

# Computer Modelling of the Process of Separation of Heterogeneous Elements (Spheres)

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**Abstract.** This scientific study considers the results of a computer experiment with heterogeneous elements (spheres) that proved to be of decisive importance during the separation process, namely their degree of activity, mobility and falling. It has been found that a detailed analysis of the Liapunov function indices allows to effectively understand and predict the dynamics of complex dynamical systems. The results obtained indicate significant changes in the physical and mechanical parameters of spherical balls under the influence of various factors and the environment. It was found that a certain accumulation of spheres occurs due to an increase in the time for simulation. It was also found that the key characteristics of the bulk mass of spherical elements significantly depend on the moulding process, surface condition and environmental conditions.

## 1 Introduction

Non-homogeneous elements, in particular spheres, can be considered as heterogeneous suspensions or mixtures of various components of any materials [1, 2]. In our context, spheres are individual particles or heterogeneous elements in a heterogeneous medium (heterogeneous system) [3, 4, 5]. In particular, spheres are circular heterogeneous particles that can be solid objects or elements that have the shape of a sphere (i.e., a circle) [6, 7, 8]. It should be noted that such elements are geometric bodies in which all points of the surface are equal in distance from a central point called the centre of the sphere [9, 10, 11]. Spherical particles are often used as a model for studying various physical and chemical phenomena in scientific research, and they are widely used in various fields [12, 13, 14].

The study of spherical particles is a mathematically convenient approach for analysis and computer modelling [15, 16, 17]. In some cases, when a circular element or object can be approximated by a sphere shape, it simplifies calculations and solving various problems [18, 19, 20]. For example, in our case, we study elements with spherical particles and the process of their separation. Modelling of such particles with a detailed study of separation can be used to analyse their behaviour, properties, and interaction in a heterogeneous system. One possible approach is to consider a heterogeneous system as a set of spheres with different physical and mechanical characteristics. Such a system may include spheres with different sizes, densities, hardnesses, shape factors, coordination numbers, etc. In order to model the separation process for such a heterogeneous system, we need to take into account the various physical and mechanical parameters of each individual sphere (element), as well as their interaction during the separation process.

Therefore, the development of an adequate and universal physical and mathematical model for such a heterogeneous system of sphere research with a combination of computer modelling includes

elements of the theory of distributed placement, medium mechanics and various interactions between spheres. It should be noted that taking into account such a large number of factors requires the use of numerical methods and computer simulations to obtain high-quality and reliable approximation solutions. It should also be noted that such an approach will allow us to take into account the diversity of components in a heterogeneous system and their interaction, which is important for understanding and optimising the processes of separation of heterogeneous media.

The relevance of the topic lies in the fact that the study of computer modelling of heterogeneous systems represented by spherical particles is of great practical importance in various fields, such as modelling, industry, science and medicine. Taking into account heterogeneities in the form of spheres can be key to understanding and improving the separation processes of any materials. Thus, the study of the interaction and separation of inhomogeneous systems consisting of spherical particles requires partial improvement, as it has wide practical applications and can lead to important scientific and technological discoveries.

## 2 Main part

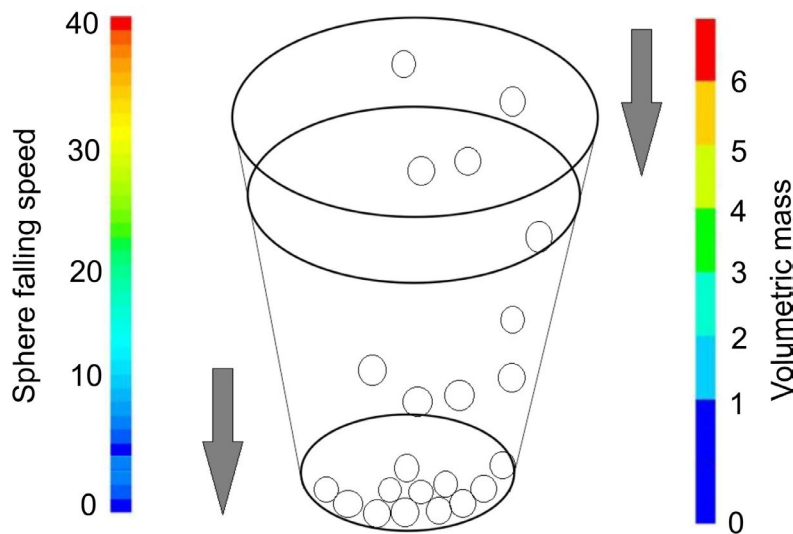
In the literature [21, 22, 23], spheres are considered as heterogeneous elements or particles in a heterogeneous medium. It has been shown that they can be solid objects that have the shape of a sphere. Also, the basic boundary conditions that need to be set in the simulation are partially covered. In [24, 25, 26], it was investigated that spheres are geometric bodies in which all surface points are equal to the distance from the centre point of the circle, i.e., the centre of the sphere. An analysis of works [27, 28, 29] has shown that spherical elements are often used as a model for studying various physical and chemical phenomena in scientific research. However, it is unclear in which fields the authors intended to use this approach. Papers [30, 31, 32] substantiate the study of mainly spherical particle shapes, and also highlight mathematical approaches, analysis and simulation of computer modelling with the possibility of approximating round elements. Research teams [33, 34, 35] describe experiments that take into account the main parameters, such as size, density, shape and hardness, which is important for the filling simulation process. It should be noted that the analysis of literature sources well defines the areas of research, methodology and practical significance of the study and justification of spherical elements in heterogeneous systems, while requiring minor improvement. Therefore, the study of the process of separation of inhomogeneous elements (spheres) based on computer modelling [36, 37, 38] is an urgent issue.

The aim of the study is to investigate the process of separation of spheres (elements) on the basis of computer modelling [39, 40, 41], as well as to analyse the dynamics of a system that includes separated spherical elements and determine the main factors that affect their behaviour.

**Materials.** The process of separation of heterogeneous elements, namely spheres, is the procedure of separating or extracting spherical particles from a heterogeneous system based on certain characteristics of the particles or the medium. This process may involve the use of a variety of methods and approaches to separate spherical elements [42, 43] from other components of the system. For example, a separation procedure may include filtration, centrifugation, sedimentation, or other methods aimed at separating spherical objects from other components of a heterogeneous system.

For the effective implementation of computer and numerical modelling, a number of physical and mechanical characteristics of heterogeneous elements (spheres) were taken into account. Among them, it is worth noting the Young's modulus of 0.1 MPa, the Poisson's ratio of 0.7, and the friction coefficient of 0.5. The volume mass of the spherical elements was in the range of 100 to 300 kg/m<sup>3</sup>. Also, the parameters of the heterogeneous medium were taken into account, in particular, the falling velocity, dynamic viscosity, average coordination number, Prandtl's coefficient of 0.4, etc. In addition, to ensure the accuracy of the numerical analysis, the grid cell size for the simulation was set to 0.01 mm. It should be noted that this approach is aimed at ensuring a reliable and accurate representation of physical phenomena in a heterogeneous environment system, allowing for reliable computer modelling results.

Figure 1 shows the results of a computer experiment of sphere separation, taking into account the main physical and mechanical parameters.



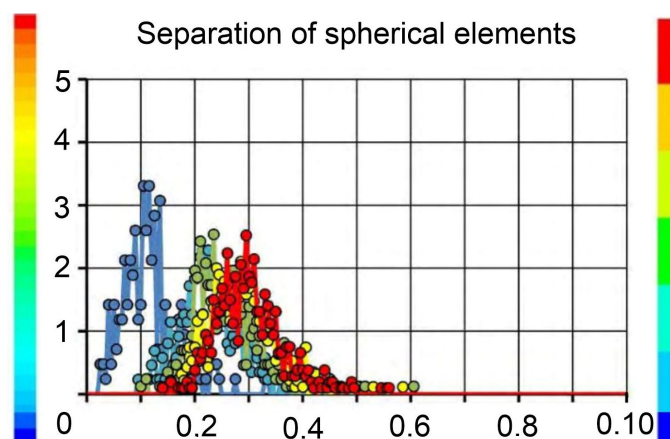
**Fig. 1.** Computer experiment of sphere separation taking into account the main physical and mechanical parameters

It should be noted that the total number of experiments in the field of numerical and computer modelling was 9. In the process of evaluating the quality of the separation process of heterogeneous elements (spheres), the mass distribution of components was used by two indicators:

- 1) by volume mass at the outputs of heavy elements, which was denoted by the symbol  $\rho(v)$ ;
- 2) by volume mass at the outputs of light components, which was denoted by the symbol  $\rho(l)$ .

During the experiment, it was found that during the analysis and simulation of the data elements, an important task arises – to identify the dependencies of the concentration of sphere components on the volume mass  $\rho$  in general, as well as on the volume mass of heavy  $\rho(v)$  heterogeneous elements and light  $\rho(l)$  sphere components in the context of various factors of computer modelling.

Figure 2 shows the developed computational scheme of the process of separation and movement of heterogeneous elements (spheres) based on modelling.



**Fig. 2.** Schematic of the process of separation and movement of heterogeneous elements (spheres) based on a computer experiment

It should be noted that as for the first stage of numerical modelling, a computational scheme was developed to study in detail the process of movement of falling heterogeneous particles, which occurs mainly under the influence of external factors. The developed computational scheme also includes complex aspects that are oriented and focused on the procedure of interaction of round

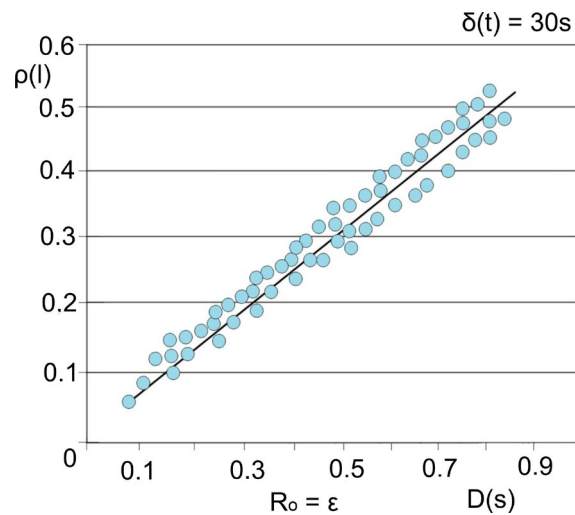
particles with a heterogeneous medium, i.e., the minimum and maximum fall of spheres, their movement and their qualitative distribution in the system.

The proposed scheme for a detailed study of the process of movement and separation of falling heterogeneous particles (in particular, spheres) shows that more attention should be paid to the coefficients of mass distribution of spherical elements. In particular, this applies to the volumetric mass of heterogeneous elements at the outlets, i.e.  $\rho(v)$  and  $\rho(l)$ . We also found out that the actual diameter of the spheres  $D(s)$  plays an important role.

**Tests.** To determine the detailed mass distribution of spherical elements in a heterogeneous system, we used one of the mathematical algorithms, the Frank-Wolfe algorithm. The Frank-Wolfe algorithm is a numerical method for solving optimisation problems. It is used to find the minimum or maximum of a function that can be differentiable or undifferentiable. It should be noted that this algorithm belongs to the class of qualitative optimisation methods, which is based on a combination of the methods of anchor points and projection methods. The main idea of our algorithm is that it uses successive projections on convex sets to approximate the optimum points. The implementation of the desired functions is a complex process and has certain limitations, but it can be easily achieved by computer modelling. That is, we consider a situation with two trajectories of the volume mass of heterogeneous elements at the outputs  $\rho(v)$  and  $\rho(l)$ , which are separated by a small distance from each other  $R_0 = \varepsilon$ . After a certain time interval  $\delta(t)$ , these trajectories reach a value in the heterogeneous system equal to  $R_1$ . For each step, the maximum Liapunov exponent was determined according to the following mathematical formula:

$$\lambda = \log |r / r| / \delta(t) \quad (1)$$

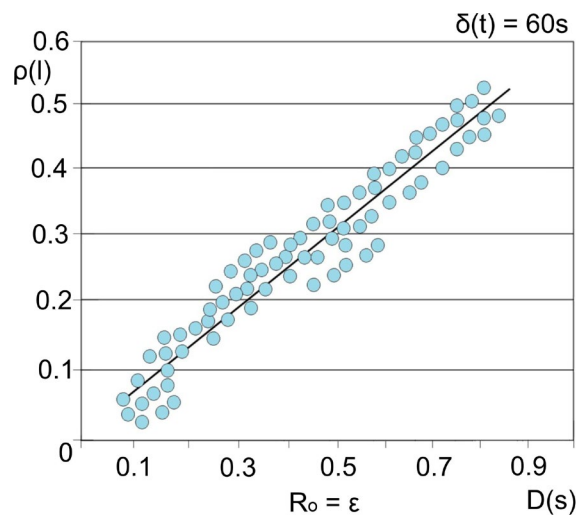
It should be noted that as the calculation time increases, the coefficient of the Liapunov exponent approaches the real value, and in this case, we can determine the stability and instability of the dynamic system. It should be noted that as the duration of the Liapunov coefficient calculation increases, its value adapts to the actual dynamics of the system, providing more accurate results. This approach allowed us not only to determine the stability of the system at a certain point in time, but also to take into account its evolution with changes in parameters or initial conditions. Such an analysis proved to be extremely useful in modelling and predicting the behaviour of systems under different conditions. It is important to note that the accuracy of the results depends heavily on the correct choice of calculation parameters and consideration of the system's characteristics. To implement this approach, we investigated the effect of the bulk mass of heterogeneous elements on the diametric size of the elements (spheres). The system under consideration is described by a separate function, to which the main parameters of the spheres and the system, the initial values of the variable parameters, and the calculation time are passed. It should be noted that the body of this function defines mainly the parameters of the right-hand side and the Jacobian determinants of the matrix of the heterogeneous system, which are used to form equations in certain variations. As a result of our computer studies, we have obtained the following dynamics of Liapunov's indicators, which is shown in Figure 3.



**Fig. 3.** Scalar indices of the mass distribution of heterogeneous elements from diametrical size of elements (spheres)

It should be emphasised that the volume mass of the lightweight components  $\rho(l)$  varied from 0 to  $0.6 \text{ kg/m}^3$  and the study lasted for 30 seconds at a remote distance from each other according to the system  $R_0 = \varepsilon$ . In turn, the diameter size of the components was 0.1-0.9 mm. The results obtained show that the degree of activity and mobility of spherical elements is important. It is worth emphasising that such a detailed analysis of the Liapunov function indices can serve as a powerful tool for understanding and predicting the dynamics of complex dynamic systems. Also, the obtained dependence of scalar products shows that under the influence of various factors and the environment, some physical and mechanical parameters of spherical balls can change significantly.

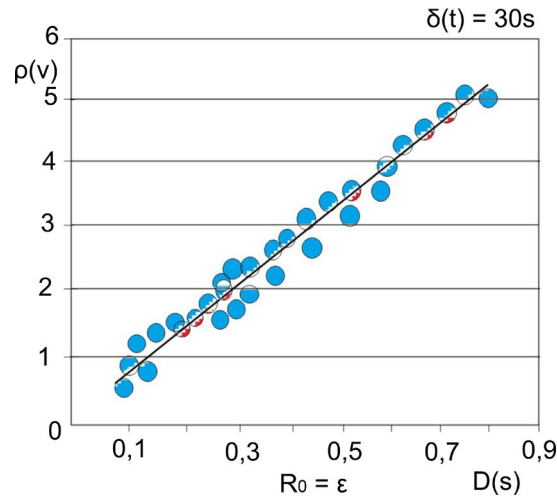
Figure 4 shows the active dynamics of computer modelling indicators within the experimental study time of 60 seconds.



**Fig. 4.** Dynamics of indicators of mass distribution of heterogeneous elements from size of elements (spheres) during  $\delta(t)=60$  seconds

It should be noted that the mass of the light components  $\rho(l)$  varied from 0 to  $0.6 \text{ kg/m}^3$ , the radius of the spheres varied from 0.1 mm to 0.9 mm, the experiment time lasted 60 seconds, and the heterogeneous system was constant and equal to  $R_0 = \varepsilon$ . The results show a much larger accumulation of spherical elements along the correlation curve. However, the spheres interact well with each other and the environment, and their accumulation is explained by the fact that more time was allocated for the experiment – 60 seconds.

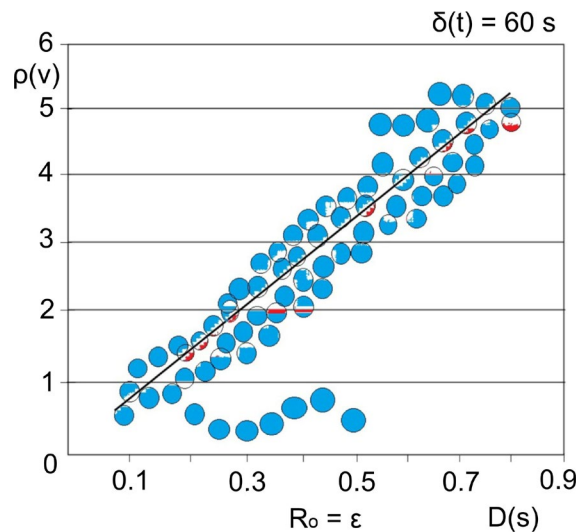
Figure 5 shows the volumetric mass of the heavy sphere elements  $\rho(v)$ , which varied from 0 to  $6 \text{ kg/m}^3$ , the simulation duration was 30 seconds, the size of the spheres varied from 0.1 mm to 0.9 mm, and the system operated within the range of  $R_0 = \varepsilon$ .



**Fig. 5.** Dynamics of the volumetric distribution of the mass of heavy heterogeneous elements  $\rho(v)$  from on the size of elements (spheres) during  $\delta(t)=30$  seconds

The obtained results of the volumetric mass distribution of heavy spheres of heterogeneous elements show that at a heavier bulk mass, the particles (spheres) also interact well with each other, but in this study we observed the separation of a small overlap of spheres on top of each other. This is most likely due to the quantitative distribution of heterogeneous elements by size. And also, by the length of time for computer modelling. It should also be noted that the main characteristics of the bulk mass of such heterogeneous spheres significantly depend on the process of its formation, the state of the surface of spherical particles, the conditions of movement and fall, as well as other factors.

Figure 6 shows again the bulk mass of heavy element spheres  $\rho(v)$ . It should be noted that the variation in the diameter dimensions of the spherical components was 0.1–0.9 mm, the volume mass was  $0\text{--}6 \text{ kg/m}^3$ , the experiment time was 60 seconds, and the inhomogeneous environment of the system was within the range of  $R_0 = \varepsilon$ .



**Fig. 6.** The dynamics of the mass distribution of heavy heterogeneous elements, determined by the function  $\rho(v)$  with respect to their size (spherical), during a time interval  $\delta(t)$  equal to 60 seconds

The results obtained show a qualitative process of separation of spheres according to their bulk mass and size variation. It should also be noted that the size of the spherical elements, in particular their radius (denoted as  $D$  (s)), is a critical and important factor in determining the contact surface area and volume. It is important to note that the mass of heavy elements or spheres has significant potential and has a much larger surface area and volume. On the other hand, a large volume can also increase the time required for numerical calculations. Thus, the choice of the optimal size of the spheres (spherical elements), taking into account their radius, depends on the specific application and requirements of the field of application, as well as on the needs and environmental effects of the heterogeneous system.

### 3 Conclusion

The results obtained indicate that the degree of activity and mobility of spherical elements is of great importance in a computer experiment. A detailed analysis of the Liapunov function indices can serve as an effective tool for understanding and predicting the dynamics of complex dynamical systems. The obtained dependences of scalar products show that the physical and mechanical parameters of spherical balls can change significantly under the influence of various factors and the environment.

Also, the generalised conclusions indicate that the volume mass of light components  $\rho$  (l), which varied from 0 to  $0.6 \text{ kg/m}^3$  with a sphere radius of 0.1 mm to 0.9 mm and an experiment duration of 60 seconds under steady-state conditions, indicates some accumulation of spherical elements. This separation process is explained by the allocation of more time for the experiment – 60 seconds.

The volumetric mass distribution of the heavy spheres of heterogeneous elements indicates their interaction, but separation is observed when the size and duration of the experiment are analysed in detail. It should be noted that the main characteristics of the bulk mass of spherical elements significantly depend on the formation process, surface condition, and environmental conditions. The results also emphasise the qualitative separation of spheres according to their bulk and size. The size of the spheres, in particular their radius, determines the contact surface and volume and is a critical factor in selecting the optimum size for a particular application and system requirements. It is important to keep in mind that the mass of heavy elements or spheres has a significant potential and depends on their volume and surface area. When selecting the size of the spheres, the specific conditions and requirements, as well as the influence of the environment in a heterogeneous system, should be taken into account.

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