CHEMICAL ENGINEERING TRANSACTIONS
VOL. 94, 2022
A publication of AIDIC
The Italian Association of Chemical Engineering
Online at www.cetjournal.it
Guest Editors: Petar S. Varbanov, Yee Van Fan, Jiří J. Klemeš, Sandro Nižetić

ISBN 978-88-95608-93-8; **ISSN** 2283-9216
DOI: 10.3303/CET2294170

Computer Simulation of Attractive Swarming Accompanied by Particles Aggregation in Dispersed Systems

Leila Musabekova[a,b,*], Kuttybek Arystanbayev[b], Madina Jamankarayeva[c], Madamin Amandikov[d]

[a]Auezov University of South Kazakhstan, Tauke Khan, 5, Shymkent, 160012, Kazakhstan
[b]South Kazakhstan Medical Academy, Al-Farabi square, 1, 160019, Kazakhstan
[c]South Kazakhstan State Pedagogical University, Baitursynov street, 13, Shymkent,160012, Kazakhstan
[d]People Friendship University named after Academic A.Kuatbekov, Tole bi street, 32, Shymkent, Kazakhstan
leila.musabekova2@auezov.edu.kz

In the previous works a systematic analysis of swarming processes, accompanied by particles aggregation with formation of high-order clusters in dispersed flows, has been carried out. As a result of the analysis, it was proposed to consider three main swarming mechanisms. However, only the inertial mechanism was previously considered in detail. In submitted work, this approach has been firstly adapted to simulating swarming according the attractive mechanism in dispersed system with allowance for the aggregation process. The research novelty, peculiarity and originality of this development lie in that the phenomenon of swarming, accompanied by aggregation, arising under influence of attraction centers, is modeled using a special probabilistic calculation scheme that is allowing to offer a universal approach to modeling attractive swarming under different physical nature of interaction. The paper presents the algorithm, results of numerical experiments and gives their brief interpretation. The results of numerical experiments have shown that the phenomenon of attractive swarming can significantly reduce the efficiency of the device, because up 4 to 50 % of the volume of the apparatus may be excluded from work during the process period.

1. Introduction

The nature of attractive swarming can be very diverse (Aibara et al., 2020). This is due to the complexity of the concept of swarming itself (Kim et al., 2015). In essence, swarming arises as a manifestation of self-organization phenomena in complex non-equilibrium systems (Carranza and Coates, 2000). In real physical systems, attractive swarming can arise due to the attraction of particles in a disperse system to certain centers (Villa et al., 2020) or regions of attraction localized in a volume (Rütschlin and Böttcher, 2020). Attractive swarming can also be caused by the concentration gradient of some substance in the area of motion of the particle system (Su et al., 2018). In biological systems (Brückner et al., 2019), attractive swarming can be caused by movement in the direction of some bait (Rocha-Gregg and Huttenlogher, 2021) or following the leader (Be'er and Ariel, 2019).

Recently, the concept of swarming has also been used to describe the phenomena of community formation in the social sciences and economics (Carrillo et al., 2010). In this context, the concept of attractive swarming seems to be the most suitable for the purposes of a formal mathematical description of the phenomenon (Bouffanais, 2016).

The most general idea for describing attractive swarming is probably the concept of a "common goal" for a system of not necessarily interacting (but able to interact with each other) moving objects (particles) of some dispersed system (Monaco et al., 2020). This implies some common nature of the objects that make up the system.

At the same time, the particles that make up the system are also subject to random drift under the influence of various factors and features of the medium in which the particles move (Weber et al., 2015). Strictly speaking, an adequate description of such a phenomenon in the form of some purposeful process (Rimer and Ariel, 2017)

Paper Received: 18 May 2022; Revised: 03 July 2022; Accepted: 03 July 2022
Please cite this article as: Musabekova L., Arystanbayev K., Jamankarayeva M., Amandikov M., 2022, Computer Simulation of Attractive Swarming Accompanied by Particles Aggregation in Dispersed System, Chemical Engineering Transactions, 94, 1021-1026 DOI:10.3303/CET2294170

requires knowledge of the specific features and details both of the phenomenon of attraction in the system and nature of the attractor itself (Jose and Singh, 2020). Swarming can be accompanied by aggregation of primary particles of the dispersed phase (Pirani et al., 2013). In this case, the primary particles form clusters-aggregates that are stable for some time (Ha et al., 2019) and move in the medium as a single particle of a higher order (Dong et al., 2021). The order of a cluster is understood here as the number of its constituent primary phase particles (Brener, 2011). Aggregation can be considered as a "strong" swarming, since swarming in any case implies an increased concentration of particles in the swarm (Tadmor and Tan, 2014), and the swarm moves as a single object with a certain velocity vector of the center of mass in the swarm.
At the same time, the forces that prevent the disaggregation of a cluster can have a different nature as well as forces responsible for attractive swarming (Sun et al., 2021). In this work, the task is to create a universal approach to modeling swarming accompanied by aggregation, and to test this approach for modeling a process in the case of an attractive swarming mechanism. For this purpose, a novel approach to modeling attractive swarming that does not use a specific attractor action mechanism has been submitted. It is probabilistic approach based on the concept of random walks on lattices (Montroll, 1965). Similar approach has previously been successfully tested to describe the complex process of liquid distribution over the packings of chemical columns (Brener, 2002). The same concept was used to model the processes of aggregation in the dispersed phase in flow devices both for the case of diffusion-limited aggregation (DLA) and for mixed kinetics (Brener et al., 2017).

2. Computer simulation

The algorithm used in this paper for the numerical study of attractive swarming is a modification of the algorithm previously proposed in the work by Brener et al. (2021), and which used early to describe swarming induced by the uneven velocity field of a continuous medium in the apparatus. The process of movement and aggregation of particles is described with the help of methods of random walk on a stochastic lattice (Brener et al., 2017).

2.1 Description of the modelling concept and the algorithm

The principal feature of the modified algorithm is that the influence of the attractor on the drift of particles is described by the prevalence of the transition probability from a given cell to that lattice cell adjacent to it, which is located closer to the attractor. The idea of the algorithm is illustrated in Figure 1.

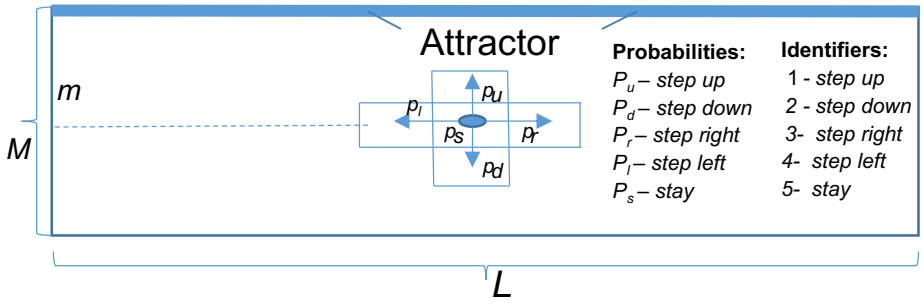


Figure 1: Illustration for the description of the random walk algorithm in the presence of an attractor on the upper wall

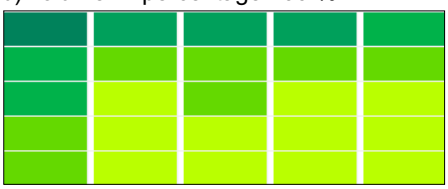
In order to implement the simplest model of an increase in particle acceleration in the direction of an attractor as it approaches it, the following scheme for choosing drift probabilities has been proposed. The choice of an identifier for calculating the drift during an acceleration that increases when approaching the attractor is carried out by random selection from a sequence of drift direction identifiers (1 - up, 2 - down, 3 - right, 4 - left, 5 - stay in place). This sequence is formed as follows for any element located in the row m. Here m is considered from top to bottom - from the attractor. That is, as the row number of the matrix is usually considered). Therefore, 1 is taken $(M - m + p_0)$ times; 2, 3, 4 and 5 - p_0 times for each digit. For example, if *M = 20, m = 8,* p_0 = 2, then the sequence for selection looks as: 11111111111111122334455. The parameter p_0 plays the role of a control parameter. To the chosen random drift is added, as before, the drift to the right by w cells (w - flow velocity). When processing the experimental data on random drift, the grid-coarsening scheme is used, as before (Brener et al., 2021). For the process of particle aggregation in the present work, the mechanism of diffusion-limited aggregation (DLA) was adopted.

2.2 Results of simulation

The *2D* scheme was used. The calculations were made for $p_0 = 1, 2, 3$ and $w = 0, 2, 4$. The nominal width of the reactor (number of rows in the calculated matrix) was taken equal to *M* = 20. The nominal reactor length (number of columns in the calculated matrix) was taken equal to *L* = 200. Some illustrative simulation results are presented in Figures 2 - 7. Figures 2, 3, 4 and 5 correspond to the situation when at the initial moment the reactor is completely filled, and each cell contains exactly one primary particle. Figures 2 - 7 show the evolution of the distribution of clusters over the volume of the apparatus through a different numbers of calculation time intervals *dt*. It can be seen that the presence of an attractor leads to a rapid redistribution, as a result of which the main number of clusters is concentrated in the vicinity of the attractor. At the same time, intensification of the aggregation process occurs in this region, and the total number of clusters of the dispersed phase decreases, but the sum of clusters orders increases.

a) volume fill percentage 100 %

b) volume fill percentage 100 %



c) volume fill percentage 92%

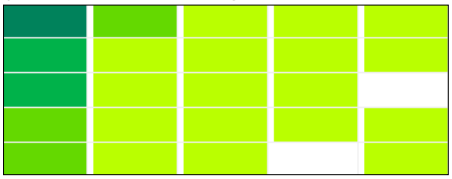
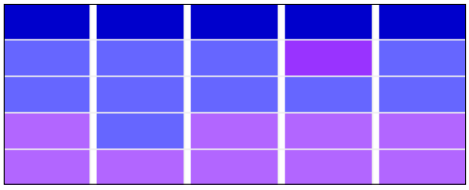
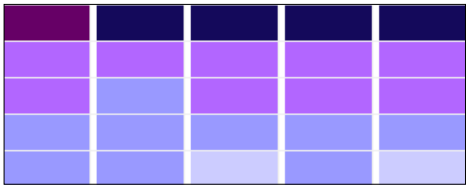


Figure 2: The number of clusters of different orders in blocks. Matrix size 200 x 20, conditional flow rate w = 2, p_0 = 1, initial number of clusters in each cell is equal to one. Time step: a) dt = 3, b) dt = 15, c) dt = 100. The number of clusters into the block (the same colours in all Figures): 0 - 20 20 - 40 40 - 60 60 - 80 80 - 100 100 - 120 120 - 140 140 - 160 160 - 180 180 - 200

a) *volume fill percentage 100 %*



b) *volume fill percentage 100 %*



c) volume fill percentage 92 %

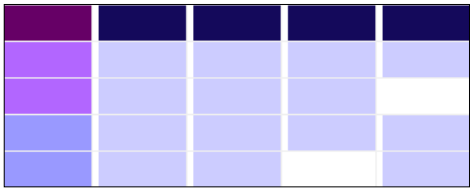
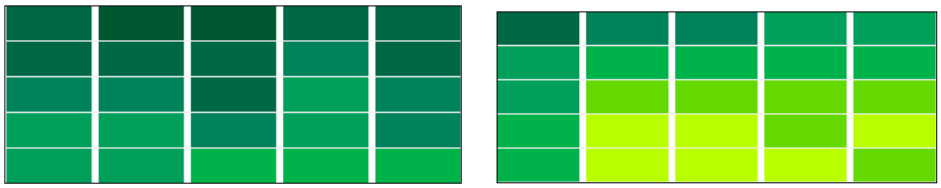


Figure 3: The sum of clusters orders in blocks. Matrix size 200 x 20, conditional flow rate w = 2, p_0 = 1, initial number of clusters in each cell is equal to one. Time step: a) dt = 5, b) dt = 15, c) dt = 100. The sum of clusters orders into the block (the same colours in all Figures): 0 - 40 40 - 80 80 - 120 120 - 160 160 - 200 200 - 240 240 - 280 280 - 320 320 - 360 360 - 400 400 - 440 440 - 480 480 - 520 520 - 560 > 560

a) *volume fill percentage 100 %*

b) *volume fill percentage 100 %*



c) volume fill percentage 100 %

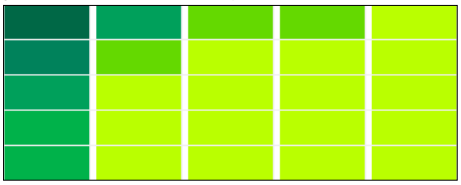
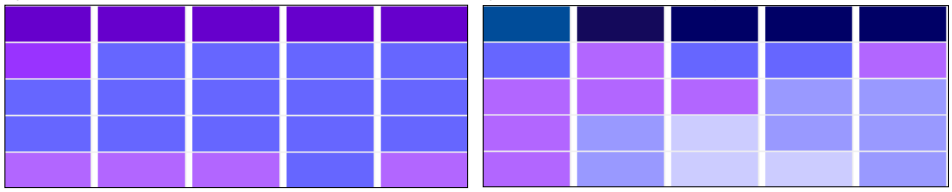


Figure 4: The number of clusters of different orders in blocks. Matrix size 200 x 20, conditional flow rate w = 4, p_0 = 1, initial number of clusters in each cell is equal to one. Time step: a) dt = 3, b) dt = 8, c) dt = 50

a) *volume fill percentage 100 %* b) *volume fill percentage 100 %*



c) volume fill percentage 100 %

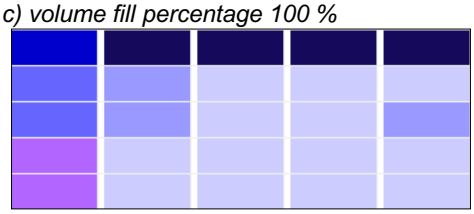
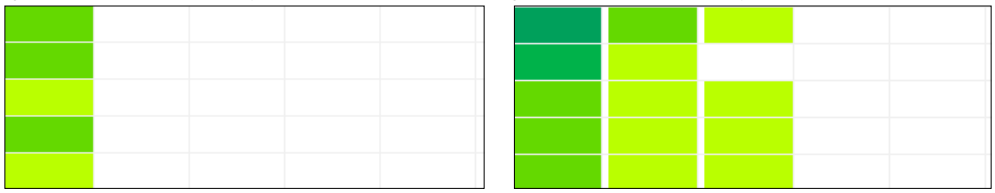


Figure 5: The sum of clusters orders in blocks. Matrix size 200 x 20, conditional flow rate w = 4, p_0 = 1, initial number of clusters in each cell is equal to one. Time step: a) dt = 3, b) dt = 8, c) dt = 50

Figures 6 and 7 correspond to the situation when at the initial moment the reactor is empty, that is, there are no primary particles in the cells.

a) volume fill percentage 20 % *b) volume fill percentage 56 %*



c) volume fill percentage 80 %

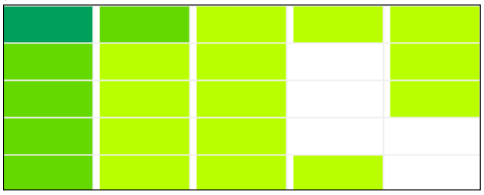
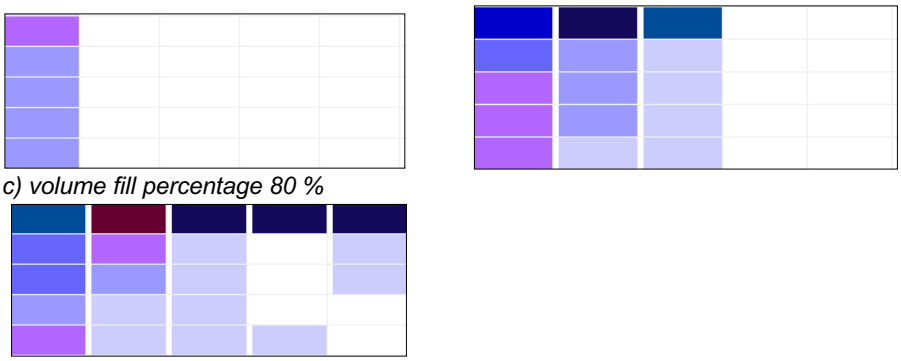


Figure 6: The number of clusters of different orders in blocks. Matrix size 200 x 20, conditional flow rate w = 2, p_0 = 3, initial number of clusters in each cell is equal to zero. Time step: a) dt = 5, b) dt = 50, c) dt = 100

a) volume fill percentage 20 % *b) volume fill percentage 60 %*



c) volume fill percentage 80 %

Figure 7: The sum of clusters orders in blocks. Matrix size 200x20, conditional flow rate w = 2, p_0 = 3, initial number of clusters in each cell is equal to zero. Time step: a) dt = 5, b) dt = 50, c) dt = 100

The calculation results clearly demonstrate the influence of the attractor distributed along the upper wall on the formation of swarms and the acceleration of particle aggregation with the formation of high-order clusters. At lower flow rates in the reactor, the formation of swarms under the influence of the attractor occurs faster at the initial section of the reactor. In an initially empty reactor, the influence of the attractor manifests itself in a slower filling of the reactor. Swarming under the influence of an attractor leads to a noticeable acceleration of DLA aggregation in the reactor. The analysis of the calculation results makes it possible to reveal some general regularities.

1. In the case where the initial number of clusters in each cell is equal to one. The total number of clusters in the calculation area first increases due to the influx of new particles into the apparatus, and then it begins to decrease due to the aggregation process. After a sufficiently large number of calculation steps (*dt* = 100), a dynamic equilibrium is established, i.e. the number of clusters becomes approximately stable. At the same time, a part of the volume of the apparatus remains weakly filled. The data on the percentage of filling of the volume of the apparatus for various flow rates are shown in Figures.
2. In general, the same picture has been observed for the case when the initial number of clusters in each cell is equal to zero. Only in this case, the initial period, when the volume of the apparatus becomes filled, is longer. The calculation results clearly show that the presence of an attractor quickly leads to localization of the process in a small region of the working volume. In this case, a significant part of the working volume of the reactor remains empty. This phenomenon can be characterized as a decrease in the efficiency of the apparatus. Apparently, more detailed studies are needed here in order to give quantitative estimates of this phenomenon. Since the algorithm is based on a stochastic process, repetition of calculations with the same set of parameters experiences some fluctuations in the results, which do not change the qualitative behavior.

3. Conclusions

The main contribution of this work is a universal approach to modelling attractive swarming accompanied by particle aggregation in a disperse system based on the apparatus of random walk statistics on mathematical lattices has been proposed. The algorithm for a numerical experiment and the corresponding code has been developed too. The calculation results clearly show that the presence of an attractor quickly leads to localization of the process in a small region of the working volume. In this case, a significant part of the working volume of the reactor remains empty (up 4 to 50 % in some calculations). This phenomenon can be characterized as a decrease in the efficiency of the apparatus. Apparently, more detailed studies are needed here in order to give quantitative estimates of this phenomenon. Although the work is theoretical, the con-ducted numerical experiments showed good interpretability of the results from the point of view of the physics of the process. The developed approach, after refinement and necessary adaptation, can be useful in designing devices and solving various engineering problems.

Nomenclature

m – current row
M – number of rows
w – flow velocity, m/s
p_0 – control parameter
L – reactor length, m
dt – time intervals, s

References

Aibara I., Huang Ch.-H., Kudo T., Bresolí-Obach R., Hofkens J., Furube A., Masuhara H., 2020, Dynamic Coupling of Optically Evolved Assembling and Swarming of Gold Nanoparticles with Photothermal Local Phase Separation of Polymer Solution, The Journal of Physical Chemistry, 124, 16604-16615.

Be'er A., Ariel G., 2019, A Statistical Physics View of Swarming Bacteria, Movement Ecology, 7(1), 1-17.

Bouffanais R., 2016, Design and Control of Swarm Dynamics, Springer-Verlag, Singapore.

Brener A.M., 2002, Adaptation of Random Walk Methods to the Modelling of Liquid Distribution in Packed Columns, In: Advances in Fluid Mechanics IV, WIT Press, 291-300.

Brener A.M., 2011, Nonlocal Model of Aggregation in Dispersed Systems, Theoretical Foundations of Chemical Engineering, 45(3), 349-353.

Brener A., Musabekova L.M., Jamankarayeva M.A., 2017, Stochastic Lattice Model of Aggregation in Heterogeneous Polydisperse Media, Chemical Engineering Transactions, 60, 79-84.

Brener A.M., Musabekova L.M., Dausheyeva N.B., 2021, On Modelling the Swarming in Dispersed Systems, Chemical Engineering Transactions, 84, 217-222.

Brückner, D.B., Fink, A., Schreiber, C., Röttgermann, P.J.F., Rädler, J.O., Broedersz, C.P., 2019, Stochastic nonlinear dynamics of confined cell migration in two-state systems. Nature Physics, 15(6), 595-601.

Carranza, P.M., Coates, P.S., 2000, Swarm modelling, Proceedings of the 3rd Generative Art Conference (GA2000), Milan: Generative Design Lab Milan, Polytechnic University, Italy.

Carrillo J.A., Fornasier M., Toscani G., Vecil F., 2010, Particle, Kinetic and Hydrodynamic Models of Swarming. In: Mathematical Modeling of Collective Behavior in Socio-Economic and Life Sciences, 297-336.

Dong Y., Wang L., Yuan K., Ji F., Gao J., Zhang Z., Du X., Tian Y., Wang Q., Zhang L., 2021, Magnetic Microswarm Composed of Porous Nanocatalysts for Targeted Elimination of Biofilm Occlusion, American Chemical Society Nano, 15(3), 5056-5057.

Ha S.-Y., Kim D., Lee J., Noh S.E., 2019, Particle and Kinetic Models for Swarming Particles on a Sphere and Stability Properties, Journal of Statistical Physics, 174, 622-655.

Jose R., Singh V., 2020, Swarming in Bacteria, J. Indian Inst. Sci., A Multidisciplinary Reviews Journal, 100(3), 515-524.

Kim S.H., Madak-Erdogan Z., Bae S.C., Carlson K.E., Mayne C.G., Granick S., Katzenellenbogen, B.S., Katzenellenbogen J.A., 2015, Ligand Accessibility and Bioactivity of a Hormone−Dendrimer Conjugate Depend on pH and pH History, Journal of the American Chemical Society, 137, 10326−10335.

Monaco J.D., Hwang G.M., Schultz K.M., Zhang K., 2020, Cognitive Swarming in Complex Environments with Attractor Dynamics and Oscillatory Computing, Biological Cybernetics, 114(2), 269-284.

Montroll E.W., Weiss G.H., 1965, Random Walks on Lattices. II, AIP Journal of Mathematical Physics, 6, 167-181.

Pirani M., Bazirat T.H., Farshad A., 2013, Study of Swarm Behavior in Modeling and Simulation of Cluster Formation in Nanofluids, Hindawi Publishing Corporation, Modelling and Simulation in Engineering, ID 142165.

Rimer O., Ariel G., 2017, Kinetic Order-Disorder Transitions in a Pause-and-Go Swarming Model with Memory, Journal of Theoretical Biology, 419, 90-99.

Rocha-Gregg B.L., Huttenlogher A., 2021, Swarming Motility in Host Defense, Science, 372(6548), 1262-1263.

Rütschlin S., Böttcher T., 2020, Inhibitors of Bacterial Swarming Behavior, Chemistry - A European Journal, 26, 964-979.

Su G., Lu G., Yan P., 2018, Improved particle swarm optimization for fast block matching with application to motion estimation in micro/nano systems, 14th IEEE/ASME International Conference on Mechatronic and Embedded Systems and Applications (MESA), Oulu, 1-6.

Sun M., Fan X., Tian C., Yang M., Sun L., Xie H., 2021, Swarming microdroplets to a dexterous micromanipulator, Advanced Functional Materials, 2011193, 31(19), 1-11.

Tadmor E., Tan C., 2014, Critical Thresholds in Flocking Hydrodynamics with Non-Local Alignment, Philosophical Transactions of the Royal Society A 372, 20130401, 1-22.

Villa K., Děkanovský L., Plutnar J., Kosina J., Pumera M., 2020, Swarming of Perovskite-Like Bi_2WO_6 Microrobots Destroy Textile Fibers under Visible Light, Advances Functional Materials, 2007073, 1-10.

Weber, C.A., Suzuki, R., Schaller, V., Aranson, I.S., Bausch, A.R., Frey, E., 2015, Random bursts determine dynamics of active filaments. Proceedings of the National Academy of Sciences (PNAS), 112(34), 10703–10707.