LOG-NORMAL AND MONO-SIZED PARTICLES' PACKING INTO A BOUNDED REGION

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Abstract Many systems can be modeled with hard and various size spheres, therefore packing and geometrical structures of such sets are of great importance. In this paper, rigid spherical particles distributed in different sizes are randomly packed in confined spaces, using a parallel algorithm. Mersenne Twister algorithm was used to generate pseudorandom numbers for initial coordination of particles. Distribution of packing densities and reproducibility of particles packing factor, with log-normal size distribution and also mono-sized particles have been compared. In addition, the effects of container size on regional particle packing density, the effect of wall on packing density and symmetry of packed structure have been investigated. The results confirm that particles in log-normal size distribution have higher packing densities, but the obtained results have less reproducibility than mono-sized particles. Also, in comparison, particles in log-normal size distribution have uniform density and regions with higher local density.

Keywords Powder Metallurgy, Porous Materials, Simulation, Packing, Log-Normal, Mono Size

چکیده بسیاری از سیستم‌ها می‌توانند به روش کره‌های سخت با اندازه‌های مختلف مدل‌سازی شوند و بنابراین فشردگی و ساختار هندسی چنین مجموعه‌هایی از اهمیت بالایی برخوردار است. در مقاله حاضر، ذرات کروی صلب در توزیع‌های اندازه مختلف به‌صورت تصادفی در یک فضای محدود با استفاده از الگوریتم موازی چیده شده‌اند. الگوریتم تویستر به منظور تولید اعداد شبه تصادفی برای مختصات اولیه ذرات استفاده شده است. توزیع چگالی‌های فشردگی و تکرار پذیری فاکتور تراکم ذرات با توزیع اندازه log-normal و ذرات هم اندازه مقایسه شده‌اند. همچنین، اثرات اندازه ظرف بر روی چگالی فشردگی ذرات و اثر دیواره بر روی چگالی قشردگی و تقارن ساختار فشرده شده مورد بررسی قرار گرفته است. نتایج بدست آمده تایید می‌کنند که ذرات در توزیع اندازه log-normal چگالی فشردگی بالاتری دارند ولی تکرارپذیری کمتری از ذرات تک اندازه دارند. همچنین چگالی ذرات در توزیع اندازه log-normal یکنواخت و نواحی با چگالی موضعی بیشتری وجود دارد.

1. INTRODUCTION

Random packing of particles has been studied for many years because of their interesting geometrical properties and technological applications in porous media [1]. The term, particle 'Packing' means 'putting together' and 'arranging' particles in a confined space. Random packing means; all particles of the same size and shape have the same probability to occupy each unit volume of the mixture [2]. Particle packing affects the efficiency of powder compaction, the final surface properties and corrosion resistance of powder metallurgy products. The porosity of powder metallurgy products can be controlled using powders with different sizes. Pore size distribution has a significant importance in production of implants and capillary porous powder metallurgy materials [3-12]. The initial step of production in powder metallurgy method is filling the mold, so it is important to simulate the loose packing of particles.

Many parameters affect the packing characteristics of particles, such as particle's size distribution, particle shape, interparticle friction, elasticity, surface chemistry (interparticle forces), agglomeration and vibration (rearrangement of particles upon shaking) [13-21]. Random packing of particles can be classified into random close packing, that is the state of maximum volume fraction of packed powders and random loose packing which is the loosest powder packing of mechanically stable condition [22,23]. Among these parameters, particles size distribution, due to its ease of adjustment in industrial applications, is probably the most significant.

One of the most important parameters in the study of granular materials is its packing factor. It is defined as the fraction of powder volume to their total occupied space.

Research on particle packing can be classified into three different approaches: experimental, theoretical, and numerical. Due to difficulties associated with experimental methods of investigating particle packing, theoretical and computational approaches are usually preferred [24].

A random variable x is said to be log-normally distributed if log(x) is normally distributed. The dispersions produced by milling, grinding or crushing provide example of powders with log-normal distribution [25]. Also it's an approximation to the expected particle size distribution for nucleation and growth process, assuming only random interactions between existing particles [26].

Packed particles can be unconfined where there are no walls to contain them, or particles can be packed in containers of various shapes. In the case of random pack, a so-called wall effect exists because the proximity of a solid surface will introduce some local order into a random packing. Thus, the particles next to the solid surface tend to form a layer of the same shape as the surface. This so-called base layer is a mixture of cluster of square and triangular units. Randomness increases by increasing distance from the base layer, which results in the disappearance of the distinct layer. Another important aspect of wall effects is the existence of a region with relatively high void next to the wall, due to the discrepancy between the radii of the wall curvature and the particles [27,28].

In this paper the packing of mono-sized powders and powders in log-normal size distribution have been investigated, using a parallel packing algorithm and reproducibility of the obtained values of packing factors, also regional packing densities of these packed structures have been compared.

2. EXPERIMENTAL

2.1. Modeling We assumed particles to be ideal rigid hard spheres with mono-sized and log-normal particle size distributions. Log-normal distribution can be expressed as:

$$f(D) = \frac{1}{D.\sigma\sqrt{2\pi}} \exp\left(-\frac{1}{2\sigma^2} \left(\log(D) - \mu\right)^2 \right) \qquad (1)$$

Two parameters are needed to specify a log-normal distribution. Traditionally, the mean μ and the standard deviation σ (or the variance σ^2) of log(x) are used. However, there are clear advantages in using 'back-transformed' values (the values in terms of the measured data):

$$\mu^*: = e^{\mu} \qquad (2)$$

$$\sigma^*: = e^{\sigma} \qquad (3)$$

Since μ is the median of log(x), the median of log-normal distribution is med(x) = $\mu^* = e^{\mu}$.

In this work, we assumed friction to be infinite. This assumption affects the obtained values for packing factor, but doesn't affect the behavior of system from standpoint of reproducibility also the assumption affects both PSD's packing factor values, so we can compare their reproducibility [29,30].

2.2. Packing Algorithm We used a time-independent model for packing particles, based on Event Dynamics (ED) model as reported in our previous paper [31]. Event dynamics method is commonly used for simulation of systems consisted of rigid spherical particles. The collisions are assumed to be instantaneous and binary. By the velocity and the coordination of the powder, their next movement could be calculated. In our model, collisions are considered to be soft. This assumption obviously requires computing each effect several times during the collision, which also increases the accuracy obtained in the model.

The particles' X-Y coordinates were randomly generated. Then in each step particles dropped a predefined distant until they reach the floor (Z=0) or collide with one another. The stability and the movements of the particles in each step is determined from the particle's coordinate and its contact points with boundary walls or other particles. The falling of particles into container was in random sequence and also no particles rearrangement was done in their stable state. The resulting state may be described as random loose packing [32].

2.3. Random Numbers We used Mersenne twister algorithm for generation random numbers which is 32-bit length number generator and complies with MT19937 standard. This algorithm produces pseudorandom numbers with very long period length. Its main advantage is rapid generation of random numbers due to bitwise operators usage, higher order of dimensional equi-distribution compared to other algorithms and passing diehard tests [33,34].

2.4. Parallel Implementation Massage Passing Interface (MPI) is a protocol for communication of computers in a cluster. This feature enables us to distribute computational tasks among computers and gather resultant data [35]. We have implemented our parallel algorithm using MPICH2 implementation of MPI library. This implementation enabled us to use Microsoft Windows operating systems and use their network enhancements. Another advantage of this MPI implementation is its complete object orientation support.

2.5. Hardware The hardware used in this simulation consisted of six dual Intel 3.4Ghz processor PCs with 512MB RAM one of which was used for distribution of jobs and gathering resultant data. These PCs were connected together in a star topology. Each simulation and analysis of data took almost 72 hours.

2.6. Calculation Parameters In this paper the friction was assumed to be infinite. For investigating relative size of particles to container effects, all dimensions are without any defined unit.

The accuracy of all calculation was 0.0001. The integration of the PSD diagrams were done by 1 unit steps in lower-Riemann method.

Minimum and maximum diameters of particles in log-normal PSD were 1 and 60, respectively. The median of Log-normal PSD was assumed to be 30. The diameter of mono-sized particles was assumed to be 30. In each case, four random seeds for Mersenne twister algorithm were used. Regional density of packing structures was calculated using 1^3 cubic elements.

3. RESULTS AND DISCUSSION

Figure 1 illustrates the reproducibility of obtained packing factors of 800 samples consisted of 500 monosized particles and 500 particles in log-normal size distribution in a $350 \times 350 nm^2$ container.

Due to the existence of the container and also because of infinite friction, our packing factor results are less than the values expected for unconfined packing. Particles in log-normal size distribution have higher packing factors but their results have broader distribution and thus lower reproducibility.

The sum of all elements with same x and y coordinates which have been occupied by particles gives a measure of regional density in that position. Non-Photorealistic Rendering (NPR) is one of the scientific visualization methods that are used for making comprehensible but simple picture of complex 3D graphs [36]. Figure 2a-c illustrates the Non-Photorealistic Rendering (NPR) of regional packing density of 500 mono-sized particles in 150×150, 250×250 and $350 \times 350 nm^2$ containers, respectively.

Figure 3a-c illustrates NPR of regional packing density of 500 particles in log-normal size distribution in 150×150, 250×250 and $350 \times 350 nm^2$ containers, respectively.

Small size and low ratio of container to particles size, causes some kind of symmetry in packing structure. This symmetry can be seen in

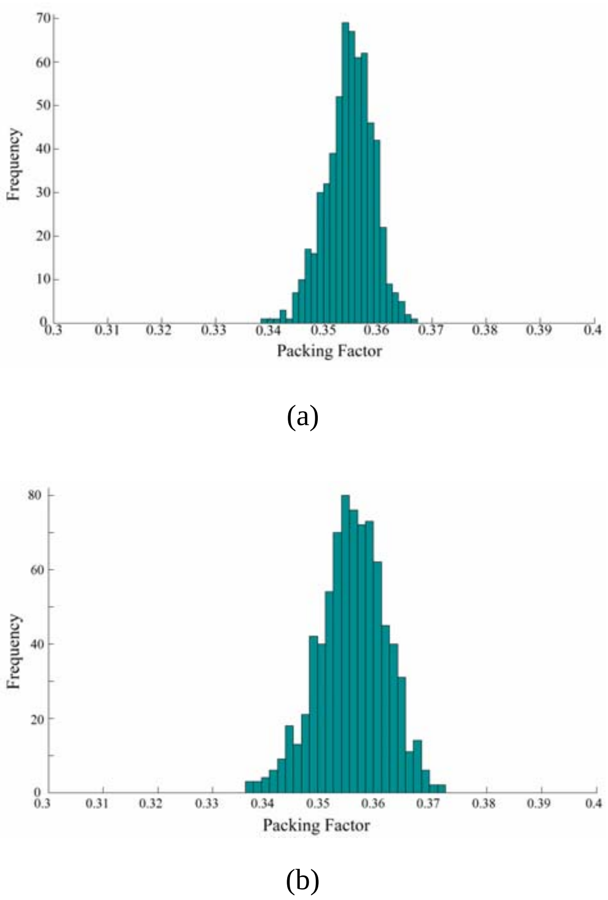


Figure 1. Reproducibility of packing factor in (a) monosized, (b) log-normal particle size distribution.

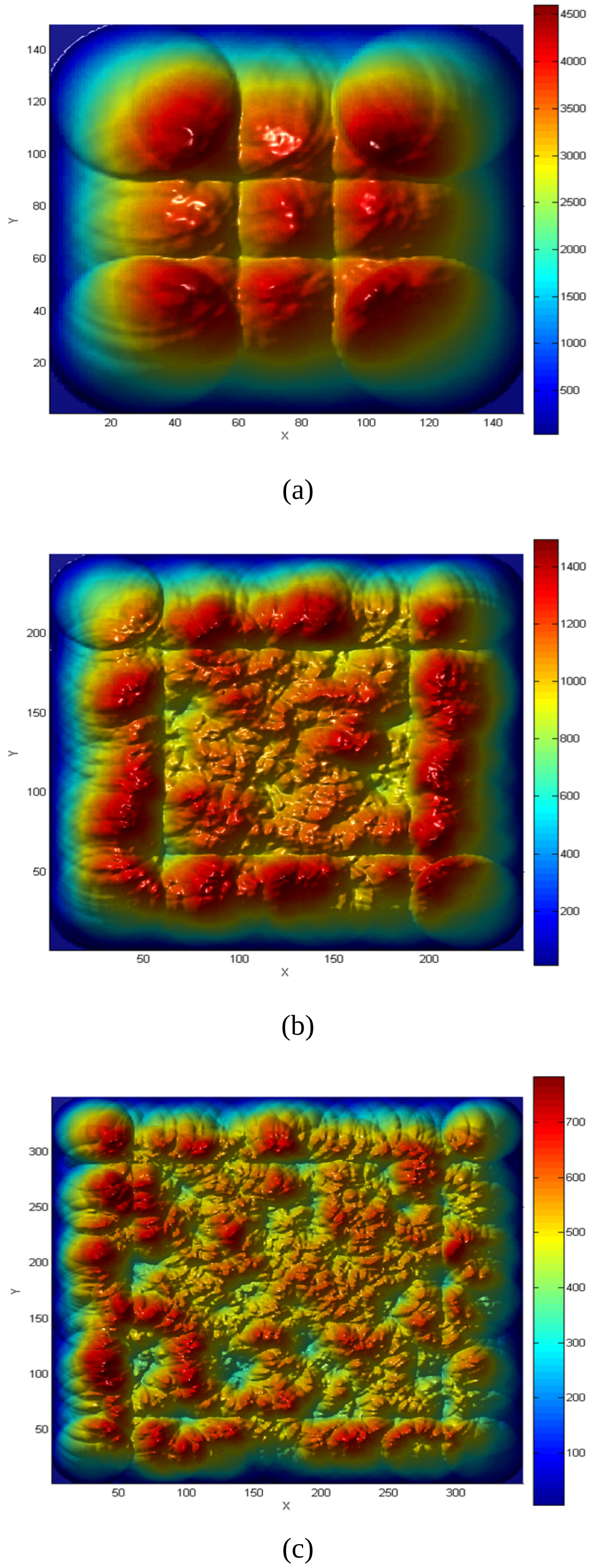
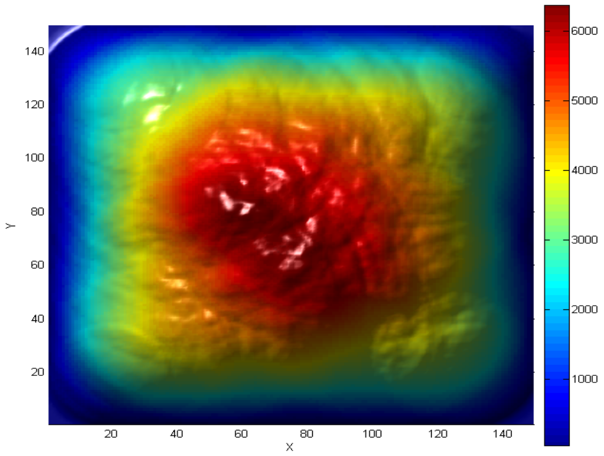
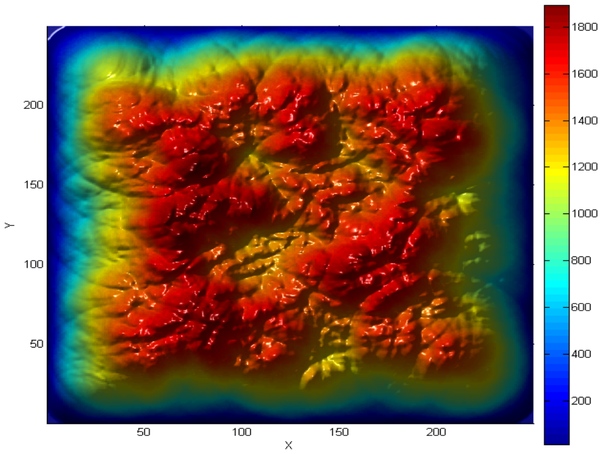


Figure 2. Regional packing density of mono-sized particles in (a) 150×150, (b) 250×250 and (c) 350×350nm^2 containers.

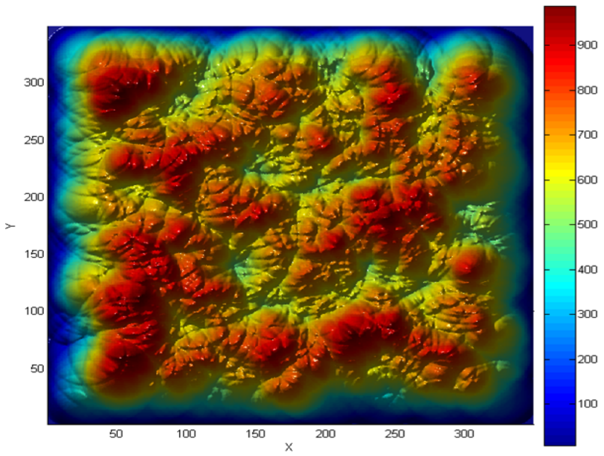
Figure 2a and Figure 3a. By increasing container size, wall effect decreases. As it can be seen in Figures 1 and 2, moving from walls to the centre of the container will increase regional density of particles packing. In comparison, particles in log-normal size distribution have higher and uniform packing density. As it can be seen in Figure 2a,b at a distance D (particles diameter) from container walls, we have the lowest packing density and the highest porosity that is in good agreement with previous studies [27] but particles in log-normal size distribution have more random regional density distribution and symmetry posed by wall decreases faster by moving to centre of the container. The edges of the container in packing particles with log-normal size distribution have



(a)



(b)



(c)

Figure 3. Regional packing density of particles in log-normal size distribution in (a) 150*150, (b) 250*250 and (c) 350*350 containers.

higher density due to the existence of smaller particles.

4. CONCLUSION

In this paper, packing behavior of mono-sized particles and particles in log-normal size distribution was compared using an Event Driven based packing model. Results confirm that particles in log-normal size distribution have higher packing factor but their results have broader distribution and thus lower reproducibility. Also, they have higher and more uniform regional density profile. Simultaneous effects of several walls cause high symmetry in low container to particle size ratios. These results provide a good starting point for the evaluation of the powder metallurgy products properties after sintering and choosing PSD for homogeneous packing and properties.

5. REFERENCES

1. Mayer, A. S. and Miller, C. T., "Influence of Porous Medium Characteristics and Measurement Scale on Pore-Scale Distribution of Residual Nonaqueous-Phase Liquids", ***J. Contam. Hydrol***., Vol. 11, (1992), 189-213.
2. Debbas, S. and Rumpf, H., "On the Randomness of Beds Packed with Spheres or Irregular Shaped Particles", ***Chem. Eng. Sci***., Vol. 21, (1966), 583-607.
3. Konakawa, Y. and Ishizaki, K., "The Particle Size Distribution for the Highest Relative Density in a Compacted Body", ***Powder Technol***., Vol. 63, (1990), 241-246.
4. Yokota, K., Murai, S. and Shinagawa, K., "Influence of Particle Size Distributions with Various Geometrical Standards Derivations on Slip-Cast Forming and Sintering Behavior in Submicron Alumina Powder Compacts", ***J. Ceram. Soc. Japan***, Vol. 114, (2006), 1138-1143.
5. Khoe, G. K., Ip, T. L. and Grace, J. R., "Rheological and Fluidization Behavior of Powders of Different Particle Size Distribution", ***Powder Technol***., Vol. 66, (1991), 127-141.
6. Liu, D. M. and Lin, J. T., "Influence of Ceramic Powders of Different Characteristics on Particle Packing Structure and Sintering Behavior", ***J. Mater. Sci***., Vol. 34, (1999), 1959-1972.
7. Subbanna, M., Kapur, P. C. and Pradip, "Role of Powder Size, Packing, Solid Loading and Dispersion in Colloidal Processing of Ceramics", ***Ceram. Int***., Vol.

28, (2002), 401-405.
8. Zheng, J. M. and Reed, J. S., “Particle and Granule Parameters Affecting Compaction Efficiency in Dry Pressing”, ***J. Am. Ceram. Soc***., Vol. 71, (1988), 456-458.
9. Zheng, J., Carlson, W. B. and Reed, J. S., “Dependence of Compaction Efficiency in Dry Pressing on the Particle Size Distribution”, ***J. Am. Ceram. Soc***., Vol. 78, (1995), 2527-2533.
10. Veta, M. C. C., Fracote, C. A., Henrique, R., Graça, M. L. A. and Cario, C. A. A., “Densification Study of Titanium Powder Compacts”, ***Mater. Sci. Forum***, Vols. 498-499, (2005), 211-216.
11. Montasser, D. M. and Lim, J. K., “Properties of Solid Core and Porous Surface Ti-6Al-4V implants manufactured by powder metallurgy”, ***J. Alloy. Compd***., (2007), Doi: 10.1016/j.jallcom.2006.12.143.
12. Sheleg, V. K. and Sabich, V. V., “Effect of the Method of Production of Porous Powder Metallurgy Materials on their Capillary Properties”, ***Powder Metall. Met. C***, Vol. 35, (1996), 244-252.
13. Yu, A. B. and Standish, N., “A Study of the Packing of Particles with Mixture Size Distribution”, ***Powder Technol***., Vol. 76, (1993), 113-124.
14. Kong, C. M. and Lannutti, J., “Effect of Agglomerate Size Distribution on Loose Packing Fraction”, ***J. Am. Ceram. Soc***., Vol. 83, (2000), 2183-2188.
15. Abreu, C. R. A., Tavares, F. W. and Castier, M., “Influence of Particle Shape on the Packing and on the Segregation of Spherocylinders Via Monte Carlo Simulations”, ***Powder Technol***., Vol. 134, (2003), 167-180.
16. Velamakanni, B. V. and Lange, F. F., “Effect of Interparticle Potentials and Sedimentation on Particle Packing Density of Bimodal Particle Distributions During Pressure Filtration”, ***J. Am. Ceram. Soc***., Vol. 74, (1991), 166-172.
17. Cheng, Y., Guo, S. and Hai, H., “Dynamic Simulation of Random Packing of Spherical Particles”, ***Powder Technol***., Vol. 107, (2000), 123-130.
18. Sikiric, M. D., Itoh, Y. and Poyarkov, A., “Cube packings, Second Moment and Holes”, ***Eur. J. Combin***., Vol. 28, (2007), 715-725.
19. Kim, J. C., Martin, D. M. and Lim, C. S., “Effect of Rearrangement on Simulated Particle Packing”, ***Powder Technol***., Vol. 126, (2002), 211-216.
20. Mason, G. and Mellor, D. W., “Simulation of Drainage and Imbibition in a Random Packing of Equal Spheres”, ***J. Colloid Interf. Sci***., Vol. 176, (1995), 214-255.
21. Pan, C., Hilpert, M. and Miller, C. T., “Pore-Scale Modeling of Saturated Permeability in Random Sphere Packing”, ***Phys. Rev. E***., Vol. 64, (2001), 066702/1-066702/9.
22. Scott, G. D., “Packing of Spheres: Packing of Equal Spheres”, ***Nature***, Vol. 188, (1960), 908-909.
23. Scott, G. D. and Kilgour, D. M., “The Density of Random Close Packing of Spheres”, ***J. Phys. D: App. Phys***., Vol. 2, (1969), 863-866.
24. Mueller, G. E., “Numerically Packing Spheres in Cylinders”, ***Powder Technol***., Vol. 159, (2005), 105-110.
25. Limpert, E., Stahel, W. A. and Abbt, M., “Log-Normal Distributions Across the Sciences: Keys and Clues”, ***Bio Sci***., Vol. 51, (2001), 341-352.
26. Kiss, L. B., Söderlund, J., Niklasson, G. A. and Granqvist, C. G., “The Real Origin of Lognormal Size Distribution of Nanoparticles in Vapor Growth Processes”, ***Nanostructured Mater***., Vol. 12, (1999), 327-332.
27. Frukawa, K., Imai, K. and Kurashige, M., “Simulated Effect of Box Size and wall on Porosity of Random Packings of Spherical Particles”, ***Acta Mech***., Vol. 140, (2000), 219-231.
28. McWhirter, J. D., Crawford, M. E. and Klein, D. E., “Wall Region Porosity Distributions for Packed Beds of Uniform Spheres with Modified and Unmodified Walls”, ***Transport Porous Med***., Vol. 27, (1997), 99-118.
29. Clarke, A. S. and Wiley, J. D., “Numerical Simulation of the Dense Random Packing of a Binary Mixture of Hard Spheres: Amorphous Metals”, ***Phys. Rev. B***, Vol. 35, (1987), 7350-7356.
30. Silbert, L. E., Erta, D., Grest, G. S., Hasley, T. C. and Levine, D., “Geometry of Frictionless and Frictional Sphere Packings”, ***Phy. Rev. E***., Vol. 65, (2002), 301-304.
31. Farzalipour Tabriz, M., Salehpoor, P., Esmaielzadeh Kandjani, A., Vaezi, M. R. and Sadrnezhaad, S. K., “Particle Size Distribution Effect on 3D Packing of Nano Particles into a Bounded Region”, ***I. J. E***., Vol. 20, No. 2B, (2007), 281-291.
32. Scott, G. D., “Packing of Spheres: Packing of Equal Spheres”, ***Nature***, Vol. 188, (1960), 908-909.
33. Matsumoto, M. and Kurita, Y., “Twisted GFSR Generators”, ***ACM Trans. Model. Comp. Simul***., Vol. 2, (1992), 179-194.
34. Matsumoto, M. and Nishimura, T., “Mersenne Twister: A 623-Dimensionally Equidistributed Uniform Pseudo-Random Number Generator”, ***ACM Trans. Model. Comp. Simul.***, Vol. 8, (1998), 3-30.
35. Gropp, W., Lusk, E., Doss, N. and Skjellum, A., “A High-Performance, Portable Implementation of MPI Massage Passing Interface Standard”, ***Parallel Computing***, Vol. 22, (1996), 789-828.
36. Markosian, L., Kowalski, M. A., Goldstein, D., Trychin, S. J., Hughes, J. F. and Bourdev, L. D., “Real Time Non-Photorealistic Rendering”, ***Proceedings of the 24th Annual Conference on Computer Graphics and Interactive Techniques***, (1997), 415-420.