Computer Simulation of Morphology and Packing Behaviour of Irregular Particles, for Predicting Apparent Powder Densities

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Abstract

This paper describes a methodology for prediction of powder packing densities which employs a new approach, designated as *random sphere construction* (RSC), for modelling the shape of irregular particles such as those produced by water atomization of iron. The approach involves modelling an irregular particle as a sphere which incorporates smaller *corner spheres* located randomly at its surface. The RSC modelling technique has been combined with a previously developed particle packing algorithm (the *random build algorithm*), to provide a computer simulation of irregular particle packings. Analysis of the simulation output data has allowed relationships to be established between the particle modelling parameters employed by the RSC algorithm, and the density of the simulated packings. One such parameter is η, which is the number of corner spheres per particle. A relationship was established between η, (which was found to have a profound influence on packing density), and the fractional density of the packing, fd. Vision system techniques were used to measure the irregularity of the simulated particles, and this was also related to η. These two relationships were then combined to provide a plot of fractional density for a simulated packing against irregularity of the simulated particles. A comparison was made of these simulated packing densities and observed particle packing densities for irregular particles, and a correlation coefficient of 0.96 was obtained. This relatively good correlation indicates that the models developed are able to realistically simulate packing densities for irregular particles. There are a considerable number of potential applications for such a model in powder metallurgy (PM), process control. In combination with on-line particle image analysis, the model could be used to automatically predict powder densities from particle morphology.

1. Introduction

1.1. Intelligent process control for powder metallurgy

Intelligent process control is a key element in the development of Computer Aided Engineering (CAE) systems for manufacturing process optimization. In the case of Powder Metallurgy (PM), where functional components are formed from metal powders, successful implementation of CAE systems requires an in-depth understanding of powder behaviour during the packing, compaction, and sintering stages of the process. Models providing quantitative descriptions of particle behaviour are necessary for generating the process related information required for development of accurate and effective process control systems. With regard to particle packing, that is to say powder behaviour prior to compaction, years of empirical research indicates that powder densities are dependent upon a number of factors relating to particle shape and size, [1]. Most of the theoretical models developed so far apply to packing of spherical particles. This has largely been due to the perceived difficulty associated with quantitative descriptions of the size and shape of irregular particles. However, particles with irregular geometries are in fact the type of particles which constitute the majority of metal powder consumed by PM industry; a typical example is water atomised iron powder, used for production of automotive structural parts. In order to build effective systems that are able to predict powder densities from information relating to particle characteristics, it is necessary to develop accurate models which relate particle morphology to packing density.

1.2. Importance of apparent density of powder

Microscopic examination of iron powder particles produced by water atomization, reveals an irregular geometry similar to that shown in Figure 1. The apparent density of such powders (i.e. the density of the loose powder), is found to be significantly lower than the packing density of spherical particles. The apparent density of a PM powder is one of its most important characteristics. In order to avoid material wastage and possible production problems, the fill depth of the PM tooling must be accurately set so that the die contains the exact weight of powder required to form the part. An incorrect setting of fill depth, resulting from an inaccurate knowledge of a powder's apparent density, could result in damage to the tool or production of an insufficiently dense part, which would be prone to structural failure. It is therefore necessary for manufacturers of metal powder parts to measure powder density using standard apparatus (e.g. Hall Flowmeter, as described in MPIF Standard 4 [2]). However, the appreciable amount of time required to perform such a test, means that this is a discrete rather than continuous approach to process measurement and quality control. This type of approach could result in undesirable process variation between measurements, consequently leading to scrap production. Such costs could be avoided by means of continuous particle

measurement and analysis through application of vision system technology and development of suitable particle packing models. For such models to accurately predict powder densities under a range of conditions, they must include some form of physical simulation of packing phenomena, which must incorporate the effects of changes in parameters such as the degree of particle irregularity.

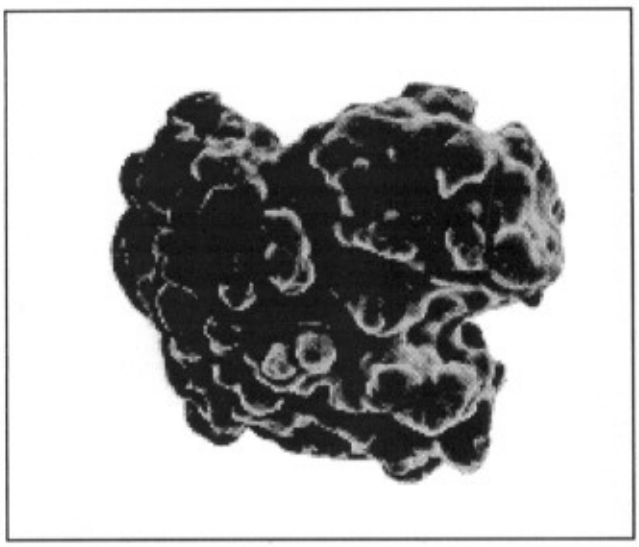

Fig. 1. Micrograph of irregular water atomised particle.

1.3. Approach for modelling irregular particles

The RSC approach for simulation of irregular particle morphology, models a given particle as a combination of spherical sub-particles. Each particle comprises a central sphere (the 'inscribed sphere'), which has smaller spheres (designated as 'corner spheres') randomly located on its surface, as can be seen in Figure 2.

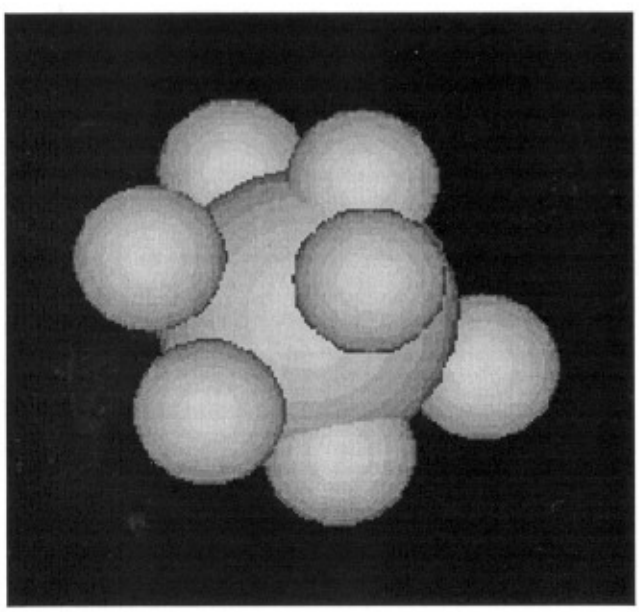

Fig. 2. RSC model of irregular powder particle.

The corner spheres act as asperities on the surface of the particles, and have the effect of increasing the distance between the centres of adjacent particles, as well as increasing inter-particle friction. These effects result in a lower apparent density for irregular powders when compared to spherical powders; water atomised iron powders typically have a fractional density (fd) of 0.38, while the accepted fd value for random close packed spheres is 0.637. This method of particle modelling, in combination with the Random Build Algorithm described previously [3], has been found to be successful for simulating packings of particles with various degrees of irregularity. In particular it is necessary to relate particle morphology to powder density, and the RSC simulation has been successfully applied to establishing such relationships. Statistical analysis provided a polynomial relationship between the degree of irregularity of the simulated particles and the number of corner spheres, (regression coefficient, $r = 0.990$), and a polynomial relationship between the number of corner spheres and the simulated packing density, ($r = 0.991$). By employing these rules, the system can take an image of a powder particle, evaluate its irregularity, simulate the packing of such particles, and calculate the predicted apparent density for the powder.

2. Modelling of Packing of Irregular Powder Particles

2.1 Approach for particle characterisation

The two particle characteristics which a characterisation methodology must address are particle size and shape, since these parameters critically influence packing behaviour. There have been a number of parameters developed for quantifying shape, such as *volume diameter*, *surface diameter*, *Stokes' diameter*, and the *light scattering diameter*, [4]. Unfortunately, for a given non-spherical particle, these methods give different values for particle size; although attempts have been made to reconcile these values through incorporation of particle shape and instrumentation information, [5]. For the present study, particle size was characterized by *sieve diameter*, which is the length of a minimum square aperture through which a particle will pass. Regarding characterisation of particle shape, a number of shape parameters have been proposed, some of which have found application in microscopy, [6]. Again, different techniques can give different shape values for the same particle; although these values can be brought into coincidence through multiplication of the value concerned by a suitable factor, [7]. The RSC particle shape simulation described here has been developed for modelling materials which have a particle shape similar to that shown in Figure 1, (depicted as 'nodular' in ISO 3252). Water atomised iron is an example of a material which is composed of particles with a generally similar morphology to the particle in Figure 1. The RSC algorithm employs a stereological approach, where the powder particles are modelled in 3d, from studies of 2d projections, and it fulfils the following requirements for stereological analysis, as specified by Exner, [8]:-

- Shape sensitivity; a change in particle irregularity results in a change in parameters of particle model, (i.e. number of corner spheres, η).

- The parameters of a modelled particle (and therefore irregularity), are not dependent upon particle size.

- Accessibility; the approach can be used to develop particle models from analysis of microscopic images of actual particles.

2.2. *Determination of particle irregularity*

A quantitative analysis of packing behaviour of irregular particles requires identification of a suitable method for evaluating particle shape. This is achieved here through use of an irregularity parameter (α), which is related to sphericity. For a given image of a particle the irregularity is given by:-

$$\alpha = \beta^2 / (4\pi\gamma)$$

Where α is the irregularity of the image of the particle, β is the perimeter of the particle's image, and γ is the area.

A sphere, for example, has an irregularity of 1. It is worth noting that to obtain an accurate value for the irregularity of a particle, it is necessary to view it from three orthogonal directions. Images of simulated particles were analysed in this way, resulting in three irregularity values for each particle. The average of these three values was calculated and assigned to the type of particle concerned. This procedure was followed for a number of simulated particles, thereby allowing the particle irregularity α to be related to the modelling parameter η.

2.3. *Previous research approaches for modelling of irregular powder packing densities*

From a review of the literature, it is evident that only a relatively small amount of research has been performed on packing of irregular particles. In 1994 Itoh and Wanibe described a stereometric method for modelling the shape of non-spherical powder particles, [9]. Their model employs an ellipsoid of revolution, and may therefore be most applicable to particles with flake-like characteristics. Suzuki *et.al.* have described a method for estimation of the void fraction for random packings of particles of three sizes, [10]. They report a close agreement with experimental data for ternary mixtures of both spherical glass beads and irregular crushed glass particles, however the model is developed through geometrical studies of spherical particles in contact, rather than a physical irregular particle model. Brown [11], has identified a non-linear relationship between the fractional packing density and the sphericity of the particles. (Brown takes sphericity to be the area of a sphere having the same volume as the particle, divided by the area of the particle.) Such relationships are of interest from the point of view of powder characterisation, but they do not provide a physical model of particle packing behaviour. They would not be able to incorporate changes in density resulting from the variations in powder parameters which are observed in practice. These limitations mean that a purely empirical approach is not a suitable simulation method for development of the powder packing models required for implementation of an intelligent process control system.

2.4. *The Random Sphere Construction Algorithm*

Numerous modelling approaches were considered as a basis for simulation of packing phenomena, leading to development of the Random Sphere Construction algorithm for modelling the morphology and packing behaviour of powder particles. This approach is analogous to Monte Carlo type methods (which have been used to simulate fluidised beds [12]), in that the particles are moved randomly, and a given move is only allowed if the specified 'acceptance criteria' are met. As shown in Figure 3, the RSC algorithm is comprised of the following key stages:-

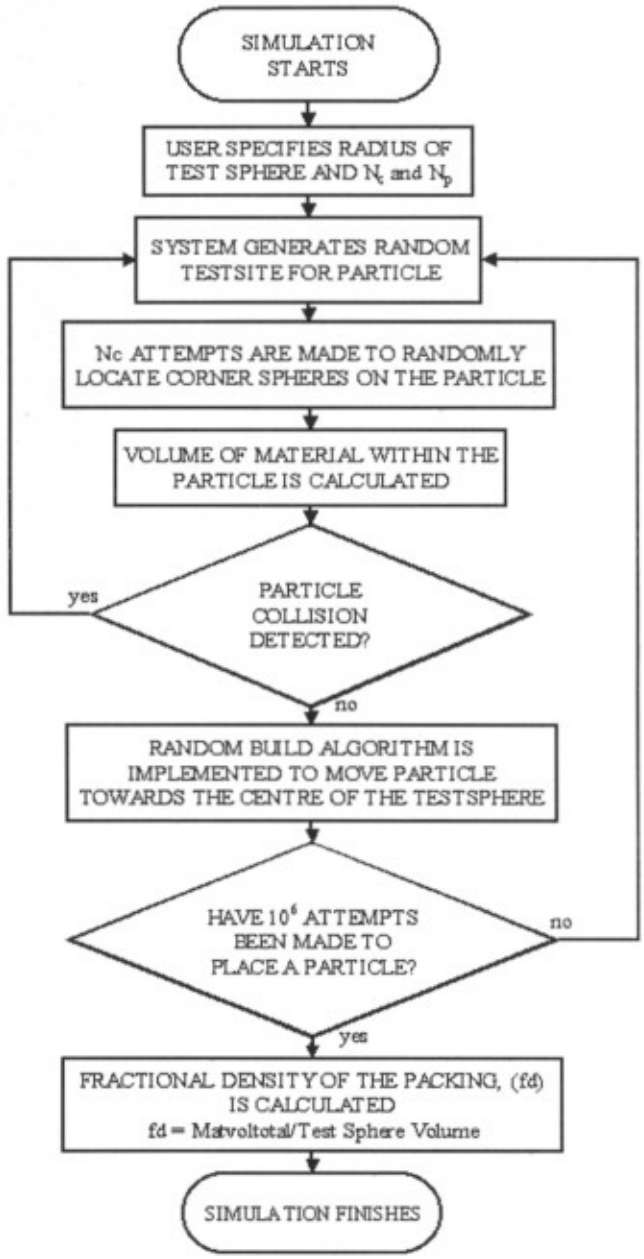

Fig. 3. Method of operation of random sphere construction algorithm for simulating packing of irregular particles.

1. The user specifies the radius of a 'test sphere' within which the particles are to be placed. Wall effects are minimised by allowing packing to occur beyond the boundaries of the test sphere, but for the calculation of packing density, only those parts of the particles are included which are within the test sphere. It is also necessary to specify the radii of the inscribed and corner spheres, the number of attempts (N_c), to be made to place a corner sphere on a given inscribed sphere, and the number of attempts (N_p), to be made to place a particle.

2 (a). A test site is chosen randomly for the centre of an inscribed sphere. N_c attempts are made to randomly locate corner spheres on the surface of the inscribed sphere. The volume of overlap of the corner spheres with the inscribed sphere is calculated, and subtracted from the total volume of all the spheres from which the particle is comprised, giving the actual volume of material for the particle.

2 (b). If any overlaps are detected (other than the necessary overlap of the corner spheres with the inscribed sphere), then the particle is not placed and the program returns to stage 2 (a).

2 (c). The random build algorithm is implemented: the particle is moved by a fixed distance, in a random direction in three dimensions. If this new test site is further from the centre of the spherical container than the old test site, or if a particle collision is detected, the particle is returned to the old test site. This attempt at random movement is repeated 10 000 times for each particle.

3. Stage 2 is repeated N_p times. Typically a value of 100 000 was used for N_p; as its magnitude increases the exact value becomes less significant. The total volume, within the test sphere, of all the particles placed (which is designated here as matvoltotal), is calculated. Matvoltotal divided by the volume of the test sphere gives the fractional density of the packing.

The part of the simulation designated as the random build algorithm (described in a previous paper [3]), moves the particle towards the centre of the test sphere in order to simulate the effects of gravitational attraction on the particles. In practice the metal powder particles move under the action of gravity to assume the lowest possible potential energy state. Their exact location is dependent upon their geometry and the frictional forces acting upon them. A simulation which placed the particles purely randomly without any subsequent movement, would give an unrealistically low packing density.

The time taken for the program to complete depends upon the size of the test sphere, the relative sizes of the inscribed and corner spheres, and N_c and N_p. The relatively fast Turbo C++® compiler was employed to keep the time needed to the minimum practicable, and the ran2() function was used for random number generation, [3]. To achieve as realistic a simulation as possible, each particle has a unique geometry, however by only recording the locations of spheres which were successfully placed, the sizes of arrays needed and number of calculations required was kept within manageable proportions.

Figure 4 shows program output data, when the following parameters were used: radius of test sphere = 70 units, radius of inscribed sphere = 10 units, radius of corner sphere = 5 units, and N_p= 100 000. The ratio of 7:1 for the test sphere and the inscribed sphere was found to offer a suitable compromise between the requirement for accurate modelling, and the time taken to run the simulation. Smaller values of test sphere radius tended to produced errors due to the size of the particle approaching that of the container. However, as the radius of the test sphere was increased beyond 70, the number of particles placed, and therefore the time needed for the simulation to run, increased rapidly. Each time the program was run a different value of N_c was employed. Regression analysis was used to fit the second order polynomial to the data, with the following results:-

$$fd = 0.0014\eta^2 - 0.0427\eta + 0.696 \qquad \ldots 1$$

Where η is the average number of corner spheres per particle, (correlation coefficient,r = 0.991). Figure 4 shows both the simulated data and the best fit polynomial.

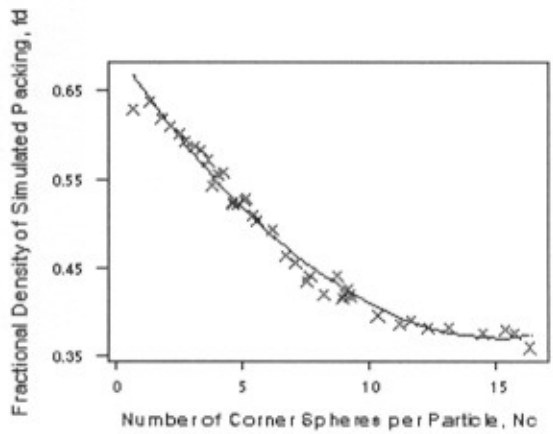

Fig. 4. Graph of Fractional Density vs. number of corner spheres per particle, for RSC simulation.

2.5. Method for relating actual particle irregularities to number of corner spheres, per simulated particle

To enable equation 1 to be usefully applied, it was necessary to find a relationship between the irregularity α, and the number of corner spheres per particle, η. This was achieved through vision system analysis of rendered images of the simulated particles. The C++ program was used to produce nine examples of simulated particles which had corner spheres in the range 1-9. For each of these particles, a record was made of the location of each of the spheres from which they were constituted. The AutoCAD® solid modeller AME™ was then used to create a solid model of each particle, by creating a solid sphere at each of the relevant locations, followed by use of the boolean UNION operation, to form them into one particle. A rendering operation was performed on the particle concerned (see Figure 2), and three images (looking from the x, y, and z directions), were created and saved to disk. Following suitable image conversion and enhancement in Paint Shop Pro, the images were loaded into the Ad Oculus image processing system. Suitable filters and feature extraction algorithms were employed in Ad Oculus to obtain a value of 'compactness' for each of the particle views, (the term compactness, as employed in Ad Oculus, has the same meaning

as irregularity α). The three values obtained for irregularity were averaged to give the value of irregularity for the simulated particle. The resulting data, which is shown in Figure 5, was used to establish the following relationship between α and η:-

$$\alpha = -0.0189\eta^2 + 0.280\eta + 1.04 \qquad ...2$$

Regression analysis gave a correlation coefficient of r = 0.990 for equation 2. This is the equation of the curve shown in Figure 5.

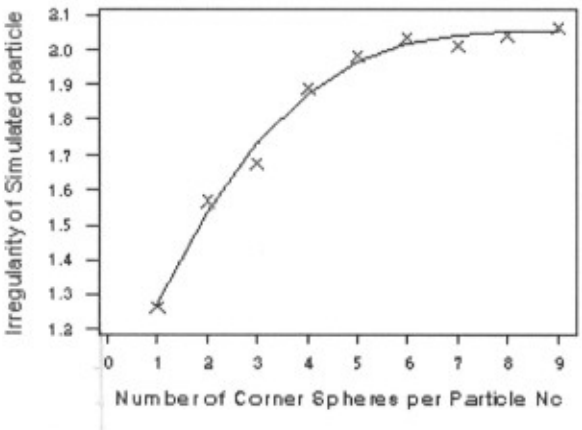

Fig. 5 Relationship between irregularity and N_c for RSC simulation.

2.6. Comparison of simulated and measured packing densities

This simulation can now be used in a powder particle analysis system to predict packing densities from analysis of particle images. A vision system is used to provide irregularity values for a number of particles of a given type. These values are averaged resulting in a value for α which is substituted into equation 2; this is then solved to generate a value for η. This value is substituted in equation 1 to give a value for the density of a packing of the particles, fd. For example, if microscopic vision system analysis of water atomised iron particles resulted in a irregularity value of 2.03, equation 2 would give a value of 5.82 for the average number of corner spheres per particle. Substituting this value for η into equation 1, gives a packing density of fd = 0.49.

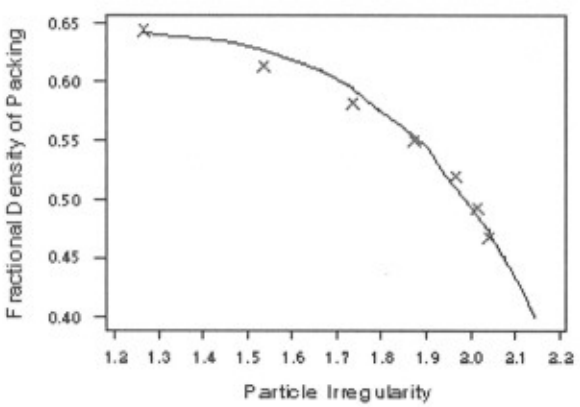

Fig. 6 Graph of fractional density vs. particle irregularity for simulated and experimental packings.

The simulation was used to predict the packing density for particles with various values of irregularity. These values for simulated packing density were plotted against particle irregularity, as shown in Figure 6. Also included in Figure 6, is a curve showing the non-linear relationship between fd and α, which was obtained experimentally by Brown [11]. Using linear regression, a coefficient of r = 0.96 was obtained for the correlation of the simulated and experimental densities.

3. Conclusion

A description has been given of a model for estimating the apparent density of a given powder by means of vision system analysis of the particles concerned, and subsequent simulation of their packing behaviour. The algorithm has been validated through comparison of simulated and experimental densities of packings of particles which exhibited various degrees of irregularity. Predicted densities were correlated with measured values to give a coefficient of 0.96. This close agreement leads to the following conclusions:-

(i) A particle modelling approach which employs a sphere combined with smaller spheres at its surface (RSC), is an effective means of quantifying the morphology of irregular particles with nodular type geometries, similar to the iron particle shown in Figure 1.

(ii) An algorithm employing numerous short-range random particle movements (RBA), is suitable for simulating packing of irregular particles.

(iii) A combination of a vision system for evaluating the particle morphology, and a computer based system employing the approach described here for modelling of particle packings, could be used to predict the apparent densities of powders as they are produced.

Further work will involve adaption of the simulation to apply it to the types of metal powders currently used in powder metallurgy. Water atomised iron is an example of a widely used PM powder which consists of particles that can have sieve diameters that are as small as 40 μm or less. When modelling the packing of such particles it will be necessary to allow for the effects of inter-particle friction, (which is itself related to particle irregularity, [1]). Inter-particle friction has a considerable influence over apparent density [13], and this effect becomes more significant as the particle size decreases. It will also be necessary to model the densities of mixtures of more than one size of irregular particle. The resulting models will then be suitable for formation into the rule base of a knowledge based system (KBS), able to advise on packing densities of irregular particles. Integration of this type of powder packing KBS with powder metallurgy KBS modules previously developed by the authors [14], offers potential for development of a comprehensive knowledge based system for PM process optimisation.

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