Packing of monosized spheres in a cylindrical container: models and approaches

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Packing of monosized spheres in a cylindrical container of a fixed diameter is a frequently discussed subject in recent studies. It is motivated by the high applicability of these models, particularly by the advances in nanomaterial science and engineering, associated with the development of hierarchically ordered matters of specific structures and properties. Their features strongly depend on the arrangement and density of the filling atoms in the channels of a nanostructured porous matrix. A special interest is devoted to a dense random packing, which by its nature is not totally random when the spheres do not overlap. In this paper, related models of packing are classified basing on the space filling method, and the densities reached theoretically as well as experimentally for those classes are given. The effects produced by some parameters on the packing density and the main properties are analyzed. The experimental techniques and computer modeling approaches are summarized.

Keywords: Packing; monosized spheres; cylinder; density; porosity; modeling.

El empaquetamiento de esferas del mismo tamaño en un contenedor cilíndrico de diámetro fijo es un tema que se discute frecuentemente en investigaciones recientes. Eso es motivado por la alta aplicabilidad de dichos modelos, debido a los avances en la ciencia e ingeniería de nanomateriales y el desarrollo de materiales jerárquicamente ordenados con estructuras y propiedades específicas. Sus características dependen estrictamente del arreglo y densidad de los átomos en canales de una matriz porosa nanoestructurada. Un interés especial está enfocado en un empaquetamiento aleatorio denso, el cual por su naturaleza no es totalmente aleatorio cuando las esferas no se traslapan. En este artículo, los modelos relacionados con el empaquetamiento son clasificados basándose en el método de llenado del espacio, y las densidades alcanzadas tanto teóricamente como experimentalmente para estas clases son dadas. Los efectos producidos por algunos parámetros en la densidad y las propiedades del empaquetamiento son analizados. Son resumidas las técnicas experimentales y los alcances del modelado por computadora.

Descriptores: Empaquetamiento; esferas iguales; cilindro; densidad; porosidad; modelado.

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1. Introduction

The three-dimensional (3D) structural model of a matter may be designed in many cases as a set of identical spheres occupying an available space. When this space is limited to a predetermined region, such as channels of a nanostructured porous matrix filled by atoms or molecules of a substance, the properties of the resulting matter strongly depend on the arrangement and density of the particles. These structures can be modeled as packings of monosized spheres in a cylindrical container.

Packing of spheres is one of the most-studied models. In 1959, Bernal first employed a random close packing of monosized spheres as a useful model for an ideal liquid [1]. Afterwards, this approach generated considerable interest of researchers as a consequence of the diversity of practical applications and the described structures depending on the materials used, the space shape, the sphere size, etc.

The investigation of non-overlapping packings of monosized spheres in the d-dimensional Euclidean space has been strongly motivated by the study of processes in chemical and nuclear reactors as well as thermal heat exchangers, see *e.g.*, [2-7]. A review of the literature describing the packing structure and effective thermal conductivity of randomly packed beds consisting of monosized particles has been recently presented in [8]. In chemical engineering and material physics, models of monosized sphere packings are applied for the description of diverse matter structures such as crystals [9-10], liquids [1], bones [11], etc. Such models are also used

for predicting properties of transport processes in gas-liquid flowing systems [12]. Monosized packing structures are appropriate models to study properties of a matter in an equilibrium state in line with the critical state of density in the transition point between two phases for diverse granular matters [13] such as powder [14-16], ceramics [17], sand [18], etc. The researchers noted some physical phenomena that occur frequently in a semi-confined space in consequence of the density increasing due to the presence of the gravitational field or an excessive external influence: fluidization, segregation, rearrangement, elastic deformation, fragmentation, plastic flow, abrasion [15,19,20], solidification [21], dilatancy [18], cohesion [22]. Such deformations affect the maximum packing density attainable as well as the desirable packing structure and properties.

The theoretical problem of the densest packing of monosized spheres in the Euclidean space belongs to the optimization problems of discrete and computational geometry and can be stated as follows: For a given set of spheres with identical radii, it is necessary to find an arrangement in a 3D packing space (the entire space, a cylinder, a cube, etc.) that has the highest density, *i.e.*, which minimizes the amount of the empty space between them. It is known that even for restricted versions with identical regular-shaped objects and domains of low-dimensional space, this problem is NP-hard, and therefore its exact solution cannot be obtained in polynomial time unless $P = NP$ [23]. There are only a few pure theoretical results due to the complexity of the geometry. The majority of works are focused on an experimental investigation and a numerical simulation of the packing structures as well as the measurement or evaluation of the parameters.

The rest of this paper is organized as follows: In Sec. 2, a classification of 3D packing models is proposed. The known densities for different models are listed in Sec. 3. Three aspects of the studies that have influenced the packing properties are described in Sec. 4: the state of the matter, the wall effects of the containers, and the aspect ratio of the diameter. The computer modeling approaches, referred to in Sec. 5, are classified into three categories: numerical simulation, pore networks, and mathematical programming. Some concluding remarks, summarizing the hot topics of modern science and technology connected with packing problems complete the paper.

The paper is directed to students and researchers in computational science and physical-chemical areas studying the material structure modeled by means of sphere packing approaches. It may also be considered as a teaching tool for students in the field of nanoscience and nanotechnology.

2. Classification of filling models

Identical particles of spherical shape packed in a closed 3D space produce a variety of models, considering different filling methods and assumptions of the problem. The interest of the researchers is focused on the prediction of the packing structure and its properties.

Initially, packing models are classified into ordered (regular) [2,24], and disordered (random) packings [3,6,22,25-29]. Ordered packing arrangements comprise rows and layers placed in cubic or hexagonal crystalline patterns. A random packing with highest density is referred to as a random close packing. The term random indicates that the packing structure remains random, even if the density increases over the commonly observed range. In the absence of a global ordering when the spheres attain a closest proximity to one another, the highest packing densities can be achieved through an agitation: shaking or jolting [14,17,17,30], vibration [2,14,24], tapping [14,15].

A packing of minimal density is referred to as a random loose packing [11,13]. It does not require any agitation or shaking. More than two of these models of packing can be defined. An infinite number of particle arrangements can be produced between these two limits. Packing may also allow trimming [31], sliding, rolling sliding [32], lifting or overlapping of the particles [5,33].

In addition, the packing models should be divided into static, dynamic and combined ones. Static models are designed to produce a fixed arrangement of spheres [12], whereas dynamic ones are capable of producing a sequence of arrangements [34]. The simplest approach to simulate a static packing is a sequential addition of the particles to an initial configuration. Physically a more realistic approach is the modeling of a sequential deposition of the spheres under the influence of gravity, by dropping them from random locations and allowing to roll until settling them on the container bottom or top of three other spheres in a gravitationally stable position. Dynamic models do not incorporate gravity effects. Mueller [28] noted that, regardless of the nature of packing, the final stable equilibrium of the geometrical structure of the packed particles is of main interest, and it greatly influences all properties of packing.

3. Known packing densities

Several works, both experimental and computational ones, deal with the description and prediction of overall and local structural properties of a packing. The primary parameters of a packed structure are the space occupation coefficient (density) and the void fraction (porosity). In 1611, Johannes Kepler conjectured that the density of a packing of congruent spheres is never greater than $\pi/(3\sqrt{2}) \approx 0.74048$ [35]. Despite the apparent simplicity of this assertion, Kepler's conjecture has been proved by Hales only recently in 1998 [36]. Kepler's space occupation coefficient implies also the lowest void fraction known to be attained. In 1955, Rankin [37] obtained $0.827\ldots$ as an upper bound for these densities and three years later, Rogers lowered it. Roger's theorem asserts that the density of an arrangement of non-overlapping equal spheres cannot exceed

$$\sqrt{18}\left[\cos^{-1}\left(\frac{1}{3}\right)-\frac{1}{3}\pi\right]=0.7797\ldots,$$

but it does not imply that this upper bound is necessarily attainable [38]. Accordingly, the void fraction cannot be less than 0.22036.

When the spheres are packed randomly, the void fraction typically lies in a region surrounding 0.38, and, according to Scott [39], it is unlikely that it can lie outside the limits of 0.36(3) and 0.39(9). In a more recent publication, Zhang *et al*. [40] affirmed that ordered structures attained a range of porosity [0.2595 ... 0.4764]. Disordered packings exhibit a much smaller porosity falling into the range [0.36 ... 0.40]. No theory is provided about an exact value, but the well-accepted limit is 0.36, plus or minus some small amount that varies according to the source consulted.

Some important sphere packing densities are as follows:

- The upper bound on the density of an arrangement of non-overlapping equal spheres is 0.7797 [38];
- The maximal density of an ordered packing is about 0.74048 (Kepler's Conjecture) [35];
- The random close packing density is about 0.6366 ± 0.0005 [30]; according to the improved data, the experimentally obtainable values of a random close packing fall into the range of 0.64 ± 0.02 [41];
- The random loose packing density of granular matter is 0.608 ± 0.006 [39];
- The random loose packing density of granular matter, at the limit of a zero gravitational force, is 0.555 ± 0.005 [42].

4. Experimental studies

The majority of the information about packing properties comes from experimental results due to the complexity of the modeling of the geometry. Experimental studies involve the construction of a physical model, and then its desired structural properties are measured. In the papers [2-4,25,40], an extensive analysis and a review of experimental techniques were given. Several techniques that have been used to determine the radial void fractions were briefly reviewed by Mueller [43].

4.1. Influence of the states of matter on the packing density

Typically, densely packed monosized spheres have a space occupation coefficient of 60%-64%. German [44] indicated that the tap (vibrated) density depends on the material, the vibration amplitude, the vibration frequency, the shear and test apparatus, and it varies with the duration of vibration. Nevertheless, McGeary [45] noted that a wide variety of materials (lead, sulfur and steel shot, steel ball bearings, glass beads, rounded sand, round California beans and poppy seeds) all produce packings within this range of density. Results for a given material and container are reproducible up to a fraction of a percent. While the sizes of the different materials tested vary considerably, the main conclusion was that neither the material density nor a difference in the size from one material to another significantly affected the ultimate packed density.

The difference in the density between the solid and the liquid states of simple monatomic substances, such as rare gases, is 15-16%, which is approximately the difference between the density of hard spheres in a regular packing and the density measured for a model of hard spheres in a random close packing [30,46]. Taking into account the state of matter, Bernal *et al*. [9] made a suggestion that the structure of a liquid may be regarded as a "heap" of molecules, in contrast to the structure of a crystalline solid which may be considered as a regular "pile". Several properties of liquids have been shown to have their geometrical counterparts in a randomly packed array of hard spheres [39].

Vandewalle *et al*. [22] studied the influence of the relative humidity on the experimental results with random packings. Millimeter-sized glass beads were used. The authors observed electrical charges on the beads when the air humidity was low. It was due to the friction between the contacting beads. When the moisture content was increasing, the charges disappeared exponentially and liquid bridges were formed between the contacting grains by a capillary condensation. The authors noted that cohesive forces like liquid bridges and electrical charges, represent a barrier for local reorganizations and could mask or modify the physical properties of granular materials. According to this study, the best condition for conducting granular experiments with glass beads corresponds to a relative humidity of about 45%, when cohesion is minimal.

4.2. The wall effect

It is known that spheres near the container wall form more ordered structures than those in the internal region of random packings. This wall effect propagates from two to four sphere diameters into the container, depending on the packing density, see *e.g.* [40]. This phenomenon makes structural properties of particles near the wall different from those far away from the wall.

The wall effect consists of two components, namely the effect of the side wall (radial direction) and the effect of the top-bottom walls (axial direction or thickness effect). The side wall effect for spheres packed in cylindrical containers was studied for many years [2,19,24,27,40,47]. It can be quantified by a radial distribution function, which is the number of spheres per unit volume at a given distance away from a fixed point [48]. The wall effect is often characterized in terms of porosity. A quantitative understanding of the porosity variation is essential for the evaluation of the wall effect on a fluid flow. Different experimental techniques have been employed to measure the variation of the packing porosity on a distance from the container wall, *e.g.*, using diverse sub-

stances like paraffin or epoxy resin as a substitute of void, or applying the X-ray radiography, a high-resolution computed tomographic scans on each assembly [47] to monitor the positions of the particles. A more recent review of the used experimental techniques was presented in Mueller's paper [43].

Due to the top-bottom wall effect, the porosity is dependent on the sphere and the cylinder diameters, d and D, respectively, but also on the ratio of the particle diameter d to the packing height H, which can be referred to as the thickness effect. This dependence can be mathematically represented by $\varepsilon(d/H,\ d/D)$ and in many studies it is implicitly assumed to be negligible. Studying the porosity behavior in dependence on $\varepsilon(d/H,\ d/D)$, Zou and Yu [4] noted that the thickness effect can be readily identified for a constant ratio d/D. For both a loose and a dense packing, increasing the d/H ratio is also increasing the porosity. It was shown that for a constant ratio d/D, the porosity $\varepsilon(d/H, d/D)$ decreases with the increase of d/H, while for a constant ratio d/H, the porosity $\varepsilon(d/H,\ d/D)$ increases with d/D for small values d/D (less than about 0.6) but it decreases with d/D for large values d/D. The authors described another phenomenon: increasing the ratio d/D within the range from 0.25 to 0.35 can decrease the porosity $\varepsilon(d/H,\ d/D)$.

4.3. The aspect ratio of the diameter

The impact that the wall effect has on the overall porosity depends on the ratio of the cylinder-to-sphere diameter D/d. It has been well established that the overall porosity decreases while this ratio increases. Various equations were empirically formulated to quantify this relationship. Analytical models and experimental measurements have clearly indicated the presence of an oscillatory radial porosity variation [4,6,8, 25,49,50]. According to the semi-empirical equations developed by Dixonn [49], a maximum overall porosity of $\varepsilon = 0.67$ occurs at $D/d \approx 1.72$.

Theuerkauf *et al*. [51] used the discrete element method (DEM) to analyze the porosity distribution of spherical particles in narrow pipes with a value D/d in the range from 3 to 20. DEM is used to create an explicit numerical model that approximates the mechanical behavior of an assembly of arbitrarily shaped particles. These particles displaced independently of each other and interact only at the contact points, where they are allowed to overlap. This is referred to as a soft contact approach. The force between the particles during a contact is calculated by mechanical elements such as springs and dash pots.

Properties of "small" packings turned out to be of special interest for researchers [27,52-54]. When the size of a sphere starts to get too close to the cylinder diameter, namely approximately in the range $1 \leq D/d \leq 8$, the density function drastically depends on the value D. A simple mechanistic modeling shows that the packing density represents a non-monotonic function of the cylinder diameter, varying in the range from approximately 0.4 to about 0.6 while the ratio D/d changes only from 2.0 to 2.5 [55-57].

Chu and Ng [52] studied the morphology of the flow in tubes with tube-to-particle diameter ratios between 2.5 and 40. A computer-generated slim tube randomly packed with spheres was first tessellated into tetrahedra in the interior and into pentahedra near the walls of the tube. Then, the pore space was represented by a network of interconnected circular and triangular sinusoidal flow channels. The authors have discovered that the presence of the walls had two counteracting effects on the fluid flow: a higher porosity promoted flow along the walls but a higher surface area per unit volume hindered it. The porosity and solid surface area per unit volume of the porous mediums were determined as a function of the distance away from the wall. For tube-to-particle diameter ratios greater than 25, the permeability was the same as that of a large diameter tube, k_∞. Between 8 and 25, the permeability was larger or smaller than k_∞; and below 8, the confining walls caused a marked increase in the overall bed porosity and the permeability was always larger than k_∞. McGeary [45] studied experimentally the packing density of arrangements, where the ratio D/d varied from 1:1 to about 200:1. He showed that the effect of the container size on the packing efficiency of monosized spheres became negligible for ratios above 50:1.

Tingate [2] considered two regions of packing: the outer region, where the thickness is equal to the sphere diameter, and the remainder, the central region. The outer region contained whole spheres touching the wall and intruding segments of a number of spheres which did not touch the wall. The central region contained the other segments of the intruding spheres, and the balance of the whole spheres located entirely within the central region. The experiments have shown that the mean occupancy fraction of the central region was remarkably constant for ratios of D/d between 5.6 and infinity. It was equal to 0.598 for $D/d = 5.6$ and increased up to 0.615 for $D/d = \infty$. This indicates that a ratio of D/d equal to 5.6 can be used for exploratory experiments without sacrificing the accuracy unduly in the central region and the homogeneity of the packing density.

When the ratio of D/d is large, the tapping of particles can be used to obtain the densest packings. The experiments of Li and Funkenbusch [15] examined container diameters that exceeded those of the powders by 51:1 to 343:1, for the purpose of a powdered material fabrication. Hence, the container size effect was considered to be negligible. The packing density was found to increase quickly with the initial taps, leveling off after several hundred taps. An increase of roughly 3% was found for typical monosized powder packings during the first 500 taps, while 500 more taps produced only an additional increase of 1% and further tapping up to 200000 taps produced less than an additional increase of 1%. That is, after the first 500 taps, the reduction of the void fraction was insignificant. The results were within 0.1% reproducibility.

5. Computer modeling approaches

A dense random packing by its nature is not totally random. The fact that particles cannot overlap and that they are placed as close as possible, introduces some structure to a dense random packing and results in the formation of ordered substructures [3,24,47,55]. The three principal lines in modeling such structures and the methods used are referred to below.

5.1. Numerical simulation methods

A numerical simulation based on the experimental data is an attractive research method for such complex physical assemblies as a packing due to the easiness of creating and reproducing for any aspect ratio of the diameter and accurately determining the parameters. On the other hand, the packing properties are highly dependent on the assumptions of the method and the generating algorithm. A short review of deterministic simulation methods was presented in [28].

Gan *et al*. [5] proposed an algorithm based on the idea of concurrently removing the worst overlap and reducing the outer radius for the calculation of the random closed packing parameters in pebble beds. Computer simulations were applied to assemblies of monosized and polydisperse spheres (nearly spherical particles). This algorithm should be used for different kinds of containers to determine packing structures in the bulk and near-wall zones. A comparison between the simulation and the X-ray tomography results was given as a verification of the method.

A computer aided design (CAD) method was presented by Lal and Sun [11] for modeling two extreme microsphere packing cases: (a) a minimum-density packing with maximum porosity for a closed-cell bone structure; and (b) a maximum-density packing with minimum porosity for an open-cell bone structure. The number of microspheres packed by these two models was then determined. Abreu *et al*. [19] employed the Monte Carlo method to describe the packing and segregation of the particles in a cylinder in the presence of a gravitational field and shaking movements. The calculation of void fraction profiles in both the axial and radial directions was realized, and some results were given. The simulations indicated that the presence of a cylindrical wall did not seem to have a strong effect on the gravitational segregation phenomenon. Wensrich [47] provided complete characterizations of various particulate assemblies with the aid of Computed Tomographic scans and Discrete Element Models, and he used this data to examine the finer details of the effect of the boundaries. A fitting algorithm based on the optimization of an objective function has been developed to direct fitting particles to Computed Tomographic scans. Discrete Element Models of each tube were created using the proprietary software PFC3D v4.0 (64-bit version) by ITASCA. Analyzing the obtained structure, the author gave some conclusions. First, he has noted that a dense random packing was far away from being totally random, and this was most evident at the walls of the container. Then Wensrich supposed that dense random packing structures were similar to the ordered packings, such as a Face Centered Cubic and a Hexagonal Close Packed, however, on small scales.

The gravitational sphere packing method based on Monte-Carlo simulation was developed and recently applied to loose packed monosized spheres by Roozbahani *et al*. [58]. The authors used a cylindrical packing approach to simulate filling of different virtual rectangular containers. The wall effect was considered. The porosity of sphere packings in the inner part of the cylinder was examined also without the effect of the boundaries to show the structure of packing in different rectangular containers with different ratios of side sizes.

The Bennet model and its modifications are frequently used to generate random packings. The packings are built by adding new spheres, one at a time, on a horizontal basal layer using iterative sequential algorithms. An added sphere is always found in contact with three other spheres. The choice of the deposition site used is varied [54,59]. In the Bennet model, the position with the lowest vertical coordinate is selected. In the "anti-Bennet" model, only the positions that are stable under gravity are considered, and the one with the highest vertical coordinate is selected. In the Eden model, the new sphere is selected at random among all the possibilities and in the stable Eden model, the random choice is limited to positions that are stable under gravity.

A packing method that used a sequential addition technique was developed by Tingate and Mueller in the works [2,3,6,27,28]. The method employs no random procedures. When $D \geq 3d$, spheres are added to the packing above the base layer utilizing two different types of positions: the wall sphere (WS) positions and the inner sphere (IS) positions. The WS positions are locations, in which newly added spheres get into contact with two other spheres and the wall of the cylindrical container. The IS positions are locations, where spheres get into contact with three other spheres but not with the container wall. The sphere to be added to the packing on an IS position must be stable under gravity. When $D < 3d$, in addition to the WS and IS locations, there exists a possibility for the third type of a position. It is the one in which newly added spheres are in contact with one sphere only and the wall. Mueller [27] provided formulas to calculate the number of spheres and the coordinates of their centers. A dimensionless packing parameter is used to determinate a stable gravity position of the spheres inside a cylinder. The experimental results showed that deterministic simulations become more inaccurate for larger diameter aspect ratios.

5.2. Network approach

The spaces within a packing form a continuous network of interconnecting pores or voids. The structure of the lattices generated by randomly packed spheres was extensively studied over a long time period because of its importance as a

predictive model in many processes involving granular materials. The research was centered principally on measuring the packing properties and the acquisition of void distribution models.

McGeary [45] described a ball-bearing model in terms of tetrahedral subunits in random close packed lattices of uniform spheres. Zou and Yu [4] and Van Antwerpen [8] analyzed the voids associated with tetrahedral structures. Each tetrahedral structure contained a central pore and four outer constrictions. Although the four connections associated with each pore varied in their sizes, nevertheless the pores joined by a common constriction were similar in size. Nolan and Kavanagh [26] simulated the packing structure as a network of cylindrical pores by applying the Voronoi-Delaunay tessellation technique that was able to predict accurately the transport properties of the porous medium for an ordinary diffusion. The Voronoi cells, or regions, are defined as the set of points closer to the selected sphere than to any other sphere. In 1998, Sean McLaughlin demonstrated that the smallest Voronoi cell is the regular dodecahedron circumscribing the sphere [35]. The volume ratio of these two figures is 0.754697, which is very close to the value of Kepler's limit (0.74048), and thus it represents an excellent upper bound on the space occupation coefficient.

The Voronoi-Delaunay approach for the analysis of the free volume, considering packing of balls confined in a cylinder, was described in [53], where a generalized Voronoi diagram was used as the underlying data structure. The edges of the Voronoi diagram are located between the objects, and they are often referred to as the Voronoi network. Two problems were considered: i) an efficient construction of the confined Voronoi diagram inside a cylindrical boundary, and ii) an analysis of the Voronoi network to study the distribution of the empty spaces (voids) in the system. An algorithm was proposed to calculate the Voronoi network for 3D systems, based on the idea of the Delaunay empty sphere: it moves inside the system so that it touches at least three objects at any time moment. In this case, the center of the sphere moves along an edge of the 3D Voronoi network. Explicit formulas to compute the coordinates of the Voronoi vertex were provided. The algorithm was implemented and tested in a 3D system for packings with disordered structure, representing a bed of spherical particles in cylinders of different radii. The models were obtained by using the Monte Carlo relaxation method.

5.3. Minimization of the cylinder size

Several papers deal with minimizing the size of a container to be filled by a fixed set of items without overlapping. Most approaches consider rectangular containers as the packing object. A generalized mathematical model for a variety of circular and spherical packing problems was proposed by Birgin and Sobral [60]. These non-linear models considered the minimization of the dimension of the container, fitting non-overlapping items inside. The authors implemented an efficient methodology based on strategies applied to the N-body problem to reduce the computational cost of computing the overlap. The N-body problem consists of the computation of the gravitational force between N particles in the 3D space, where each particle exerts a force on all the other particles, implying pairwise interactions. This kind of a physical system occurs in several fields, like celestial mechanics, plasma physics, fluid mechanics and semiconductor device simulations. By using this strategy, packing problems with a large number of items were solved. Several models were summarized for distinct forms of the objects (container).

A solution for the optimization problem of identical sphere packing in a cylinder of minimal height was proposed by Stoyan and Yaskov [29]. This problem is a multi-extremal one and NP-hard. A mathematical model was offered and its characteristics were pointed out. Based on those characteristics, a strategy of searching for an approximation to a global minimum was proposed: generation of a special search tree to obtain the starting points leading to different local minima; a modification of the Zoutendijk feasible direction method to calculate the local minima, and a modification of the decremental neighborhood method to search for an approximation to a global minimum. Numerical examples and a performance analysis of the solutions were given. On the basis of the mathematical model and the numerical experiments, a number of analytical conclusions were drawn. The numerical examples illustrated that the run time increased dramatically if the number of spheres was more than 200. In this case, the offered approach became ineffective.

6. Concluding remarks

Finding the densest packing is important in several different areas. First, a densest packing means the best utilization of space. Therefore, it is a basic problem of mathematics, physics and engineering, and one of the most important computational problems over centuries.

Nowadays, there are many modern applications and industrial branches, beginning from the bundle of nuclear fuel rods for a thermonuclear reactor to crystal engineering in the design of functionalized solids, nanoparticles, materials with predetermined microporous, chemical and physical properties, where the problem of filling an available restricted empty space with characteristic matrix porosity starts to be a key issue. At a fundamental level, there is a need to achieve a general 3D control over the packing of components in a volume.

Hierarchically structured hybrid nanocomposite materials demonstrate outstanding properties, see, *e.g.* [61,62]. The manufacture of these materials requires to realize the design and successful processing of a new generation of smart ingredients which are important for the development of heterogeneous catalysis, photocatalysis, light harvesting, hybrid organic/inorganic surface chemistry, etc. The physicochemical properties of such materials start to be size-dependent,

and they are strongly influenced by the confinement in nanoporous matrices [63-65].

The confinement in molecular sieves is a promising strategy for fabricating nanostructured assemblies with a highly uniform size distribution. So, nanomaterials based on nanoparticles stabilized inside of zeolite matrices have been widely searched. Existing approaches to the procedure of packing of idealized hard spheres inside a zeolite framework were recently reviewed in [66].

Some experimental results, which deal with the processes of stabilizing clusters and nanoparticles into different zeolite matrices, their optical, electrical, magnetic properties and theoretical approaches to the properties of obtained systems, revealed that the physicochemical properties of nanomaterials start to be size-dependent, and they are strongly influenced by the confinement in nanoporous matrices [67-70]. It was shown that the diffusion in ultrathin channels depends on their size [71,72].

Careful attention is paid to biomedical applications of nanomaterials. For example, a bone is a nanocomposite, which consists of organic and inorganic components, with a hierarchical structure ranging from nano- to macroscale. The development of nanomaterials for bone repair and regeneration was reviewed in [73]. As interesting examples of the papers dedicated to sphere packings, some medical applications can be mentioned [11,74].

Another example of a new application of the packing approach to design the structure was found in the corrosion of materials. The porosity of reinforced concrete structures are the paths for a migration of chloride ions from the saline environment to the carbon steel reinforcement, causing severe corrosion damage. To avoid this problem, the pores are sealed using monosized spheres as it has been demonstrated by modeling spherical and cylindrical particles [75].

The packing approach permits to organize nanostructured materials not only by an ordering of a nanosized matter, but as well by organizing nanosized voids. Metal foams are an example of those materials, which currently attract a concentrated interest due to their outstanding properties [76]. In this sense, the foam materials with the packing of empty spheres or other kinds of bubbles of emptiness start to become a challenge in the synthesis of nanomaterials.

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