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Mathematical Model of the Dynamics of Spherical Elements

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Abstract. This paper presents a study in the field of modelling the dynamics of spherical elements. The results obtained indicate the successful use of the discrete element method (DEM) as a numerical tool for analysing the behaviour of the system studied with the help of spheres. The results are based on the importance of correct consideration of the boundary conditions for the spheres, which determine the key aspects of modelling with the developed three-dimensional model. The developed model solves a number of important tasks, expanding the field of scientific research. Firstly, it allows studying the main parameters of the formation of a heterogeneous medium by analysing the compaction of spherical elements in different media. Next, the three-dimensional model is used to study the process of changing the structure of a heterogeneous medium from a static to an oscillatory state, which allows for a deeper understanding of this process. By modelling the mathematical behaviour of spherical elements under the influence of external and additional factors, a detailed understanding of their dynamics and contact interaction can be obtained. The application of the developed model to analyse the contact interaction of spherical elements in heterogeneous media allows predicting the main parameters of spheres and their heterogeneous environment with a reliable accuracy of up to ±1 %. It should be noted that the results obtained on the basis of the three-dimensional model are effective and indicate a number of practical applications in various fields.

1 Introduction

In modern scientific research, spherical elements have become the subject of in-depth analysis using mathematical models [1, 2, 3]. Understanding the dynamics of these elements is a key aspect in various fields of science and technology, from astrophysics to molecular biology [4, 5, 6]. It should be noted that the abstract concepts of mathematical models and their practical application in specific situations are a modern and urgent task of today. Therefore, it is important and necessary to carefully analyse various properties of spherical elements, in particular their motion characteristics based on their dynamics, interaction in various conditions, and the interaction of contacts with each other [7, 8, 9].

Mathematical models based on the discrete element method (DEM) are defined as an important tool for considering the real dynamics of these objects [10, 11, 12]. The DEM is becoming the main approach to modelling spheres and studying their motion and interaction in a general dynamic environment [13, 14, 15]. It should also be noted that the practical aspects of using such mathematical models in modern research, including their role in predicting and optimising various processes where spherical elements are key participants, are not well established [16, 17, 18]. There is also little research on how these models can influence the development of new technologies and innovations in various scientific fields [19, 20, 21]. By systematically analysing mathematical models of the dynamics of spherical elements, we aim to uncover the deep connections between theory and practice, identify new opportunities for research and technology development, and contribute to understanding the nature of various phenomena in which these elements are involved. Therefore, an important issue is to implement a mathematical model of the dynamics of spherical elements based on the developed three-dimensional model, revealing its application and importance in solving the challenges associated with their motion and interaction in various research contexts.

2 Main Part

Literature sources [22, 23, 24] shows that modern studies of spherical elements are based on the use of mathematical models. The key aspect of understanding the dynamics of spherical elements in various fields of science and technology is emphasised [25, 26, 27]. The method of discrete elements as the main tool for modelling the real dynamics of spherical elements has been partially substantiated [28, 29, 30]. Concerns have also been expressed about the insufficiently substantiated practical aspects of the use of mathematical models in modern research [31, 32, 33]. It is noted that an important issue is to study the impact of such models on the development of technologies and innovations in various scientific fields [34, 35, 36]. The importance of systematic analysis of mathematical models of the dynamics of spherical elements to reveal the deep connections between theory and practice, etc. is emphasised in [37, 38, 39]. Thus, it can be concluded that the above works have not sufficiently investigated a number of issues, including the study of the influence of three-dimensional models on the nature of various phenomena involving spherical elements. Therefore, from the analysis of literature sources, there is a great need for further research and improvement of the practical use of mathematical models [40, 41] of the dynamics of spherical elements in various fields of science and technology.

The purpose of the study is to implement a mathematical model of the dynamics of spherical elements based on the developed three-dimensional model, as well as to investigate the procedure of heat transfer between spherical elements at different temperatures [42, 43] and different ball radii.

Materials. The closest to describing the real dynamics of spherical elements is the discrete element method (DEM), which is the main approach to modelling spheres, as well as their motion and dynamics in general. The discrete element method is based on the study of the interaction of individual particles, as well as qualitative dynamics with all other elements in the layer of the dispersed medium. It should also be noted that this method uses mainly the Lagrangian reference frame, which allows taking into account the motion of each spherical element as a separate entity.

In the DEM, the balance of mechanical motion and dynamics of spheres is determined by considering the forces and qualitative interconnection between individual elements. Typically, the motion of the elements is modelled in three-dimensional space, and for each particle, its coordinates and velocity must be determined. Another important aspect of this method (DEM) is the consideration of non-static conditions, such as collisions, deformation and fracture. Our proposed discrete element method is as follows:

$$\begin{cases} m_i \cdot \dfrac{dv_i}{dt} = m_i \cdot b + \sum_{j=1}^{k} \cdot F_{ij} \, , \\ I_i \cdot \dfrac{dw_i}{dt} = \sum_{j=1}^{k} \cdot (T_{il} + M_{ij}) \, , \end{cases} \tag{1}$$

where: $m_i -$ mass of elements (mm); t – time (c); i – spherical element index; $v_i -$ linear velocity vector; $I_i -$ moment of inertia; $F_{ij} -$ external factors (force) affecting the elements i through the interaction of contacts with elements j; k – the total number of spheres that interact with each other with elements i; $T_{ij}-$ external torque, which is directly connected through the interaction of the contacts of the spherical elements i and j; $M_{ij}-$ falling moment (top to bottom).

It should also be noted that the above proposed mathematical model of element dynamics allows for a detailed study of the behaviour and motion of spherical elements under the influence of external factors. Moreover, such a discrete description of the movement (dynamics) of elements based on the DEM allows obtaining more accurate and realistic results, taking into account their internal structure and interaction of elements with each other.

In the discrete element method (DEM), where each elemental particle is modelled as a sphere of radius R_i, it is important to define the interaction between these elements using mathematical relations. Hence, we propose to use the following mathematical approach to describe the contact interaction, in particular:

$$n_{ij}\cdot F=\frac{4}{3}\cdot E\sqrt{R_i\cdot R_j}\cdot\delta^{3/2}\,, \tag{2}$$

$$t_{ij}\cdot F=\frac{8}{3}\cdot G\sqrt{R_i\cdot R_j}\cdot\delta^{1/2}\cdot v_{ij}\,, \tag{3}$$

where: E – Young's modulus of a heterogeneous medium; G – shear modulus of spherical elements; δ – the amount of deflection (immersion) of spherical elements during contact interaction; v_{ij} – maximum and minimum speed of the spheres i and j.

Figure 1 shows the dynamics of spherical elements interacting with each other.

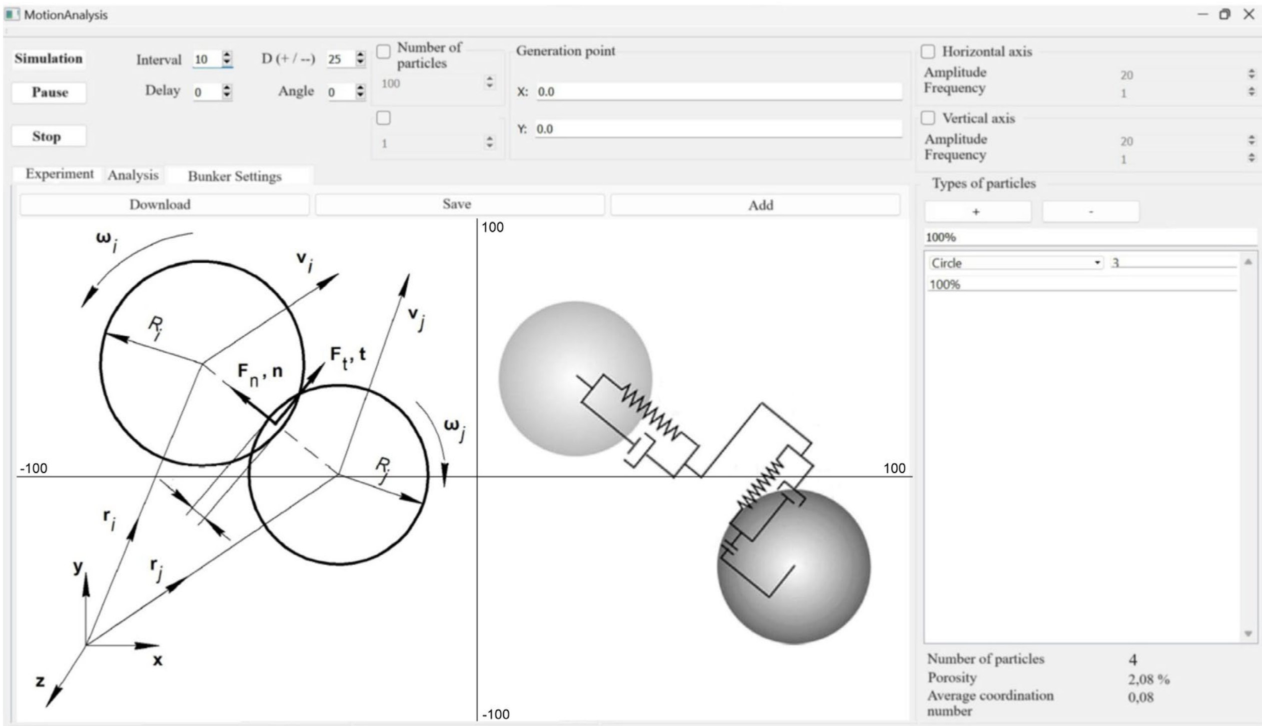

Fig. 1. Dynamics of spherical elements interacting with each other, where: diagram of vector interaction of contacts and velocity vector of a spherical element

It should be noted that this approach allows us to study the main details of the contact interaction between elements in heterogeneous media, taking into account their geometry and basic properties. We also found that for a more detailed proposed description of the discrete element method (DEM), an analysis of boundary conditions is also necessary. In this case, the DEM mainly determines the interaction between individual elements of the system and the environment that affects the system itself. For spherical element modelling with a DEM description, the boundary conditions can be described as follows:

1) **Node anchoring**: one or more nodes of the spherical element can be anchored to account for real boundary conditions at the structure boundaries;

2) **Loads:** the boundary conditions also include the introduction of external forces or moments acting on the spherical element. These loads can be caused by external factors or actions, or internal, such as thermal loading;

3) **Contact conditions:** for cases where spherical elements are in contact with each other, an important aspect is the definition of contact boundary conditions. This includes conditions regarding displacements, forces or other parameters that determine the interaction between the elements;

4) **Boundary conditions at the boundaries:** for spherical elements, it is important to define how they interact with the boundaries of the system under analysis. This may involve the introduction of boundary conditions on displacements, stresses or other parameters within the permissible limits of the system.

Tests. Since the mathematical modelling of the behaviour of spherical elements under the influence of external and additional factors by the discrete element method allows us to obtain a detailed understanding of their dynamics and the interaction of contacts with each other, we have modelled spherical elements with a ball radius of 0.1 mm to 0.7 mm.

Figure 2 shows the simulation of spherical elements based on the developed three-dimensional model.

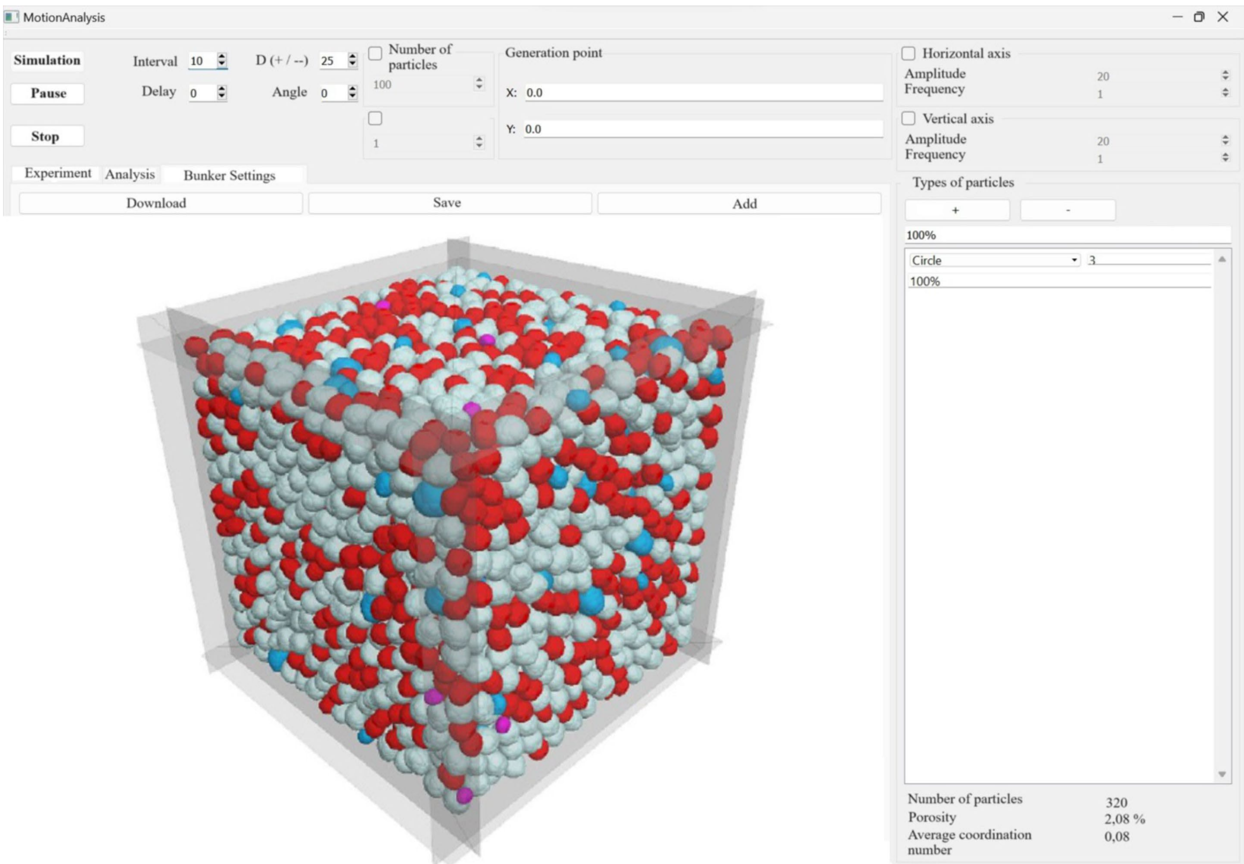

Fig. 2. Modelling spherical elements (spheres)

It follows from the study that the DEM is used as a numerical method to analyse the behaviour of a system considered with the help of spherical elements. The boundary conditions for spheres are important, in particular:

1) one or more nodes of the spherical element can be fixed, taking into account the real boundary conditions at the boundaries of the structure;

2) additional external forces or moments acting on the spherical element are introduced, including external and internal loads, such as geometrical parameters, pressure or thermal load;

3) for qualitative cases of mutual contacts between spherical elements, additional contact boundary conditions are defined, which mainly include conditions on displacements, forces and other physical parameters that determine the interaction;

4) it is important to determine how the spherical elements interact with the boundaries of the system, including the introduction of boundary conditions on displacements, stresses and other parameters within the system.

Figure 3 shows a study of heat transfer between spherical elements at a constant temperature *t*=20 °C with a ball radius *R*=0.1 mm.

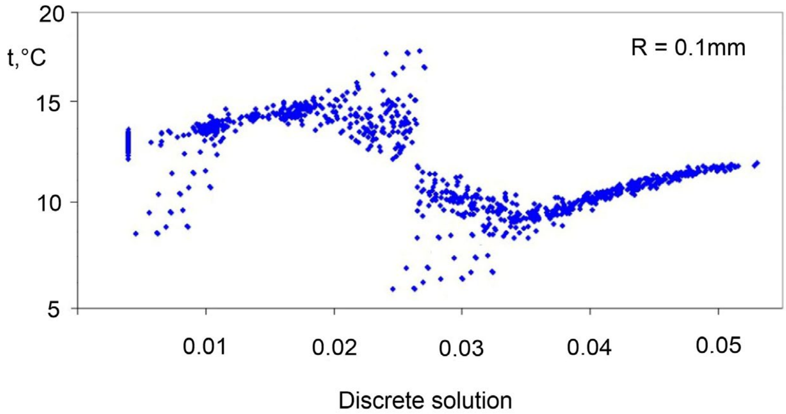

Fig. 3. Results of the study of heat transfer between spherical elements with a size of 0.1 mm

It should be noted that the results of the study of heat transfer between spherical elements at a constant temperature *t*=20 °C and with a given ball radius *R*=0.1 mm are justified by several key aspects that are important for understanding and optimising heat transfer in such systems:

1. **Geometrical characteristics of spherical elements:**

o The size of the spherical elements, in this case their radius R, is an important parameter for determining the contact surface area and volume, which affect the heat transfer rate. It should be noted that large spherical elements can have a larger surface area and volume, which in turn can facilitate efficient heat transfer.

2. **Thermal properties of the heterogeneous medium:**

o The thermal properties of the heterogeneous medium in which the spherical elements are modelled (e.g. thermal conductivity) determine how efficiently heat is transferred through the surface and how well the spheres are contacted. These properties are important for understanding and predicting heat transfer.

3. **Stability of the temperature regime:**

o Setting a steady-state temperature of *t*=20 °C defines the thermal gradient between the spherical elements and their surroundings. It is important to note that this temperature regime affects the heat transfer and thus affects the efficiency of the entire environment in which the ball dynamics are modelled.

4. **Heat transfer mechanisms:**

o Consideration of heat transfer mechanisms such as conduction, convection and radiation is important to determine the dominant heat transfer factors in a given system.

5. **The influence of the environment:**

o Environmental properties, such as pressure and atmospheric composition, also have a partial influence on the heat transfer process.

It should also be noted that the specified radius of the balls *R*=0.1 mm also affects the thermal resistance and the overall heat transfer efficiency. It follows that the study of heat transfer between spherical elements under these specific conditions can lead to important conclusions regarding the optimisation of thermal processes in microscopic systems, as well as find application in microelectronics manufacturing, biomedicine and other areas.

Figure 4 shows a study of heat transfer between spherical elements at a constant temperature of *t*=50 °C with a ball radius of *R*=0.5 mm.

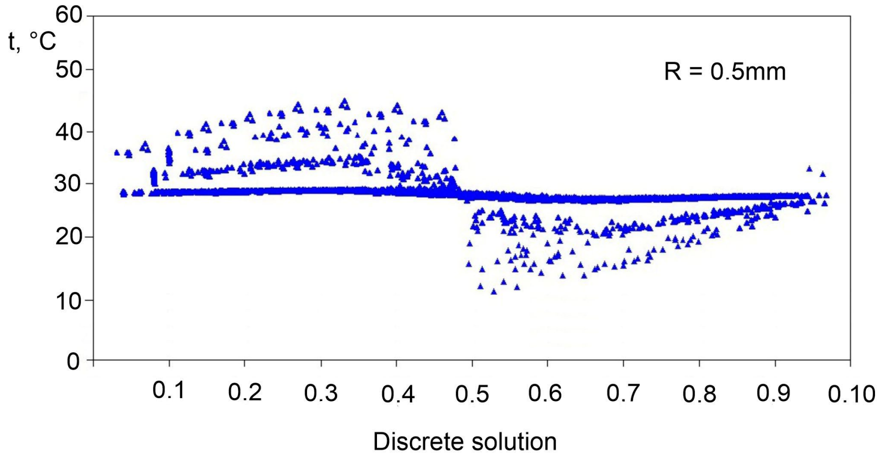

Fig. 4. Results of the study of heat transfer between spherical elements at a constant temperature *t*=50 °C with a ball radius *R*=0.5 mm

It should be noted that setting a constant temperature of *t*=50 °C determines the thermal gradient between the spherical elements (spheres), which is important for determining heat fluxes and heat transfer properties. A given ball radius of *R*=0.5 mm affects the geometric configuration and surface area interacting with the environment, determining the overall heat transfer efficiency. In turn, the analysis of heat transfer mechanisms, such as conduction, convection and radiation, helped us to establish in more detail the contact between the elements and their interaction at a given temperature.

3 Conclusion

Thus, it can be concluded that the results of the study indicate that the discrete element method (DEM) is successfully used as a numerical method for analysing the behaviour of a system considered with spherical elements. The rationale for the results is based on the importance of boundary conditions for the spheres, which determine the key aspects of modelling based on the developed three-dimensional model. It is important to note that the developed model solves a number of key tasks, expanding the horizons of scientific research:

1. **Study of moulding properties of heterogeneous products:**

o As part of the analysis of the compaction process of spherical elements, the three-dimensional model allows for the study of both monodisperse and polydisperse heterogeneous media.

2. **Study of the structure change process:**

o By modelling the changes in the structure of a heterogeneous medium from a static to an oscillatory state, using mathematical modelling methods, a deep understanding of this process can be obtained.

3. **Modelling the mathematical behaviour of elements:**

o By modelling the mathematical behaviour of spherical elements under the influence of external and additional factors, it is possible to study in detail their dynamics, the interaction of contacts between elements, etc.

4. **Discrete element method based on a three-dimensional model:**

o The calculation based on the discrete element method (DEM) has proven to be effective for analysing the contact interaction of spherical elements in heterogeneous media. It is noted that a detailed description of the DEM requires additional analysis of boundary conditions, which play an important role in modelling the interaction between elements and the environment.

5. **Prediction of the main parameters of elements:**

o The application of the model allows predicting the main parameters of spherical elements and their heterogeneous environment with a reliable accuracy of ±1 %.

Thus, such an extended approach through the implementation of a mathematical model of the dynamics of spherical elements is a powerful tool for the study and optimisation of heterogeneous processes, as well as for the study of the basic parameters and dynamics of spheres in different conditions.

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