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On Modeling the Swarming in Dispersed Systems

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The paper is devoted to modeling the swarming of micro and nanoparticles in dispersion flows. A systematic analysis of the swarming phenomenon is presented, and approaches to the creation of generalized swarming models for describing the mentioned phenomena are offered for discussion. Based on the review of various works and speculative analysis, for the first time it is proposed to distinguish three main different mechanisms of swarm formation in dispersed mixtures. These mechanisms determine the swarming processes in wide range of particles sizes: from nanoparticles to small dust particles. The results of computer simulation and numerical experiments for describing swarming phenomenon proceeding by the inertial mechanism using both the computer fluid dynamics (CFD) simulation and the stochastic lattices approach adapted especially in the submitted work for describing swarming phenomenon have been also submitted.

1. Introduction

Since the term swarming is used in the study of various issues (Carrillo et al., 2010, Naldi et al., 2010), it is necessary to clarify that in this work, swarming is understood as the formation of moving areas with an increased concentration of the dispersed phase in flows (Bouffanais, 2016). This problem is clearly poorly understood from the point of view of creating generalized models and universal approaches (Rimer & Ariel, 2017). The swarming phenomenon can occur in various processes in which the particles of the dispersed phase are entrained by the flow of a continuous medium. Swarming is observed both in flows of microparticles and in nano-dispersed systems (Pirani et al., 2013). Applying to nanosystems the following examples can be noted: when modelling processes in intracellular environments (Weber et al., 2015), in biology and biotechnology when modeling the migration and aggregation of cellular systems (Brückner et al., 2019,), under modeling and design of mechatronic systems too (Su et al., 2018).

1.1 Speculative analysis of the phenomenon

Hypothetically, three main different mechanisms of the formation of a swarm of particles in a continuous flow of a dispersed mixture can be proposed.
The first swarming mechanism may be due to a change in the structure of the flow of a continuous carrier medium in the volume of the apparatus (Schmidt et al., 2006). Such a mechanism can apparently be called as inertial swarming. The second mechanism is due to the influence of singularities or attracting (repulsive) centers in the volume of the apparatus (Satyobroto Talukder, 2011). Such a mechanism can be called as attractive swarming. And, finally, the third mechanism of this phenomenon is due to the presence of interaction forces acting between the particles of the dispersed mixture in the flow of a continuous medium (Carranza & Coates, 2000). This mechanism can be called as interacting swarming. Each of the noted mechanisms has its own characteristic features (Bees et al., 2000).
Inertial swarming can be accompanied by separation of the dispersion flow, i.e. (*id est*), by creating several swarms with different particle size and masses (orders) distribution functions. By this the initial general distribution function transforms into several functions for different swarms (Figure 1 (A)). The inertial swarming mechanism is used for the separation of polydisperse systems with microparticles and larger particles (Carranza & Coanes, 2000). Attractive swarming, in turn, can proceed according to various scenarios. The first, force scenario, is realized by the influence of the force changing particles trajectories in direction to or from the singularity dot (Figure 1 (B)). The second scenario can be called a signal scenario. In this case, the

singularity generates signals that affect the behavior of particles in the flow. Under the signal scenario, it is necessary to consider the characteristic time of the particle reaction to the signal. The formation of a swarm during the movement of its constituent particles in the direction of the concentration gradient of some substance in the continuous phase can be attributed to the same type. Another scenario of attractive swarming is possible when information signals are transmitted from particle to particle with indicating the direction to the attractor. Such a scenario may, in particular, be realized in the case of particles in biotechnological systems (Bees et al., 2000, Brückner et al., 2019). Simulation of the interacting swarming leads to the classic many-body problem (Fellner & Raoul, 2011).

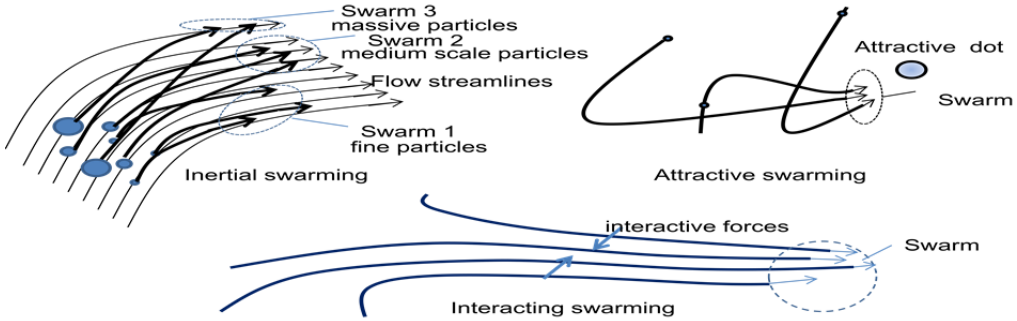


Figure 1: Illustration of the behaviour of dispersed phase particles in inertial and attractive types of swarming

Of course, in the given system, various mechanisms and swarming scenarios can be implemented simultaneously. The swarming process can be accompanied by the aggregation of particles with the formation of clusters with a complex internal structure (Brener, 2006), or it can occur without aggregation. In the first case, i.e., when aggregated clusters are formed, their aggregation activity may depend on both the order of the clusters and of their ages too (Mogliner & Edelstein-Keshet, 1999). The term "age of a cluster" (Brener & Dil'man, 2016) is here understood as the time that elapsed from the moment of completion of its primary formation to the moment of changing its size or order, i.e., to the moment of changing the number of its constituent nanoparticles or the internal structure. Cluster age plays an important role in the aggregation process, because affects its morphology and aggregation activity (Brener & Dil'man, 2016). In this case, the kinetic equations for aggregation process should be non-Markovian (Zabrocki et al., 2006). The manifestation of memory effects in non-Markov processes can significantly transforms the kinetic equations, which, in particular, leads to the appearance of nonlinear wave solutions. This problem applying to the swarming phenomenon will be the subject of further research by the authors.
At the same time, the swarming process itself can be considered as a version of weak (correlative) aggregation, when the connection between the particles that make up the swarm is determined by correlating the spatial coordinates and velocities of the swarm particles (Kim & Brener, 1986). Further in this work, the main attention is paid to the inertial type of swarming, the description of which is very important for the correct calculation of many technological processes. The contribution of the work lies also in that two approaches to modeling this phenomenon are presented, and their features, advantages and disadvantages are shown.

2. Theoretical details and simulation of the inertial swarming

2.1 Governing equations for CFD approach

It is hard to propose in any form a satisfactory generalized model of inertial swarming, since the intensity and mechanism of this process depend on the hydrodynamic picture in the apparatus and the size and mass distribution functions of the dispersed phase particles. However, if the dispersed phase consists of particles of the same composition and similar morphology and geometrical shapes, then it can be assumed that the difference in the vectors of the relative velocities of particles of different sizes plays a decisive role in the swarm formation in inertial swarming. It is this factor that leads to the separation of particles and the formation of swarms of particles with close relative velocities. A convenient model for tracking the modulus and direction of the relative velocity of the dispersed phase particles in a continuous medium flow was proposed in the longstanding article by Brener et al., 1987. This model makes it possible to calculate the temporal evolution of the relative velocity of particles using a simple numerical algorithm, even in flows with a complex structure (Balabekov et al., 2016).
In the case of absence of particles aggregation or their decay the equation of a particle motion in a flow can be written as follows

$$\frac{d}{dt}\left(m_p\vec{W}_p\right)=-\xi\frac{\rho_g}{2}\pi d_p^2 W_{rel}^2\vec{e}+\vec{F}_\perp+m_p\vec{g} \tag{1}$$

Here $\vec{g}$ is the vector of gravity acceleration, d_p is the diameter of a particle, $\vec{e}$ is the unit vector along the relative velocity, m_p is the mass of a particle, t is the time, $\vec{F}_\perp$ is the lifting force, $\vec{W}_p$ is the vector of the particle velocity, $\vec{W}_{rel}$ is the vector of relative velocity of the particle in the continuum medium stream, ρ_g is the continuum medium density, ξ is the resistance coefficient.

According to the mentioned model, the basic equation of motion of a particle is transformed into the form of a system of equations for calculating the modulus of the particle relative velocity and the angle between the unit vector of the relative velocity direction and the selected coordinate axis (usually in the direction of the axis of the apparatus). The advantage of this transformation is the ability to immediately determining the relative velocity of the particle at any moment of motion.

Using Lagrangian approach equation (1) can be rewritten as

$$\vec{e}\left(\frac{dW_{rel}}{dt}+k_1W_{rel}^2\right)+\frac{d\vec{e}}{dt}W_{rel}=-\frac{d\vec{W}_g}{dt}+k_2W_{rel}e_\perp+\vec{g} \tag{2}$$

Here

$$k_1=\frac{3\xi\rho_g}{4\rho_p d_p}\ ;\ \ k_2=\frac{3K\mu_g}{4\pi\rho_p d_p}\sqrt{\frac{1}{\nu_g}\left|\frac{\partial\vec{W}_g}{\partial\vec{n}}\right|} \tag{3}$$

Complete time-derivative of gas velocity reads

$$\frac{d\vec{W}_g}{dt}=\frac{\partial\vec{W}_g}{\partial t}+\left(\frac{\partial\vec{W}_g}{d\vec{r}},\frac{d\vec{r}}{dt}\right)=\frac{\partial\vec{W}_g}{\partial t}+\left(\frac{\partial\vec{W}_g}{\partial\vec{r}},\vec{W}_g\right)+\left(\frac{\partial\vec{W}_g}{\partial\vec{r}},\vec{e}\right)W_{rel} \tag{4}$$

The term $\frac{\partial\vec{W}_g}{\partial\vec{r}}$ denotes the spatial tensor-derivative. The general form of this term reads

$$\frac{\partial\vec{W}_g}{\partial\vec{r}}=\begin{bmatrix}\partial W_{g,x}/\partial x & \partial W_{g,x}/\partial y & \partial W_{g,x}/\partial z\\ \partial W_{g,y}/\partial x & \partial W_{g,y}/\partial y & \partial W_{g,y}/\partial z\\ \partial W_{g,z}/\partial x & \partial W_{g,z}/\partial y & \partial W_{g,z}/\partial z\end{bmatrix} \tag{5}$$

After certain transformations, equation (4) is reduced to the following system

$$\frac{dW_{rel}}{dt}=-k_1W_{rel}^2-\left(\vec{e}',\vec{e}\right)W_{rel}-\left(\vec{V},\vec{e}\right)+\left(\vec{g},\vec{e}\right) \tag{6}$$

$$\frac{d\alpha}{dt}=\frac{1}{W_{rel}}\left(\left(\vec{g},\vec{e}_\perp\right)-\left(\vec{V},\vec{e}_\perp\right)\right)-\left(\vec{e}',\vec{e}\right)+k_2 \tag{7}$$

Here

$$\vec{e}'=\left(\frac{\partial\vec{W}_g}{\partial\vec{r}},\vec{e}\right)\ ,\ \ \vec{V}=\frac{\partial\vec{W}_g}{\partial t}+\left(\frac{\partial\vec{W}_g}{\partial\vec{r}},\vec{W}_g\right) \tag{8}$$

The use of this approach makes it possible to perform calculations with a previously unknown profile of the carrier flow velocity, since the hydrodynamic calculation can be performed in parallel with the calculation of the trajectories of the dispersed phase particles. At the same time, this approach does not take into account the possibility of particles aggregation. Computer simulation of the trajectories of spherical liquid particles of various sizes in a gas flow with a transverse flow around a cylinder in 2-D model approximation were carried out by B.Ch. Balabekov et al., 2016. A similar study based on the proposed model can, of course, be carried

out for solid particles in a liquid or gas flow. The difference in this case will consist only in different criterion dependences for the resistance coefficients, as well as in different physical characteristics of the media. Figure 2, which is drawn on the basis of the results of this work, demonstrates the appearance of a swarm of larger particles with close diameters, while particles with smaller diameters are involved in complex motion in vortex zones in the vicinity of streamlined bodies. These particles also form swarms, which linger near the streamlined body. Larger particles are grouped into a swarm, moving in the direction of the main stream. In contrast to the cited work, here the capabilities of the developed model are demonstrated precisely for identifying areas of particle accumulation with the formation of a swarm. The disadvantage of the cited work is that the influence of Brownian motion on the motion of micro and nanoparticles is not considered. Of course, in order to correctly take into account the formation of a swarm of micro- and nanoparticles in the zones of vortex formation, it is necessary to add the effect of Brownian motion. This can be done without fundamentally complicating the described model, since taking into account the Brownian motion does not change the tensor derivative of the velocity of the main carrier flow. The influence of random particle drift is fully taken into account in the stochastic lattice model used for the simulation in the next section of the article.

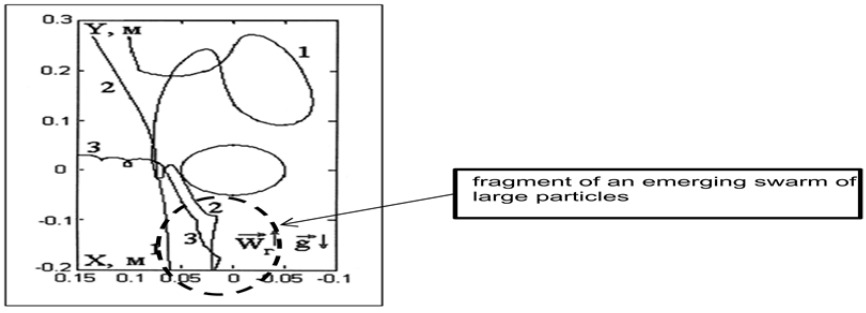


Figure 2: Particles trajectories for a non-stationary vortex street with different particles diameters (Balabekov et al., 2016): 1 - 2x10^{-4} m, 2 - 5x10^{-4} m, 3 - 7x10^{-4} m; diameter of the cylinder is D_{cyl}=0.2 m; average velocity of the gas flow is W_g = 3 m/s.

Analysis of the results shows that this behavior is characteristic for different cases of flow around both a single cylinder and a packed layer with different mutual arrangement of cylindrical bodies. Typical trajectories of particles with different diameters are shown in Fig. 2. Note that small particles (Fig. 2, curve 1) fly into the vortex wake zone while moving, and larger particles (Fig. 2, curves 2, 3) fly past the cylinder, but some of them move on certain sections of theirs trajectories transversely to flow direction (Fig. 2, curve 3) along a loop-like trajectory. As a result, the residence time of particles in this zone increases.

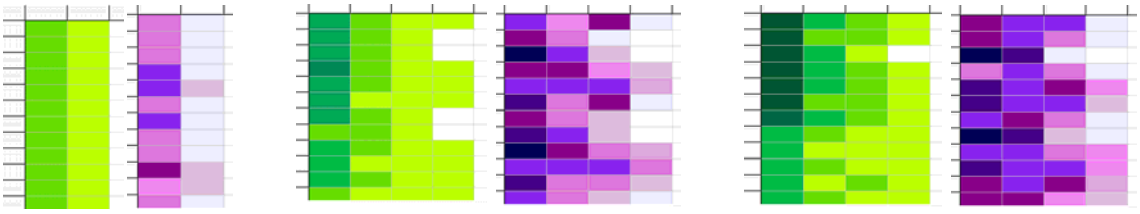
2.2 Stochastic lattice model approach

Further, a numerical experiment was carried out on the basis of the stochastic lattice model (Brener et al., 2017) at various velocity profiles of the incoming flow of the carrier phase. Such an approach requires preliminary specification of the profile of the carrier flow velocity, but at the same time it becomes possible to effectively take into account the kinetics of aggregation processes including the many-particles collisions, that is principal applying to aggregation in dense nanodispersed systems (Brener, 2014). Previously, the algorithm and the main part of the code for the stochastic lattice method were published. The results of testing this approach to calculating the aggregation processes in dispersed systems in cases of diffusion-limited aggregation (DLA) and with mixed kinetics were submitted too (Brener et al., 2017). In order to adapt this method to swarming simulation especially with allowance for the aggregation process and random drift influence, a special lattice coarsening algorithm was developed, and it is presented in this work firstly. The main steps of this algorithm in the case of DLA are described below.

Step 1. The following matrices are created: the main concentration matrix $C(I,J)$ and the coarse matrix of the total number of clusters in blocks $CO(X,Y)$, where dimensions of the matrix $C(I,J)$ are M,N, and dimensions of the matrix $CO(X,Y)$ are R,T. Here $R=M/a$; $T=N/b$; and a,b are the dimensions of the coarse lattice block (i.e., the number of rows and columns of the matrix $C(I,J)$ captured to the block for generating the matrix $CO(X,Y)$. Step 2. The block with specific coordinates (X_s,Y_s) in the coarse matrix $CO(X,Y)$ is built from the elements of the matrix $C(I,J)$, which make up rows with numbers from (aX_{s-1} +1) and to aX_s and columns with numbers from (bY_{s-1} +1) and to bY_s. Step 3. The matrix element $CO_{X_sY_s}$ should

be calculated as the sum of all numbers d_{kl}, defined from the matrix elements $c_{X_sY_s}$ that fall into the block (X_s, Y_s). Namely: $co_{X_sY_s} = \sum_{bY_{s-1}+1}^{bY_s} \sum_{aX_{s-1}+1}^{aX_s} d_{kl}$. Here elements d_{kl} should be calculated by the following algorithm: if $c_{X_sY_s} \neq 0$ then $d_{kl} = 1$, else $d_{kl} = 0$. The coarse matrix of the total number of the clusters orders in blocks $CO1(X,Y)$ should be calculated by the analogous manner as the matrix $CO(X,Y)$. The only difference is that items $co1_{X_sY_s}$ are calculated using the formula $co_{X_sY_s} = \sum_{bY_{s-1}+1}^{bY_s} \sum_{aX_{s-1}+1}^{aX_s} c_{kl}$.

Some of the results of this simulation are shown in Figure 3. Various intensity of colors for blocks of the coarse matrices corresponds to different concentration of clusters (cold colors) and to different sum of orders of cluster aggregates (warm colors). The known additive color model RGB code was used for blocks coloring. The step of variation was 20 units both in the number of clusters and in the sum of their orders. The dimensions of the computational matrix were 20x200, the dimensions of any block of the coarse matrix were 4x40. The calculations were carried out for three different initial profiles of the carrier flow velocities: uniform stream, symmetrical uneven stream and asymmetric uneven stream. Conditional flow rates ***W*** for these three cases are: 1- ***W***=2; 2- $\boldsymbol{W}_w$ =2 nearby the walls, $\boldsymbol{W}_c$ =6 at the stream central axis; 3- $\boldsymbol{W}_{w1}$ =2 nearby the top wall, $\boldsymbol{W}_c$ =6 at the stream central axis, $\boldsymbol{W}_{w2}$ =4 nearby the bottom wall. Flow direction is from left to right. The order of all particles introduced by the carrier flow into the contour is taken equal to 1. Then, particles of different orders appear due to DLA aggregation.



1 **2** **3**

Figure 3: Illustration for calculating swarming using the stochastic lattice model. Explanation of symbols is given in the text above

As a result of visualization of the simulation results, it is possible to clearly identify two swarms of particles formed in a reactor with an uneven profile of the velocity of the carrying flow. These swarms are formed in the regions above and below the central axial zone of the reactor, and in the case of an asymmetric uneven flow, the average concentration of particles in the swarm zone turned out to be 40 percent higher. Comparison of the results of swarming taking into account the total number of clusters without regard to their orders and the results of estimation by summing the orders of the clusters convincingly shows an increase in the intensity of aggregation in the zone of swarm formation. This conclusion is quite consistent with the known regularities of aggregation (Brener et al., 2017). In an even (piston) profile of the flow velocity, no obvious swarms are formed, and the observed local differences in concentrations can be explained by the influence of random particle drift.

3. Conclusions

Simulation based on the CFD model, modified for a step-by-step calculation of the relative velocity of the dispersed phase particles in a flow of a complex structure, demonstrated the efficiency of the model for calculating the trajectories of particles and identifying the zones of swarms formation. The advantage of this approach is the possibility of modeling with a previously unknown carrier flow velocity profile, and the disadvantage is the difficulty of taking into account the particle aggregation process. Simulation has shown that numerical experiment based on the stochastic lattice model can be performed with allowance for the particles aggregation and multi-particles collisions. This model added by the new lattice coarsening algorithm makes it possible to clearly visualize the formed swarms of micro and nanoparticles and estimate their scales, the distribution of particles by orders in the swarm, as well as to evaluate the average swarm drift along the stream. However this model requires a preliminary definition of the carrier flow velocity profile. Experiments based on the lattice model demonstrate a clear effect of the uneven velocity profile of the carrier flow on the rate of particles swarm formation of the dispersed phase. Several swarms can be formed, especially in the

case of an asymmetric profile. The concentration of particles in the swarm in the experiments performed with an asymmetric profile exceeded the average for the flow by an average of 40 percent. In the swarm, the intensity of DLA aggregation increases sharply, and the sum of orders of clusters in the swarm region is more than twice that in the rest of the reactor.

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