoparticle incidence (expressions (20) and (21)) and the equation of the open surface of the logjam.

The open surface of the logjam has a complex shape, and to date, there are no dependencies describing this boundary. The comparison between the experimental and calculated values, with an accuracy sufficient for engineering calculations, showed that when determining the time of the nanoparticle fall from the blade, the equation of the open surface of the logjam can be taken in the following form:

$$ y = x \cdot \tan \alpha_f $$

where $\alpha_f$ is the angle between the open surface of the logjam and the horizon.

Solving equations (20), (21) and (28) jointly, we can obtain the following dependencies to determine the coordinates of the point of the intersection of the trajectory of the falling nanoparticle with the open surface of the logjam and the time of the nanoparticle fall.

$$ x = -h_i \sin \alpha - v_i \cos \alpha \left( M + \sqrt{M^2 - N} \right) $$

$$ y = h_i \cos \alpha - v_i \sin \alpha \left( M + \sqrt{M^2 - N} - \frac{g}{2} \left( M + \sqrt{M^2 - N} \right)^2 \right) $$

$$ \tau = M + \sqrt{M^2 - N} ; $$

$$ M = \frac{1}{g} \left( v_i \cos \alpha + \tan \alpha_f - v_i \sin \alpha \right) $$

$$ N = \frac{2}{g} \left( h_i \cos \alpha - h_i \sin \alpha \cdot \tan \alpha_f \right) $$

$$ \alpha_f = \arctan \frac{y}{x} $$

Substituting the values of $v_i$ and $h_i$, obtained for the nanoparticles moving along the upper and lower boundary of the flow, into expression (31), we can find the upper integration limit for expression (27). In this particular case, the lower limit is equal to 0.

To determine the particle incidence rate, when they fall from the blade, it is necessary to differentiate equations (20) and (21) by time:

$$ V_H = v \cos \alpha $$

$$ V_V = v \sin \alpha + g \tau $$

where $V_H$ and $V_V$ are the horizontal and vertical components of the nanoparticle motion rate, respectively.

The absolute modulus $v$ of the nanoparticle motion rate is defined as follows:

$$ v = \sqrt{V_H^2 + V_V^2} $$

To assess the motion rate of the nanoparticle when it passes through the horizontal section 1-1, lagging behind the falling-off edge directed at distance $H$ (figure 3), it is required to substitute the value $y=H$ into equation (22), find the value of $\tau$, and determine the values of $V_H$ and $V_V$ using equations (32) and (33).
Figure 3. Determining the loosening coefficient for the NDM in the fan.

Earlier, it was noted that when falling off the lead blade, the NDM flow is loosened. By analogy with the loosening coefficient in the rolling layer, the loosening coefficient $K$ for the NDM flow falling off the blade can be represented as a ratio of the volume $V_g$ of the NDM amount $Q$ in motion, to the volume $V_P$ occupied by the lead blade.

To clarify the causes of the loosening of the incident NDM flow, we consider the loosening of the flow in the horizontal and vertical directions. When determining the loosening coefficient $K_H$ for the horizontal direction, it is necessary to take into account the fall of nanoparticles 1 and 2 located in different rate sublayers on the blade.

The distance $L_2$ between the centers of gravity of the nanoparticles in the horizontal direction, when they pass through the section $P-P$ held horizontally through the falling-off edge of the lead blade, can be determined from the following expression:

$$L_2 = \frac{V_2^2 \cos \alpha \cdot \sin \alpha}{g} + V_2 \sqrt{\frac{V_2^2 \cdot \sin^2 \alpha}{g^2} + 2h \cdot \cos \alpha}$$ \hspace{1cm} (35)$$

where $V_1$ and $V_2$ are the motion rates of nanoparticles 1 and 2, respectively, at the time of their detachment from the lead blade; $\alpha$ is the angle between the rate vectors and the horizon; $h$ is the distance between the center of gravity of nanoparticle 2 and the falling-off edge of the blade, in the direction normal to the nanoparticle motion rate vectors. The distance $L_1$ between the points of the intersection of the trajectories of the nanoparticle incidence with the horizontal section 1-1 can be determined as follows:

$$L_1 = \frac{V_2^2 \sin \alpha}{g} + V_2 \sqrt{\frac{V_2^2 \sin^2 \alpha}{g^2} + 2 \cdot (h \cos \alpha + H)} + V_1 \sqrt{\frac{V_1^2 \sin^2 \alpha}{g^2} + 2H}$$ \hspace{1cm} (36)$$

Given that the loosening of the NDM at the falling-off edge of the blade is insignificant, the numerical value of the loosening coefficient $K_H$ for the section 1-1 can be obtained from the following relation:

$$K_H = \frac{L_1}{L_2}$$ \hspace{1cm} (37)$$

To determine the loosening coefficient $K_V$ for the vertical direction, it is necessary to consider the fall of nanoparticles 2 and 3 detached from the blade one by one from the same sublayer. At the moment of the detachment from blade, the nanoparticles have the same motion rate, but nanoparticle 3 is detached later than nanoparticle 2. The lag time $\tau_{32}$ can be determined from the following expression:

$$\tau_{32} = \frac{L_{32}}{V_3}$$ \hspace{1cm} (38)$$
where $L_{32}$ is the distance between the centers of gravity of the nanoparticles in the direction of their motion at the moment of the detachment of nanoparticle 2.

For some time $\tau$ passed from the moment of the detachment of nanoparticle 3 from the lead blade, the distance between the centers of gravity in the horizontal direction can be determined as follows:

$$L_\tau = v_2 \cdot \tau_{32} + \frac{g \tau_{32}^2}{2} + g \tau_{32}$$  

(39)

From equations (37) and (39), it follows that the loosening of the NDM in the fan varies in width and height.

When carrying out practical calculations, it is more convenient to use the volume loosening coefficient $K$:

$$K = \frac{V_M}{V_R}$$  

(40)

where $V_M$ is the volume occupied by a certain amount of the moving material; $V_R$ is the volume occupied by the same amount of the material at rest.

Let us consider in more detail the definition of the volume loosening coefficient. Let for some time $\tau$, the NDM amount $q$ falls off the blade. This amount, being on the lead blade, occupied the volume $V_R$ according to equation (17):

$$V_R = L \int_S dS$$  

(41)

When passing through the section 1-1, the volume $V_M$, occupied by the material amount $q$ in motion, can be determined from the following expression

$$V_M = L_1 \cdot L \cdot v_{av} \cdot \tau$$  

(42)

where $L_1$ is the width of the fan in the section 1-1; $v_{av}$ is the vertical component of the average motion rate of the material when it passes through the section 1-1. After substituting equations (41) and (42), expression (40) takes the following form:

$$K = \frac{L_1 \cdot v_{av} \cdot \tau}{\int_S dS}.$$  

(43)

3. Discussion

Analyzing the NDM motion from the bunker, first along the vibration bottom, then, along the lead blade, and finally, when falling in the fan, a number of conclusions and assumptions were made as for the properties of the moving layer of the material. In this regard, one can say that the nanoparticle motion rate along the height of the material flow fan will increase. The flow loosening coefficient (porosity of the nanoparticle flow) will be directly proportional to the height and rate of the nanoparticles when the NDM falls. The acceleration rate of the flow on the lead blade will be affected by the inclination angle, apart from the physical and mechanical properties of the NDM. The width of the opening of the NDM flow fan will change only to a certain height, and after that, it will remain almost constant; the area of the gap and the angle of the lead blade inclination will affect the performance of the feeder, whereas the effect of the NDM physical and mechanical properties will be reduced due to the vibration.
4. Conclusion

Thus, when analyzing the NDM behavior, a conventional approach was used for the first time to calculate the industrial technological equipment. Besides, the features of the behavior of a nanodispersed layer and single nanoparticles were considered as applied to single elements of the technological equipment. Moreover, again for the first time, dependencies were formulated and recommendations were given for designing a bunker assembly used for the functionalization of the NDMs. As a result, a general approach to the optimization synthesis of equipment for feeding nanodispersed materials based on a three-stage method is proposed. The features of the behavior of the nanodispersed layer at each stage when feeding the NDMs from the hopper to its subsequent processing are established.

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