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

Bakhtiyar Rashidovich Ismailov1, Leyla Mukhamedjanovna Musabekova2, Zhanat Rysbayevna Umarova1, Khairulla Bakhtiyarovich Ismailov1, Kuttybek Arystanbayev3
1Department of Information Systems and Modeling, M. Auezov South Kazakhstan University, Tauke Khan Avenue 5, Shymkent, Kazakhstan
2Department of Computing Technology and Software, M. Auezov South Kazakhstan University, Tauke Khan Avenue 5, Shymkent, Kazakhstan
3South Kazakhstan Medical Academy, Al-Farabi Square 1, Shymkent, Kazakhstan

Article Info

Article history:
Received Nov 21, 2021
Revised Jul 22, 2022
Accepted Aug 12, 2022

Keywords:
Aggregation algorithm
Computer simulation
Droplet
Mathematical model
Stochastic lattices
Swarming model

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.

This is an open access article under the CC BY-SA license.

Corresponding Author:
Zhanat Rysbayevna Umarova
Department of Information Systems and Modeling, M. Auezov South Kazakhstan University
Tauke khan avenue 5, Shymkent, Kazakhstan
Email: zhanat.umarova@auzeov.edu.kz

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, i.e. 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 is the two-dimensional Navier-Stokes equations in variables, the stream function \( \psi (x,y,t) \) and vorticity \( \omega (x,y,t) \) [9]-[14].
\[
\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} = \omega \tag{1}
\]
\[
\frac{\partial \psi}{\partial t} + u \frac{\partial \psi}{\partial x} + \vartheta \frac{\partial \psi}{\partial y} = \psi \left( \frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} \right) \tag{2}
\]

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](image_url)  
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:

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

where \(R_n\) 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:

\[
\begin{align*}
\psi_{i,j}^{n+1,s+1} &= \psi_{i,j}^{n+1,s} + \alpha_0 \left[ \frac{1}{4} \left( \psi_{i+1,j}^{n+1,s} + \psi_{i-1,j}^{n+1,s} + \psi_{i,j+1}^{n+1,s} + \psi_{i,j-1}^{n+1,s} - h^2 \psi_{i,j}^{n+1,s} \right) - \psi_{i,j}^{n+1,s} \right], \\
\psi_{i,j}^{n+1,s} &= \frac{\psi_{i,j}^{n+1,s+1} - 2 \psi_{i,j}^{n+1,s} + \psi_{i,j}^{n+1,s+1}}{h^2} + \frac{\psi_{i+1,j}^{n+1,s} - 2 \psi_{i,j}^{n+1,s} + \psi_{i-1,j}^{n+1,s}}{h^2} - \omega
\end{align*} \tag{4}
\]

where is the \(\alpha_0\) - iterative parameter defined through the grid parameters.

\[
\sigma, h \left( \alpha_0 = 4\sigma/h^2 \right) \tag{5}
\]

The \(\sigma\) 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):

---

*Mathematical and computer simulation of particle redistribution and ... (Bakhtiyar Rashidovich Ismailov)*
Algorithm 1. Fragment of the algorithm for calculating the flow of gas around the plate

Begin { Calculating derivatives }

\[ a_1 := \frac{f[i,j+1] - f[i,j]}{h}; \quad \{ u \} \]
\[ a_2 := -\frac{f[i+1,j] - f[i,j]}{h}; \quad \{ V \} \]
\[ a_3 := \frac{w[i+1,j] - w[i,j]}{h}; \quad \{ \frac{\partial w}{\partial x} \} \]
\[ a_4 := \frac{w[i,j+1] - w[i,j]}{h}; \quad \{ \frac{\partial w}{\partial y} \} \]
\[ a_5 := \frac{w[i+1,j] - 2w[i,j] + w[i-1,j]}{h^2}; \quad \{ \frac{\partial^2 w}{\partial x^2} \} \]
\[ a_6 := \frac{w[i,j+1] - 2w[i,j] + w[i,j-1]}{h^2}; \quad \{ \frac{\partial^2 w}{\partial y^2} \} \]
\[ a_7 := a_1a_3 + a_2a_4; \]
\[ a_8 := a_5 + a_6; \quad a_{10} := \tau (a_8/Re - a_7); \]
\[ w[i,j] := w[i,j] + a_{10}; \]
\[ \text{if} \; \text{maxw} < \text{abs}(a_10) \quad \text{then} \; \text{maxw} := \text{abs}(a_10); \]
\[ l_{3}: \text{iterf} := \text{iterf} + 1; \quad \{ \text{start of inner loop for stream function} \} \]
\[ \text{writeln}('\text{iterf}=', \text{iterf}, ':3); \]
\[ \text{for} \; i := 0 \text{ to } n \text{ do } \{ \text{updating} \} \]
\[ \text{for} \; j := 0 \text{ to } m \text{ do } \{ \text{stream and vorticity functions at the plate boundaries} \} \]
\[ \text{begin} \]
\[ \text{if} \; (i = n1) \text{ and } (j = m1) \text{ and } (j = m2) \text{ then} \]
\[ f[i,j] := 0.5; \text{ begin} \]
\[ w[i,j] := (2*(f[i,m1+1]-f[i,m1]))/h/h; \text{ end} \]
\[ \text{else} \]
\[ \text{begin} \; \{ \text{vorticity function calculation} \} \]
\[ b_1 := (f[i+1,j]-2f[i,j]+f[i-1,j])/h/h; \]
\[ b_2 := (f[i,j+1]-2f[i,j]+f[i,j-1])/h/h; \]
\[ b_3 := b_1 + b_2 - w[i,j]; \]
\[ f[i,j] := f[i,j] + \sigma * b_3; \]
\[ \text{if} \; \text{maxf} < \text{abs}(\sigma * b_3) \quad \text{then} \; \text{maxf} := \text{abs}(\sigma * b_3); \]
\[ f[i,j] := f[i,j]; \]
\[ \text{end}; \text{ end}; \]
\[ \]
2.3. Modeling and calculation of droplet trajectories

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

\[ m_d \frac{dW_d}{dt} = -\frac{\xi_d}{2} \rho g f_d W_{rs}^2 \vec{e} + m_d \vec{g} \]  

(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 \( W_{rs} \); \( \vec{g} \) - 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 - \( x = 0,8 \)
Mathematical and computer simulation of particle redistribution and ... (Bakhtiyar Rashidovich Ismailov)
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 \((aX_s+1)\) to \(aX_s\) and columns with numbers from \((bY_s+1)\) to \(bY_s\); iii) The element of the matrix \( CO(X,Y) \) must be calculated as the sum of all numbers \( d_{kl} \), determined from the elements of the matrix \( c_{X_sY_s} \) that fall into the block \((X_s,Y_s)\). Namely: \( CO(X_s,Y_s) = \sum_{bY_s+1}^{bY_s+1} \sum_{aX_s+1}^{aX_s+1} c_{kl} \). Here the elements \( d_{kl} \) should be calculated according to the following algorithm (A): If \( c_{XY} \neq 0 \), 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 \( CO1_XY \) are calculated using a formula: \( CO1_XY = \sum_{bY_s+1}^{bY_s+1} \sum_{aX_s+1}^{aX_s+1} c_{kl} \). 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,j]:= vg[l,i,j]+w1;
  if uw.ItemIndex=1 then // unequable distribution, the №1 type
    begin if (i>=wn1) then vg[l,i,j]:= vg[l,i,j]+w1;
    if (i<wn1) and (i<=wn3) then vg[l,i,j]:=vg[l,i,j]+w1;
    if (l>=r1_4) then vg[l,i,j]:= vg[l,i,j]+w1; end;
  if uw.ItemIndex=2 then // unequable distribution, the №2 type
    begin if (i>=wn1) then vg[l,i,j]:= vg[l,i,j]+w1;
    if (i<wn1) and (i<=wn3) then vg[l,i,j]:=vg[l,i,j]+w1;
    if (l>=r1_4) then vg[l,i,j]:= vg[l,i,j]+w1; end;
  if uw.ItemIndex=3 then // unequable distribution, the №3 type
    begin if (l>=r1_4) and (i=w3) then vg[l,i,j]:= vg[l,i,j]+w1;
    if (l<w3) then vg[l,i,j]:= vg[l,i,j]+w1; end;
  if uw.ItemIndex=4 then // unequable distribution, the №4 type
    begin if (l>=r1_4) and (i<w3) then vg[l,i,j]:= vg[l,i,j]+w1;
    if (l<wn3) then vg[l,i,j]:= vg[l,i,j]+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](image-url)
The conditional flow rates \( W \) for these three cases are equal: 1- \( W=2 \); 2- \( W_c=2 \) at the baffles, \( W_c=6 \) on the central axis of the flow; 3- \( W_{a1}=2 \) at the upper baffle, \( W_c=6 \) at the central axis of the flow, \( W_{a1}=4 \) 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 velocities 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

Mathematical and computer simulation of particle redistribution and behavior (Bakhtiyar Rashidovich Ismailov)
BIOGRAPHIES OF AUTHORS

Bakhtiyar Rashidovich Ismailov
Doctor of Technical Sciences (2006), Professor of the Ministry of Education and Science of the Republic of Kazakhstan (2010). Currently, he works as a full professor at the Department of Information Systems and Modeling of the M. Auezov South Kazakhstan University. Research interests are represented in the following areas: mathematical and numerical modeling of phase interaction in contact devices of chemical technology devices; modeling and calculation of gas distribution in case of man-made emergencies; alternative energy. He can be contacted at email: ismailovb@mail.ru.

Leyla Mukhamedjanovna Musabekova
Doctor of Technical Sciences (2010), In 2010, on December 27, she successfully defended her doctoral dissertation in the specialty 05.17.08. Processes and apparatus of chemical technologies on the topic “Scientific foundations of modeling chemical devices with moving fronts of separation of kinetic zones.” Currently she works as a professor at the Department of Computing Technology and Software at the Auezov South Kazakhstan University. Research interests: computer modeling of reaction-diffusion processes, aggregation and swarming processes. She can be contacted at email: mleyla@mail.ru.
Zhanat Rysbayevna Umarova received her PhD degree in Informatics, Computer Engineering and Control from Ministry of Education and Science, in 2013. Currently she works as an Associated Professor of Information Systems and Modeling department at M. Auezov South Kazakhstan University. She has supervised and co-supervised more than 20 masters students. She has authored or coauthored more than 100 publication. Her research interests include Mathematical modeling, Computer simulation, Information security and data protection in information systems, web-programming, renewable recourses. She can be contacted at email: zhanat.umarova@auezov.edu.kz.

Khairulla Bakhtiyarovich Ismailov Candidate of Technical Sciences, Associate Professor of the Department of Information Systems and Modeling of M. Auezov South Kazakhstan University. In 2006 he defended his Ph.D. thesis on "Hydrodynamics and Mass Transfer in an Apparatus with Regular Vibrating Spiral Nozzles". Research interests: mathematical and computer modeling of chemical technology processes. He can be contacted at email: ismailovkhb@mail.ru.

Kuttybek Arystanbayev In 2007, on February 27, he successfully defended his Ph.D. thesis in the specialty 05.17.08 - Processes and apparatus of chemical technologies on the topic "Modeling the high-temperature process of the afterburning of toxic substances in the cooled zones of multicomponent steam-gas flows." Currently he works as a professor at the Department of "Technology of pharmaceutical production" at the South Kazakhstan Medical Academy. Research interests: computer modeling of the fuel combustion process in thermal power plants. He can be contacted at email: arystanbayev74@mail.ru.