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Mathematical and computer simulation of particle redistribution and inertial swarming in dispersed systems

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ABSTRACT

This work is devoted to modeling the motion of a dispersed phase in a gas flow in two cases: i) the dynamic characteristics of the gas flow (velocity components, stream functions and vorticity, ii) are found by numerically solving the Navier-Stokes equations with the subsequent construction of the droplet trajectory; study of the coalescence of droplets in a given model gas flow with analysis of the swarming of dispersed particles. In the first approach, the size and location of vortex and stagnant zones in a channel with a streamlined plate and with a turning flow are determined by numerically solving the equations of gas dynamics in Helmholtz variables. To study the coalescence of drops that occurs when the trajectories of two or more drops come into contact, a second approach has been developed-a computer model of inertial swarming in dispersed systems using the Delphi10 programming environment based on stochastic lattice algorithms and computable lattice enlargement. This approach is needed to pre-define the media flow rate profile. Also in this article, were analyzed the grouping and redistribution of particles for the manifestation of the "swarm of drops" effect.

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1. INTRODUCTION

Physical phenomena of aggregation (for example, coalescence and fragmentation of droplets and bubbles in a gas stream) form the basis of many processes of chemical, oil refining, food and pharmaceutical technologies and are mainly associated with a change in the spectrum and number of particles per unit volume, which determine the value of the interfacial surface of mass and heat transfer. Theoretical and experimental studies of the processes of coalescence, fragmentation and deformation of drops and bubbles are presented in many works. For example, in [1], a review of works of a certain importance in the modeling of problems in petrochemistry is carried out. The results of theoretical studies of the phenomena of coalescence of two-particle collisions of small droplets in the approximation of Brownian particles in a homogeneous unbounded system on the simplest models were first carried out in [2], [3], the frequency and time of coalescence, inversely proportional to the molecular diffusion coefficient of Brownian particles, were determined. It should be noted that in rarefied gas-droplet flows the probability of collision of droplets is

small, but their consequences are important for the correct calculation of mass transfer processes. Therefore, the problem of modeling the phenomena after the collision of drops in general, and swarming, in particular, is relevant.

The swarming process can be accompanied by the aggregation of particles with the formation of clusters with a complex internal structure [4] or proceed without aggregation. In the first case, i.e. when aggregated clusters are formed, their aggregation activity can depend on both the order of the clusters and their age [5]. The term "cluster age" [6] here means the time elapsed from the moment of completion of its primary formation to the moment of changing its size or order, ie. change in the number of its constituent nanoparticles or internal structure. The age of a cluster plays an important role in the process of aggregation, since it affects its morphology and aggregation activity [6]. In this case, the kinetic equations for the aggregation process must be non-Markovian [7]. The manifestation of memory effects in non-Markov processes can significantly transform the kinetic equations, which, in particular, leads to the appearance of nonlinear wave solutions.

At the same time, the swarming process itself can be considered as a kind of weak (correlative) aggregation, when the connection between the particles that make up the swarm is determined by the correlation of the spatial coordinates and velocities of the swarm particles [8]. 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 main formulation of the problem of this work is to study the redistribution of the dispersed phase in terms of the size and mass of particles during its interaction with the flow of a continuous medium. Particles of one size can be in one area of the flow, and of another size in another area of the flow, i.e. swarms of particles of different average sizes are formed. In contact zones, where vortices are formed, small particles can be trapped, while large ones fly by. The paper shows two approaches to calculating this phenomenon, each of which has its own advantages and disadvantages.

The first approach describes the structure of the flow of a continuous medium and the motion of particles in this flow using the equation of continuum mechanics and a numerical algorithm developed in [9], [10], [11]. The movement of particles in this complex-structured flow is described. To ensure the convergence of the numerical algorithm for the implementation of the mathematical model, the method of hydrodynamic establishment is used, which is described in the most complete form in [12]. The mathematical model of the trajectory of liquid droplets is based on the ideas of [13], in particular, on the relative velocity of the droplets. The uniqueness of the solution of the differential Navier-Stokes equations, the convergence of our numerical algorithms for their solution are ensured by the fulfillment of the corresponding conditions given in [14]-[17]. This approach is quite strict, but it has drawbacks in the interpretation of numerical results. For example, additional difficulties arise for taking into account possible aggregation due to the difference in volumes and masses of particles. In the processes of aggregation of nanoparticles, intermolecular forces prevail [18], and in this problem these are the mass forces of gas and droplets, the force of interaction of continuous and dispersed flows. It should be noted as a disadvantage of this approach that it is difficult to solve the equations of gas dynamics, especially in a turbulent regime.

To overcome the disadvantages of the first approach, a second approach has been developed: the flow structure is presented in a model form. It can be taken from theory or from experiment. The structure then describes the formation of the swarm. At the same time, accounting for aggregation and the formation of a swarm becomes easier. A flow was modeled, the dynamic characteristics of which are specified, its structure is simplified, and another calculation concept was applied-the method of stochastic lattices. In papers [19]-[22] aggregation is described and a swarming algorithm is given. The key point in the swarming algorithm is the idea of coarsening or coarsening of the lattice, which makes it possible to describe the change in concentration in separate regions of the flow, and two points are studied: the total change in the concentration of particles of different sizes and the total change in the order of particles. Using them, the average particle size can be calculated. The results of computer modeling and numerical experiments are presented to describe the phenomenon of swarming [23], [24], proceeding according to an inertial mechanism, using both computer hydrodynamic modeling and the approach of stochastic lattices, specially adapted in the presented work to describe the phenomenon in swarms [25], [26].

2. ALGORITHM FOR FINDING THE DYNAMIC CHARACTERISTICS OF A GAS

2.1. Gas velocity distribution

To simulate and generate an inhomogeneous gas flow, two cases are considered (Figure 1): Figure 1(a) flow around the plate; Figure 1(b) a turning stream. The basis of the mathematical model of gas dynamics in is the two-dimensional Navier-Stokes equations in variables, the stream function $\psi(x,y,t)$ and vorticity $\omega(x,y,t)$ [9]-[14].

$$\frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2\psi}{\partial y^2}=\omega \quad (1)$$

$$\frac{\partial\omega}{\partial t}+u\frac{\partial\omega}{\partial x}+\vartheta\frac{\partial\omega}{\partial y}=\upsilon\left(\frac{\partial^2\omega}{\partial x^2}+\frac{\partial^2\omega}{\partial y^2}\right) \quad (2)$$

When specifying the initial and boundary conditions, the geometry of the channel and the shape of the nozzles are taken into account.

2.2. Solution domain and finite difference scheme

To solve problem (1)-(6), we use the finite-difference method. The area of the numerical solution of the problem is shown in Figure 1, therefore the area for solving the equations of gas motion is the flow around the plate in case Figure 1(a) and the Figure 1(b) case is a turning stream.

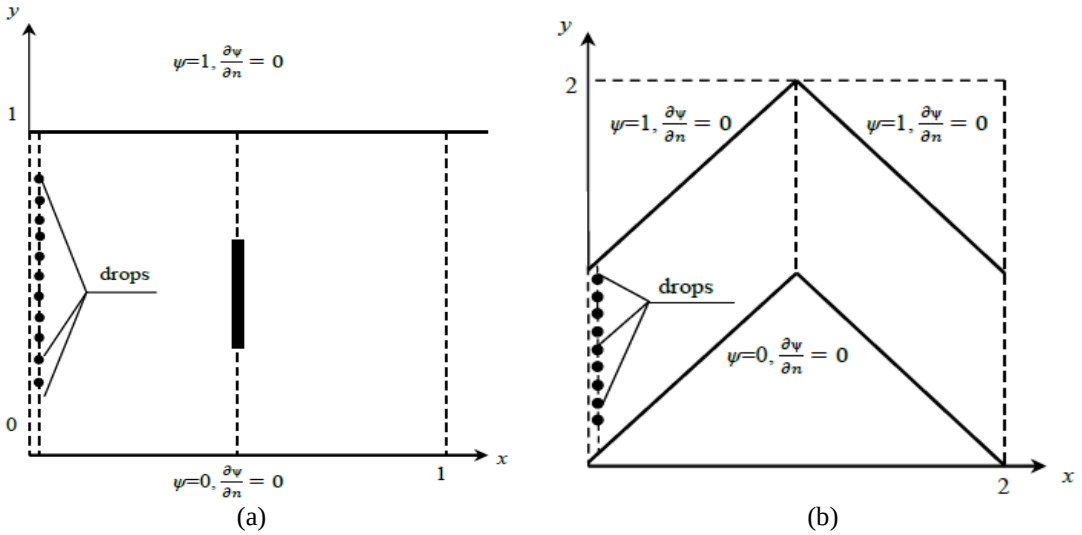

Figure 1. The area for solving the equations of gas motion, (a) the flow around the plate and (b) a turning stream

Let's use the following explicit scheme for the vortex equation:

$$\frac{\omega_{i,j}^{n+1}-\omega_{i,j}^{n}}{\tau}+u_{i,j}^{n}\frac{\omega_{i+1,j}^{n}-\omega_{i,j}^{n}}{h}+v_{i,j}^{n}\frac{\omega_{i+1,j}^{n}-\omega_{i,j}^{n}}{h}=\frac{1}{R}\left(\frac{\omega_{i+1,j}^{n}-2\omega_{i,j}^{n}+\omega_{i-1,j}^{n}}{h^2}+\frac{\omega_{i,j+1}^{n}-2\omega_{i,j}^{n}+\omega_{i,j-1}^{n}}{h^2}\right)+R_n \quad (3)$$

where R_h- is the remainder whose order is *O(h)*.

We now turn to solving the Poisson equation for the stream function (1). Let us denote by *s* the index of the inner cycle and write down the scheme for solving this equation on the time layer *n+1* in the form:

$$\psi_{i,j}^{n+1,s+1}=\psi_{i,j}^{n+1,s}+\alpha_0\left[\frac{1}{4}\left(\psi_{i+1,j}^{n+1,s}+\psi_{i-1,j}^{n+1,s+1}+\psi_{i,j+1}^{n+1,s}+\psi_{i,j-1}^{n+1,s+1}-h^2\psi_{i,j}^{n+1,s}\right)-\psi_{i,j}^{n+1,s}\right],$$

$$\frac{\psi_{i,j}^{n+1,s}+\psi_{i,j}^{n+1,s}}{\sigma}=\frac{\psi_{i+1,j}^{n+1,s}-2\psi_{i,j}^{n+1,s}+\psi_{i-1,j}^{n+1,s+1}}{h^2}+\frac{\psi_{i,j+1}^{n+1,s}-2\psi_{i,j}^{n+1,s}+\psi_{i,j-1}^{n+1,s+1}}{h^2}-\omega \quad (4)$$

where is the α_0 - iterative parameter defined through the grid parameters.

$$\sigma, h\ (\alpha_0=4\sigma/h^2) \quad (5)$$

The *z* values of the iterative parameter depend on the Reynolds number and are selected according to the recommendations [12].

A fragment of our algorithm in the ABC Pascal language, which implements the method of hydrodynamic settling, as applied to the problem of gas flow around a plate, has the following form (Algorithm 1):

Algorithm 1. Fragment of the algorithm for calculating the flow of gas around the plate

```
Begin { Calculating derivatives }
a1:=(f[i,j+1]-f[i,j])/h; {u}
a2:=-(f[i+1,j]-f[i,j])/h; {V}
a3:=(w[i+1,j]-w[i,j])/h; {dw/dx}
a4:=(w[i,j+1]-w[i,j])/h; {dw/dy}
a5:=(w[i+1,j]-2*w[i,j]+w[i-1,j])/h/h; {d^2w/dx^2}
a6:=(w[i,j+1]-2*w[i,j]+w[i,j-1])/h/h; {d^2w/dy^2}
a7:=a1*a3+a2*a4;
a8:=a5+a6; a10:=tau*(a8/Re-a7);
w[i,j]:=w[i,j]+a10;
if maxw<abs(a10) then maxw:=abs(a10);end;
l3: iterf:=iterf+1; { start of inner loop for stream function }
writeln('iterf=',iterf:3);
for i:=0 to n do { updating }
for j:=0 to m do
f1[i,j]:=f[i,j];
if iterf>nf then stop;
for i:=1 to n-1 do { stream and vorticity functions at the plate boundaries }
 for j:=1 to m-1 do
begin
if (i=n1) and (j>=m1) and (j<=m2) then
f[i,j]:=0.5; begin
w[i,j]:=(2*(f[i,m1-1]-f[i,m1]))/h/h;end;
 else
begin { vorticity function calculation }
b1:=(f[i+1,j]-2*f[i,j]+f1[i-1,j])/h/h;
b2:=(f[i,j+1]-2*f[i,j]+f1[i,j-1])/h/h;
b3:=b1+b2-w1[i,j];
f1[i,j]:=f[i,j]+sigma*b3;
if maxf<abs(sigma*b3) then maxf:=abs(sigma*b3);
f[i,j]:=f1[i,j];
end; end;
```

2.3. Modeling and calculation of droplet trajectories

The differential equation of the droplet motion is written in the form [27]:

$$m_d \frac{dW_d}{dt} = -\frac{\xi_d}{2} \rho_g f_d W_{rs}^2 \vec{e} + m_d \vec{g} \quad (6)$$

where $\xi_d = f(Re, We)$ - coefficient depending on the Reynolds and Weber numbers; f_d- drop cross-sectional area; W_{rs}- relative droplet velocity; $\vec{e}$- unit direction vector W_{rs}; g–free fall acceleration vector.

After transformation of the last equation and reduction to dimensionless form, a system of equations for the relative velocity of the drop and the angle between the direction of the drop and the gas was obtained [27]. This system was solved numerically by the Runge-Kutta method with automatic step selection. Dynamic characteristics of an inhomogeneous gas flow - numerical values of stream functions and vorticity at the nodes of the finite-difference grid. The solution continues until the drop hits the channel boundary, plate surface, or meets another drop. Figures 2 and 3 show the contour lines obtained for the Reynolds number equal to 100 in the channel with the plate and in the turning channel. In vortex zones, the maximum values of the vertical component of the velocity are twice or higher than the average flow rate, due to the thickening of the streamlines.

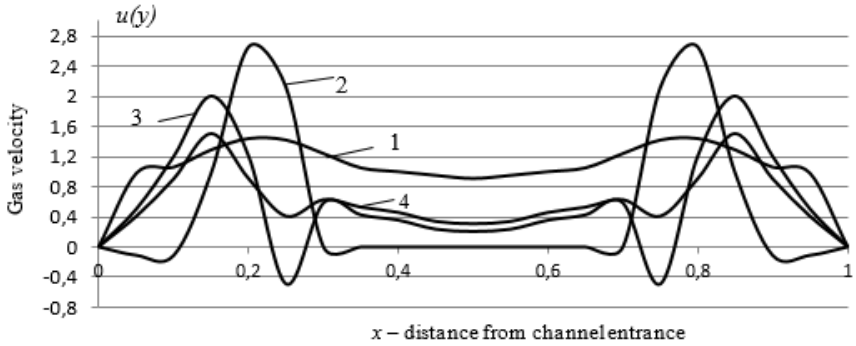

Figure 2. Profiles of the longitudinal gas velocity when flowing around the plate, Re = 100.
x – distance from channel entrance 1 – *x* = 0,3; 2 – *x* = 0,5; 3 – *x* = 0,6; 4 – *x* = 0,8

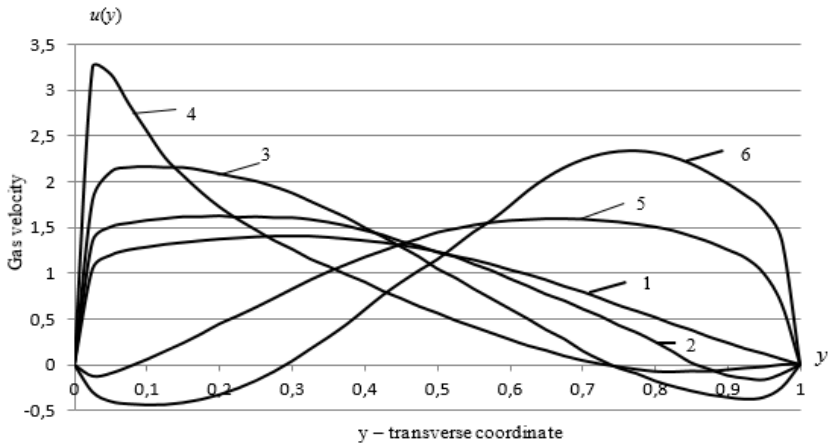

Figure 3. Profiles of the longitudinal gas velocity in a turning flow, Re=100.
x–distance from channel entrance, 1–*x*= 0,3; 2–*x*=0,5; 3–*x*=0,6;4–*x*=0,8

Figure 4 shows the calculated trajectories of drops with a diameter of 3 mm in a channel with a plate. Single drops are "placed" on the first vertical line, after the gas enters. The dotted line shows the isolines of the gas flow function. Under the influence of the forces of gravity and the inhomogeneity of the gas flow, a swarm of particles is formed in zones 1 and 2 with an average velocity directed to the upper and boundary, respectively. Zones 1 and 2 can be called zones of "swarm" of drops, falling into which the drops lose their spherical shape and flow into the film. In these zones, the probability of droplet aggregation increases: in zone 1, due to the thickening of streamlines, in zone 2, due to the accumulation of drops. Because, in these zones, the probability of particle aggregation increases due to an increase in their local concentration and a decrease in relative velocities.

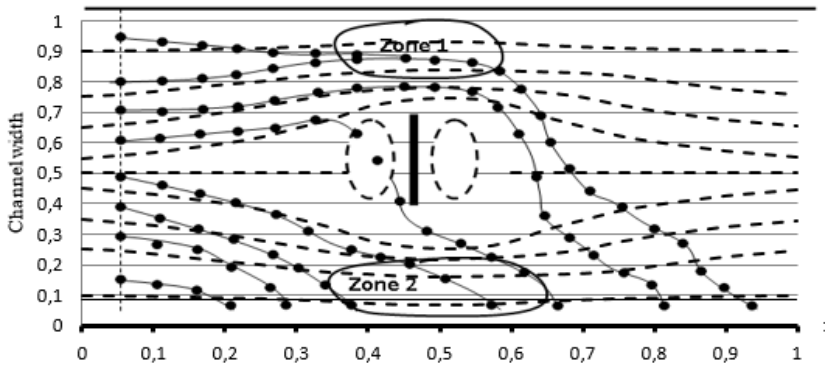

Figure 4. Trajectories of drops in an inhomogeneous gas flow, d=3mm

3. STOCHASTIC LATTICE SWARMING MODEL

The above approach has sufficient completeness and rigor in theoretical and computational terms. It is difficult to generalize this approach to create a conjugate model taking into account particle aggregation in collisions. Therefore, a numerical experiment was carried out on the basis of a stochastic lattice model [19], [20], [21] at different profiles of the carrier phase flow velocity. This approach requires preliminary specification of the carrier flow rate profile, but at the same time it becomes possible to effectively take into account the kinetics of aggregation processes, including collisions of many particles, which is fundamentally applicable to aggregation in dense disperse systems [22]-[26], [27]-[30]. The algorithm and the main part of the code for the stochastic lattice method have been published earlier [19]-[21]. Also presented were the results of testing this approach to the calculation of aggregation processes in dispersed systems in cases of diffusion-limited aggregation (DLA), and with mixed kinetics [19]-[21]. Special algorithms are used for computer simulation of swarming processes [31]. To adapt this method to simulating swarming, especially taking into account the aggregation process and the influence of random drift, a special lattice enlargement

algorithm was developed, which is presented in this paper. The main steps of this algorithm in the case of DLA are described below. i) The following matrices are created: the main matrix of concentrations $C(I,J)$ and a rough matrix of the total number of clusters in blocks $CO(X,Y)$, where M, N the dimensions of the matrix $C(I,J)$ and $R,T$the dimensions of the matrix $CO(X,Y)$. Here $R = M/a$; $T = N/b$; and a,b - the dimensions of the coarse lattice block (that is, the number of rows and columns of the matrix$C(I,J)$, captured in the block to generate the matrix.$CO(X,Y)$; ii) The block with specific coordinates (X_s,Y_s) in the rough 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) to aX_s and columns with numbers from (bY_{s-1} +1) to bY_s; iii) The element of the matrix $CO(X,Y)$ must be calculated as the sum of all numbersd_{kl}, determined from the elements of the matrix $c_{X_sY_s}$, 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 the elements d_{kl} should be calculated according to the following algorithm (A): If $c_{X_sY_s} \neq 0$, then $d_{kl} = 1$, Else $d_{kl} = 0$. A rough matrix of the total number of orders of clusters in blocks $CO1(X,Y)$ should be calculated similarly to the matrix $CO(X,Y)$. The only difference is that positions $co1_{X_sY_s}$ are calculated using a formula$co_{X_sY_s} = \sum_{bY_{s-1}+1}^{bY_s}\sum_{aX_{s-1}+1}^{aX_s} c_{kl}$. That is, it is not necessary to pre-calculate by Algorithm 1.

A fragment of the program for calculating the flow rate by the horizontal component for four types of uniform and non-uniform distribution of flows, the principles of which were described in [24] (Algorithm 2).

Algorithm 2. Fragment of the algorithm for calculating the horizontal component of the velocity

```
If uw.ItemIndex=0 then// equable distribution
If l>=w1 then vg[l,i]:= vg[l,i]+w1;
If uw.ItemIndex=1 then // unequable distribution, the №1 type
 begin if (i<=wn1) then vg[l,i]:= vg[l,i]+w1;
 if (i>wn1) and (i<=(wn1+wn2)) then vg[l,i]:=vg[l,i]+w2;
 if (i>(wn1+wn2)) and (i<=n1) then vg[l,i]:=vg[l,i]+w1; end;
if uw.ItemIndex=2 then // unequable distribution, the №2 type
 begin if (i<=wn1) then vg[l,i]:= vg[l,i]+w1;
 if (i>wn1) and (i<=(wn1+wn2)) then vg[l,i]:=vg[l,i]+w2;
 if (i>(wn1+wn2)) and (i<=n1) then vg[l,i]:=vg[l,i]+round(w3); end;
if uw.ItemIndex=3 then // unequable distribution, the №3 type
 begin if (l>=r1_4) and (i>wn3) then begin vg[l,i]:= vg[l,i]; end;
 if (i<=wn3) and (l>r1_4) then vg[l,i]:= vg[l,i]+3*w1;
 if (l<r1_4) then vg[l,i]:= vg[l,i]+w1;end;
if uw.ItemIndex=4 then // unequable distribution, the №4 type
 begin if (l<=r1_4) then vg[l,i]:= vg[l,i]+w1;
 if (l>=r1_4) and (i<=wn3) then begin vg[l,i,j]:= vg[l,i]; end;
 if (l>=r1_4) and (i>(wn3+wn1*2)) then begin vg[l,i]:= vg[l,i]; end;
 if (i>wn3) and (i<=(wn3+wn1*2)) and (l>r1_4) then vg[l,i]:= vg[l,i]+3*w1;end;
```

Some results of this simulation are shown in Figure 5. Different color intensities of different blocks of rough matrices correspond to different concentrations of clusters, both without taking into account their orders (cold colors) and different sums of orders of cluster aggregates (warm colors). To color the blocks, we used the RGB code of the additive color model [32]. The step of change was 20 units, both in the number of clusters and in the sum of their orders. The overall range observed during the simulation was from 0 to 200 units.

The dimensions of the computational matrix are 20x200, the dimensions of any block of the coarse matrix are 4x40. The calculations were performed for three different initial carrier flow velocity profiles: uniform flow, symmetric irregular flow, and asymmetric irregular flow.

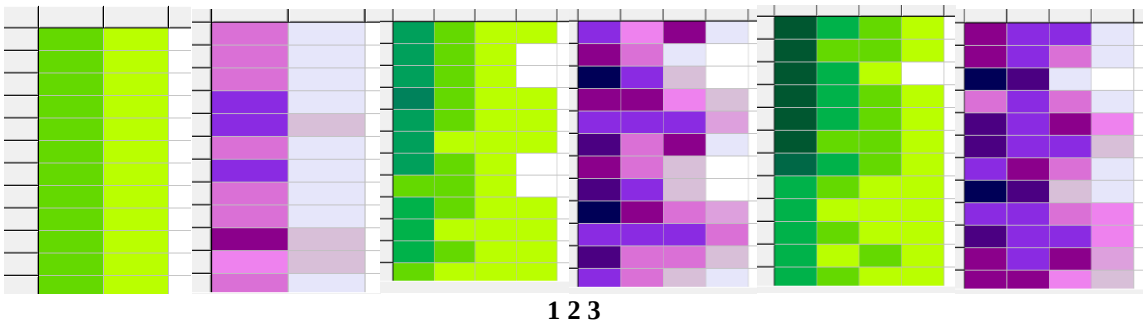

Figure 5. Illustration for calculating swarming using a stochastic lattice model. Explanation of symbols in the text above

The conditional flow rates W for these three cases are equal: 1-W=2; 2-W_w=2 at the baffles, W_c=6 on the central axis of the flow; 3- W_{w1}=2 at the upper baffle, W_c=6 at the central axis of the flow, W_{w1}=4 at the lower baffle. Flow direction from left to right. The order of all particles introduced by the carrier flux into the circuit is assumed to be 1. Then particles of different orders appear due to DLA aggregation [19].

4. CONCLUSION

The analysis of the results of the first approach showed that when the gas flows around the plate, the streamlines become thicker, respectively, at the edge of the plate, the horizontal and vertical components of the velocity increase by 1,5-2 times. Getting into this zone, small drops rise up, and large ones-down due to the prevalence of gravity forces. This means that the droplet size distribution function changes. Thus, the distribution function becomes dependent on the coordinates of the points of the region of gas and droplet flow. If the drops were initially evenly distributed in size, then passing a certain path and staying in motion for a certain time, they fall into the zones in which they accumulate (the "swarm" effect). This fact must be taken into account when calculating mass transfer in chemical technology devices, since at each point of the region, the droplet size distribution function is different.

The analysis of the second approach showed that the comparison of the results of swarming taking into account the total number of clusters without taking into account their orders and the results of the assessment by summing the orders of the clusters shows an increase in the intensity of aggregation in the swarm formation zone. This conclusion is quite consistent with the known laws of aggregation. With an even (piston) flow velocity profile, no obvious accumulations are formed, and the observed local differences in concentrations can be explained by the influence of random particle drift. Experiments based on the lattice model demonstrate a clear effect of the non-uniform profile of the carrier flow velocity on the rate of formation of a swarm of particles of the dispersed phase. Several swarms may form, especially in the case of an asymmetrical profile. The concentration of particles in the swarm in experiments carried out with an asymmetric profile exceeded the average value for the flow by an average of 40 percent.

REFERENCES

[1] G. I. Kelbaliyev and S. R. Rasulov, "Mathematical modeling of coalescence and breakage of droplets and bubbles in an isotropic turbulent flow: A review," *Vestnik Samarskogo Gosudarstvennogo Tekhnicheskogo Universiteta, Seriya Fiziko-Matematicheskie Nauki*, vol. 23, no. 3, pp. 541–581, 2019, doi: 10.14498/vsgtu1664.

[2] V. G. Levich, "Physicochemical hydrodynamics, Prentice-Hall international series in the physical and chemical engineering sciences," in *Physicochemical hydrodynamics*, Englewood Cliffs, N.J., Prentice-Hall, 1962, p. 700.

[3] S. L. Soo, *Fluid Dynamics of Multiphase Systems*, vol. 788, no. 1965. Blaisdell, Waltham, MA, 1967.

[4] A. M. Brener, "Nonlocal equations of the heat and mass transfer in technological processes," *Theoretical Foundations of Chemical Engineering*, vol. 40, no. 6, pp. 564–572, Dec. 2006, doi: 10.1134/S0040579506060029.

[5] A. Mogilner and L. Edelstein-Keshet, "A non-local model for a swarm," *Journal of Mathematical Biology*, vol. 38, no. 6, pp. 534–570, Jun. 1999, doi: 10.1007/s002850050158.

[6] A. M. Brener and V. V. Dil'man, "Concept of building an aggregation kinetic model taking into consideration the dependence between aggregation activity and cluster ages," *Theoretical Foundations of Chemical Engineering*, vol. 50, no. 4, pp. 439–443, Jul. 2016, doi: 10.1134/S0040579516040321.

[7] K. Zabrocki, S. Tatur, S. Trimper, and R. Mahnke, "Relationship between a non-Markovian process and Fokker-Planck equation," *Physics Letters, Section A: General, Atomic and Solid State Physics*, vol. 359, no. 5, pp. 349–356, Dec. 2006, doi: 10.1016/j.physleta.2006.06.063.

[8] L. A. Kim and A. M. Brener, "On the time nonlocality in the heat- and mass-transfer equations for high-rate processes," *Theoretical Foundations of Chemical Engineering*, vol. 30, no. 3, pp. 233–235, 1996.

[9] L. P. Kholpanov, B. R. Ismailov, and N. P. Bolgov, "Modeling of turbulent flow of incompressible liquid in channels of complex shape," *Theoretical Foundations of Chemical Engineering*, vol. 24, no. 4, pp. 313–319, 1991.

[10] B. Ismailov, K. Ismailov, A. Urmatova, and T. Koyshieva, "Mathematical modelling, dynamic and mass-transfer calculation of gas-drop mixture in the mass-transfer apparatus multistage channels," *Applied Mathematical Sciences*, vol. 8, no. 89–92, pp. 4561–4570, 2014, doi: 10.12988/ams.2014.46471.

[11] B. Ismailov, A. Urmatova, and K. Ismailov, "Modeling and calculation of the trajectory of droplets in a multistage channel mass-transfer apparatus," in *AIP Conference Proceedings*, 2014, vol. 1611, pp. 63–66, doi: 10.1063/1.4893805.

[12] P. Roach, *Computational Fluid Dynamics.* Moscow: Mir, 1980.

[13] B. C. Balabekov, A. M. Brener, and O. S. Balabekov, "Numerical modeling of heat and mass transfer processes upon the flowing of regular structures by gas-droplet stream," *Theoretical Foundations of Chemical Engineering*, vol. 50, no. 3, pp. 273–285, May 2016, doi: 10.1134/S0040579516030039.

[14] A. Ashyralyev, A. S. Erdogan, and N. Arslan, "On the modified Crank-Nicholson difference schemes for parabolic equation with non-smooth data arising in biomechanics," *International Journal for Numerical Methods in Biomedical Engineering*, vol. 26, no. 5, pp. 501–510, 2010, doi: 10.1002/cnm.1190.

[15] A. Ashyralyev, A. S. Erdogan, and O. Demirdag, "On the determination of the right-hand side in a parabolic equation," *Applied Numerical Mathematics*, vol. 62, no. 11, pp. 1672–1683, Nov. 2012, doi: 10.1016/j.apnum.2012.05.008.

[16] A. Ashyralyev and A. S. Erdogan, "Finite difference method for the estimation of a heat source dependent on time variable," *Malaysian Journal of Mathematical Sciences*, vol. 6, no. SUPPL., pp. 139–150, 2012.

[17] A. S. Erdogan and A. Ashyralyev, "Stability of Implicit Difference Scheme for Solving the Identification Problem of a Parabolic Equation," in *Lecture Notes in Computer Science (including subseries Lecture Notes in Artificial Intelligence and Lecture Notes in Bioinformatics)*, vol. 8236 LNCS, 2013, pp. 271–278.
[18] B. Ismailov, Z. Umarova, K. Ismailov, A. Dosmakanbetova, and S. Meldebekova, "Mathematical modeling and algorithm for calculation of thermocatalytic process of producing nanomaterial," *Indonesian Journal of Electrical Engineering and Computer Science*, vol. 23, no. 3, p. 1590, Sep. 2021, doi: 10.11591/ijeecs.v23.i3.pp1590-1601.
[19] A. M. Brener, L. M. Musabekova, and M. A. Jamankarayeva, "Stochastic lattice model of aggregation in heterogeneous polydisperse media," *Chemical Engineering Transactions*, vol. 60, pp. 79–84, 2017, doi: 10.3303/CET1760014.
[20] L. Musabekova, N. Zhumataev, A. Yunussova, N. Dausheyeva, and A. Zhidebayeva, "Development of the stochastic lattice model for describing aggregation processes in the polydisperse systems (3D case)," *Chemical Engineering Transactions*, vol. 76, pp. 823–828, 2019, doi: 10.3303/CET1976138.
[21] L. Musabekova, N. Zhumatayev, N. Dausheyeva, and M. Jamankarayeva, "Discrete-event simulation of aggregation processes in batch and flow tubular reactors based on the stochastic lattice models," *Chemical Engineering Transactions*, vol. 81, pp. 1135–1140, 2020, doi: 10.3303/CET2081190.
[22] P. C. Miranda and P. Coates, "Swarm modeling," 2000.
[23] J. M. Z. Maningo, G. E. U. Faelden, R. C. S. Nakano, A. A. Bandala, R. R. P. Vicerra, and E. P. Dadios, "Formation control in quadrotor swarm aggregation using Smoothed Particle Hydrodynamics," in *2016 IEEE Region 10 Conference (TENCON)*, Nov. 2016, pp. 2070–2075, doi: 10.1109/TENCON.2016.7848390.
[24] A. Brener, L. Musabekova, and N. Dausheyeva, "On modeling the swarming in dispersed systems," *Chemical Engineering Transactions*, vol. 84, pp. 217–222, 2021, doi: 10.3303/CET2184037.
[25] O. Rimer and G. Ariel, "Kinetic order-disorder transitions in a pause-and-go swarming model with memory," *Journal of Theoretical Biology*, vol. 419, pp. 90–99, 2017, doi: 10.1016/j.jtbi.2017.02.009.
[26] J. A. Carrillo, M. Fornasier, G. Toscani, and F. Vecil, "Particle, kinetic, and hydrodynamic models of swarming," in *Modeling and Simulation in Science, Engineering and Technology*, vol. 51, Boston: Birkhäuser Boston, 2010, pp. 297–336.
[27] A. M. Brener, N. P. Bolgov, M. T. Kaziev, and E. M. Orymbetov, "Simplified model of drop motion in a gas flow," *Theoretical Foundations of Chemical Engineering*, vol. 21, no. 1, pp. 126–131, 1987.
[28] S. Talukder, "Mathematical Modelling and Applications of Particle Swarm Optimization," School of Engineering Blekinge Institute of Technology, 2011.
[29] S. Yaseen and G. A. Mansoori, "Asphaltene aggregation due to waterflooding (A molecular dynamics study)," *Journal of Petroleum Science and Engineering*, vol. 170, pp. 177–183, Nov. 2018, doi: 10.1016/j.petrol.2018.06.043.
[30] X. H. Zhou, B. C. Huang, T. Zhou, Y. chen Liu, and H. chang Shi, "Aggregation behavior of engineered nanoparticles and their impact on activated sludge in wastewater treatment," *Chemosphere*, vol. 119, pp. 568–576, Jan. 2015, doi: 10.1016/j.chemosphere.2014.07.037.
[31] N. S. Kanianthara, S. P. Ang, A. F. K. Sulayman, and Z. bin Hj. Abd. Hamid, "Optimising monthly tilt angles of solar panels using particle swarm optimisation algorithm," *Indonesian Journal of Electrical Engineering and Computer Science*, vol. 23, no. 1, p. 75, Jul. 2021, doi: 10.11591/ijeecs.v23.i1.pp75-89.
[32] C. Poynton, *Digital Video and HD: Algorithms and Interfaces*. Waltham MA USA: Morgan Kaufmann Publication, 2012.

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