Advances in Science and Technology
ISSN: 1662-0356, Vol. 156, pp 15-25
doi:10.4028/p-Xm5pzL
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Submitted: 2024-03-28
Accepted: 2024-05-18
Online: 2024-09-09

Use of the Boundary Element Method for Solving Problems of Predicting the Regularities of Formation of the Structure of Non-Isometric Components

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Keywords: boundary element method, modelling, constants, component simulation, potential, dynamics, boundaries, angles.

Abstract. In this paper, the boundary element method (BEM) is investigated and computer simulations are conducted to study the patterns of structure formation of non-isometric elements. The modelling of this study covered various aspects, including shape, radius, angle from the stable radius, porosity, average coordination number, simulation time, component falling force, and electrostatic constant. The simulation results provided important information about the properties and interaction of non-isometric components under different conditions. It was found that the obtained parameters can be effectively predicted for further research. It should also be noted that important processes, such as deformation and material behaviour, colloidal aspects, dynamic modelling of the movement of components with complex shapes, and features of nanotechnology, were observed in parallel with computer simulation.

1 Introduction

In the context of modern scientific progress and the expanding use of analysis and modelling methods [1, 2], especially in the field of research related to the structure of the formation of non-isometric components, the boundary element method is one of the key tools for solving problems of predicting patterns in the formation of the structure of non-isometric elements [3, 4, 5].

It should be noted that the boundary element method (BEM), also known as the boundary integral method or the contour element method, is a numerical method for solving various physical problems, such as mechanics, modelling, and heat transfer problems [6, 7, 8]. The main idea of the BEM is [9, 10] that the system or domain to be studied is divided into subdomains, which in turn are called boundary elements [11, 12, 13]. Instead of studying the properties of the entire system, attention is focused on the boundary elements, analysing their interaction and impact on the entire object [14, 15]. It is also important that the main property of the BEM is the use of boundary conditions to solve equations describing the behaviour of the system and non-isometric components, which require a lot of attention [16, 17]. Boundary elements are chosen so that their properties are easily computable, and they are often located along the boundary of the study area [18, 19, 20].

One of the key stages of the BEM is the Green's functions [21, 22], which reflect the interaction between the system elements in general [23, 24, 25]. These functions take into account mainly the impact of point loads on the entire system and their elements located in it, and are also used to calculate those values that require further study [26, 27].

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Therefore, in this scientific study, we will consider the importance and advantages of using the boundary element method in the context of solving problems of predicting patterns in the formation of the structure of non-isometric particles and components. In turn, using the boundary element method and its basic research concepts, in particular, the analysis of the formation of the structure of components, we will be able to obtain accurate and efficient results in the study and prediction of the properties of non-isometric particles. Another important advantage is the efficiency of working with complex geometric shapes and the ability to model various physical phenomena in systems with a complex structure.

2 Main Part

The basic principles of the boundary element method are covered in [28, 29, 30]. The authors consider in detail the principles and basic concepts of the boundary element method. They also argue that special emphasis should be placed on its application to forecasting problems. The work [31, 32] is based on the study of non-isometric components and focuses on the use of BEM. Boundary conditions and the selection of boundary elements required for forecasting are described in [33, 34]. An analysis of the literature describing the importance of boundary conditions using the BEM for solving mathematical problems is presented in [35, 36]. The role of Green's functions in the boundary element method is described in [37, 38]. The need to use the BEM in specific cases is presented in scientific experiments [39, 40, 41]. It should be noted that analysing aspects of the literature, it can be concluded that they are incompletely substantiated and require further substantiation and research. Therefore, it is important to use the boundary element method in solving forecasting problems, as well as to substantiate the main regularities that occur in the formation of the structure [42, 43, 44] of non-isometric components.

The aim of the study is to improve the boundary element method for computer simulation of the regularities of the structure formation of non-isometric elements. To investigate the parameters of shape, radius, porosity, average coordination number, angle from the stable radius, as well as to record the simulation time, particle incidence force and electrostatic constant.

Materials. The boundary element method (BEM) is a numerical method used to solve various boundary value problems in areas with complex geometry. It should be noted that the application of this method allows you to approximate the solution of a differential equation or any mathematical model on the boundary by replacing the boundary region itself with a set of boundary elements. The main idea of the BEM is to divide the region of non-isometric components into a certain number of elements (usually boundary elements), where the solution of the equation will be solved quite simply. After that, the solution of the mathematical equation will be determined at the boundary of these elements, and their internal link values will be calculated using approximation methods, such as the finite element method or the finite difference method. It should also be noted that this method is effective in modelling systems that include particles with inhomogeneous shapes, i.e., non-isometric components. In such modelling, the main idea of the BEM will be to focus on the boundaries of the region where the inhomogeneities are mainly located, and to approximate the solution only at these boundaries.

We offer the following recommendations for justifying the BEM for modelling non-isometric components with inhomogeneous shapes:

1) geometric complexity (for systems containing non-homogeneous components with complex geometry, analytical or numerical solution of the internal regions can be extremely difficult. In this case, the BEM allows us to focus on the problematic boundaries where the main physical processes occur);

2) reducing the amount of computation (approximation of the solution only at the boundaries can significantly reduce the amount of computation compared to other mathematical methods that require solving equations over the entire volume of the system);

3) suitability for heterogeneous materials (BEM easily takes into account inhomogeneities in non-isometric components, since it can establish different physical relationships and properties for each component at the boundary);

4) consideration of interactions between particles or components (boundaries of non-isometric elements are key points of interaction between components of complex shape. It should be noted that the MGE effectively models the interaction, focusing on the boundaries where it is most significant);

5) generalisation for different shapes (the BEM can be adapted to different shapes of components, including their heterogeneous structures that are formed in the course of modelling. By applying approximation methods at the boundaries, it is possible to avoid the detailed description observed inside non-isometric components);

6) use of local properties (BEM allows to take into account local properties of heterogeneous components, such as shape, size and physical properties, focusing mainly on their boundaries).

Figure 1 shows the non-isometric components depicted as an ellipse.

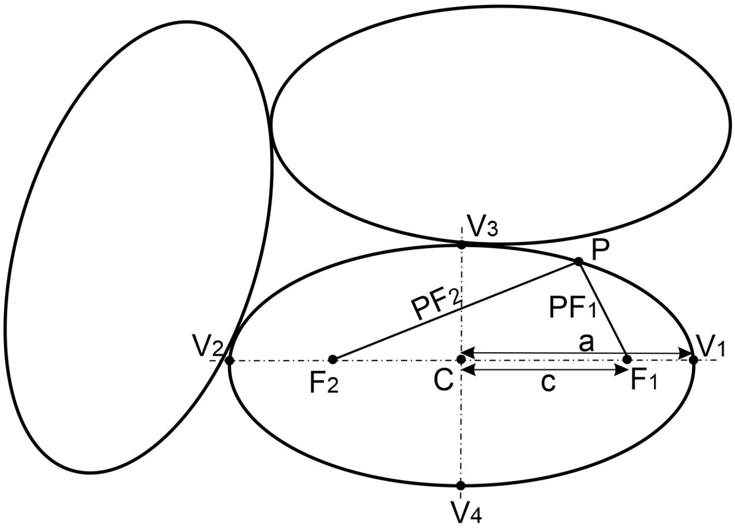


Fig. 1. Non-isometric components depicted as an ellipse

It should be noted that an ellipse (in this case, non-isometric components) is a geometric figure that can be described as a set of points in two or three dimensions that have specific properties with respect to two fixed points, which are generally called foci. Let us denote an ellipse by the distances from each point P to the foci F_1 and F_2. The set condition for non-isometric components, in particular, the ellipse, will be given as follows:

$$\left|P \cdot F_1\right| + \left|P \cdot F_2\right| = 2a \tag{1}$$

where: a – is half of the major axis of the non-isometric component (ellipse), and it is assumed that $2a > \left|F_1, F_2\right|$. In order to avoid the special case of a linear segment. More formally, an ellipse can be defined and described as a set of points P in the plane R^2. Then we have:

$$E = \left(P \in R^2 \left\| P \cdot F_2 \right| + \left| P \cdot F_1 \right| = 2a\right) \tag{2}$$

In turn, the center of the ellipse (non-isometric component), denoted as C, is located in the middle of the segment that connects the foci. It should be noted that the major axis of the ellipse is the line that passes through the foci, and it is also called the major axis. The minor axis of the non-isometric component is a line perpendicular to the major axis and passes through the center of the ellipse.

It should be noted that the major axis also contains the vertices V_1 and V_2, the distance from which to the center is equal to a. The distance from the foci to the center of the ellipse, c, is called the focal length or also called the linear eccentricity. The eccentricity, denoted by an exponent e, is defined by the mathematical relation $\frac{c}{a}$. The mathematical theorem described above allows you to describe the geometric properties of the non-isometric components of an ellipse as accurately as possible and is used to analyses its shape and dimensions.

Tests. In order to predict the qualitative regularities of the structure formation of non-isometric components, it is necessary to perform modelling of ellipsoidal particles with a detailed description of their formation. It should be noted that the study of non-isometric components is an important task in many scientific fields, such as physics, chemistry, biology, materials science, modelling, etc. These components can be molecules, colloidal elements, or even objects in nanotechnology. To obtain a high-quality result of such a cumbersome study, we propose several aspects of modelling non-isometric (ellipsoidal) components:

1. geometric modelling (ellipsoidal elements can be described by parameters such as length and width of axes, orientation in space, etc. Also, the geometrical parameters can be determined experimentally or theoretically, depending on the nature of the components;
2. behavioural models (various models can be used to reasonably describe the interaction between ellipsoidal non-isometric components, such as the hard disk model, the Van der Wals model, or models that take into account electrostatic interactions);
3. molecular dynamics (for a more detailed study of the movement and interaction of such components, it is necessary to use partially molecular dynamics (MD) and boundary element methods (BEM). In turn, molecular dynamics allows taking into account various interactions between elements of complex shape and reproducing their dynamics in time);
4. reaction kinetics (if ellipsoidal elements are involved in chemical or biological reactions, then modelling the kinetics of these reactions can be an extremely important aspect. For this purpose, it is necessary to use various reaction models and numerical integration methods);
5. electrodynamics (if particles with this shape have an electric charge, it is important to take into account the electrodynamic properties of the system in which the modelling is performed. It should be noted that electrostatics and electrodynamics models can be used to describe the charge and motion of non-isometric components in electric fields).

Figure 2 shows the modelling of components with a non-isometric shape.

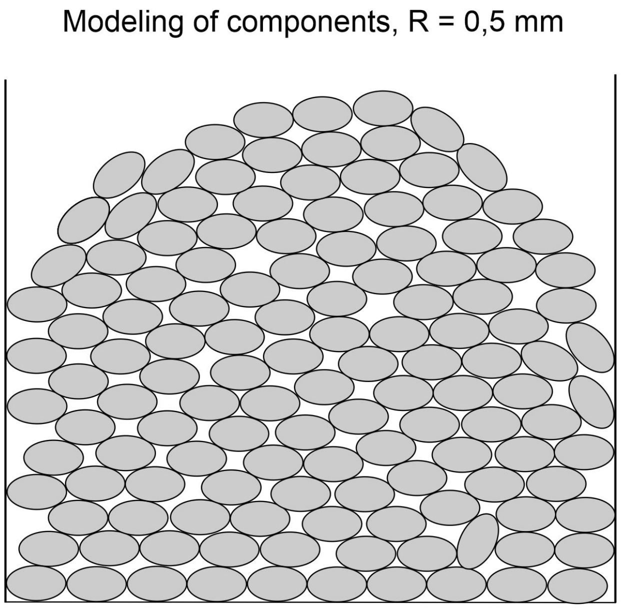


Fig. 2. Modelling components with non-isometric shapes

It should be noted that such modelling is a simple physical model that mainly describes the interaction between molecules of non-isometric components in a heterogeneous state. The proposed model (Fig. 2) is used to simulate the interaction between ellipsoidal elements or particles, in particular in the study of colloidal systems or in the field of soft materials.

To perform this type of modelling, we include two main aspects in the potential energy of a heterogeneous system:

1) The potential energy of attraction (a):

- this part of the model describes the attraction between non-isometric particles and arises as a result of the interaction of dipole moments;

- for ellipsoidal components, additional effects related to their shape and orientation in space can be modelled.

Figure 3 shows the potential energy of attraction of elements with a non-isometric shape.

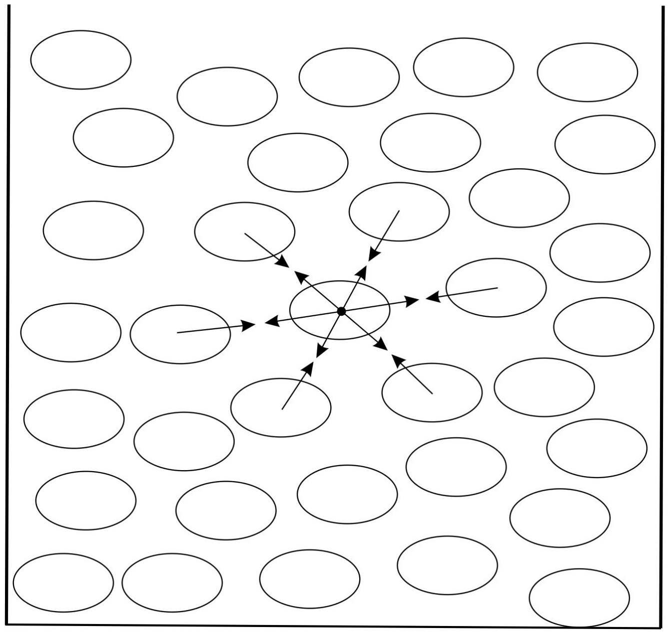


Fig. 3. Scheme for attracting elements with non-isometric shapes

It should be noted that the attraction of non-isometric elements is directly related to the ability of a system or object to attract components according to the basic principles of gravity or electrostatics. The main aspects of the attraction of non-isometric components include:

- gravitational potential energy (gravitational energy basically attracts objects to each other through the force of gravity. This energy depends on the mass of the objects and the distance between them. The formula for the gravitational potential energy (*U*) in a free field of gravity is as follows:

$$U = m \cdot g \cdot h \tag{3}$$

where:

m – mass of the object;

g – acceleration of free fall (approximately 9,2-9,8 m/s^2);

h – height above the surface.

- electrostatic potential energy (electrostatic energy of attraction of components occurs between charged particles (i.e., elements) due to electrostatic forces and their bonds. The mathematical relation for the electrostatic potential energy (*U*) between two charged components is as follows, get:

$$U = \frac{k \cdot q_1 \cdot q_2}{r} \quad (4)$$

where:

k – the electrostatic constant (8,98×10^9 Н·м^2/C^2 in an inhomogeneous medium);

q_1 and q_2 – are the charge values of the non-isometric components;

r – the distance between these non-isometric components.

2) Potential repulsive energy (b):

- this part of the model represents mainly the repulsion between components arising from the interaction of the electron shells of elements or particles;
- the potential repulsion energy can also be adapted to account for the shape and orientation of non-isometric components.

The general form of the model developed by us can be written in the form of an energy potential (U) between two components (particles) as follows:

$$U(r) = \frac{a}{r^{12}} - \frac{b}{r^6} \quad (5)$$

where:

r – distance between the centres of non-isometric components;

a and b – constants determined by the characteristics of the heterogeneous system.

It is important to note that our proposed model for the formation of the structure of non-isometric components helps to take into account both the attraction and repulsion between particles (components), which is important for studying their phase behaviour and structural parameters. If necessary, their orientation and shape can also be further modelled within this developed model to study non-isometric components.

Figure 4 shows the ejection scheme of non-isometric elements.

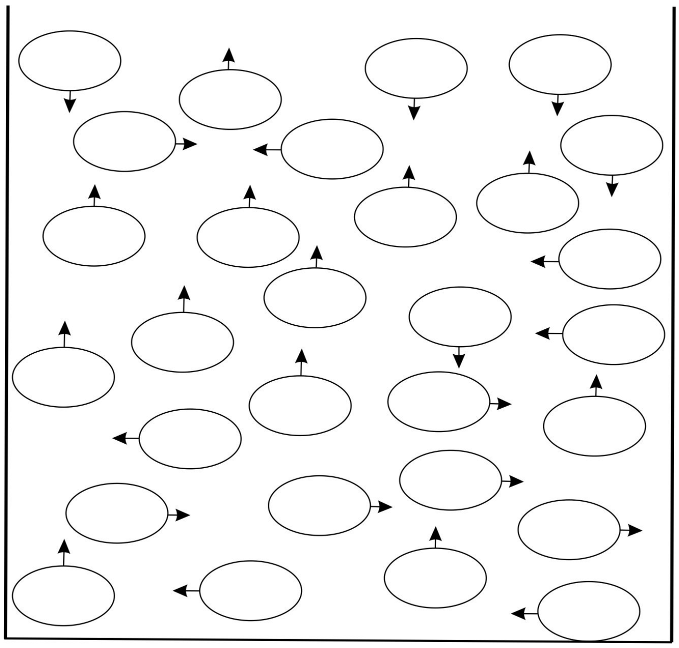


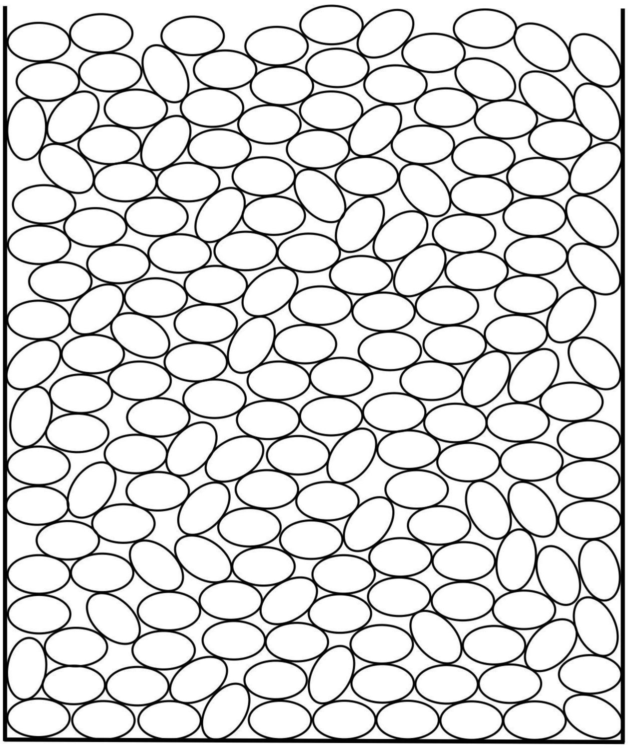
Fig. 4. Modelling the repulsion scheme of components with a non-normal structure

It should be noted that the modelling of this scheme of repulsion of elements with non-standard shapes is closely related to the potential energy that arises between objects or components that repel each other due to repulsive forces. Hence, the two main types of repulsive energy that can occur in different situations are electrostatic potential energy and repulsive energy between components and their reactions. In particular:

- electrostatic potential repulsive energy (this type of energy occurs between non-isometric elements with the same charges due to the repulsive forces in electrostatics. If two particles (two elements) have the same positive or negative charge, their electrostatic potential repulsive energy will increase as they come closer together. Mathematical calculations for the electrostatic potential repulsive energy between two charged elements will be carried out according to the formula for the energy of attraction (equation 4));
- the repulsive energy between components and their reactions (in this case, the repulsive energy can be converted into other forms of energy, such as heat or light, etc.).

Based on the above material on the use of the Boundary Element Method (BEM) and the regularities of the formation of the structure of non-isometric elements, we conducted a computer simulation of the formation of elements with a non-isometric shape. We studied such indicators as: the shape of the components, the radius of the non-isometric components, the formation of the angle from the stable radius of the non-isometric elements, the fixed porosity in the formation of the structure of ellipsoidal elements, the average coordination number, the time for simulation, the force of particle incidence, and the electrostatic constant.

The results of the computer simulation are shown below in Figure 5.



Modeling:

1) Radius of components: R, mm = 0,5;
2) Radius angle of the components: α,° = 0,2-0,5;
3) Porosity of components: P,% = 0,3-1,2;
4) Average coordination number: ACN = 2,1;
5) Simulation time: T, minutes = 20;
6) Falling force: S, m/s² = 9,2-9,8;
7) Electrostatic constant: C, N·m²/c² = $8{,}98 \cdot 10^9$;
8) Form - a ellipse.

Fig. 5. Results of computer simulation of non-isometric components

It should be noted that the obtained indicators presented in Figure 5 can be easily predicted for further research. It should also be noted that in parallel with the results of the computer simulation, we were able to observe a number of other equally important processes, including:

1) deformation and behaviour of the material (simulation of non-isometric particles showed us how the material deforms under the influence of external forces or pressure);
2) colloidal aspects (particle distribution in a heterogeneous medium. Simulation of this process allowed us to record the distribution and interaction of ellipsoidal particles in colloidal systems);
3) dynamic modelling of the movement of non-isometric components (simulation allowed to consider in detail the process of dynamics of components movement and interaction of ellipsoidal particles in heterogeneous systems);

4) features of nanotechnology (self-organisation of components. The simulation was also aimed at studying the self-organisation of non-isometric components in nanoscale systems, which is important for the development of new materials and devices).

Therefore, it can be concluded that modelling ellipsoidal components requires taking into account various physical and chemical aspects of the interaction of these objects in a particular environment or system. It is also important to choose approaches and methods that depend on the specific characteristics of the system and the tasks at hand.

3 Conclusion

In this study, the boundary element method (BEM) was improved and the regularities of the structure formation of non-isometric elements were studied by computer simulation. The simulations covered various aspects such as the shape of the components, the radius of the non-isometric particles, the angle from the stable radius, the porosity in the formation of the structure of ellipsoidal elements, the average coordination number, the simulation time, the particle incidence force, and the electrostatic constant. It should be noted that the simulation results provided important information about the properties and interaction of non-isometric components under different conditions. This study has the potential for further applications in materials development, biological systems, graphic modelling and other areas where the interaction of non-isometric structures is important.

It should also be emphasised that the results presented in Figure 5 indicate the possibility of predicting the obtained parameters for further research. In parallel with the computer simulation, a number of important processes were observed. These include material deformation and behaviour, colloidal aspects, dynamic modelling of the movement of non-isometric components, and nanotechnology features through simulation of self-organisation of non-isometric components. The results obtained indicate the wide potential of simulation for further research in the development of new materials and devices in various fields of science and technology.

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