On the sphericity of coal and char particles

A. Luckos, A. Koekemoer
Sasol Technology, Research and Development, Sasolburg, South Africa

Keywords: fixed bed, fluidization, particle, sphericity, laser scanning

Abstract—Most solid particles of practical interest are irregular in shape. In fixed-bed and fluidized-bed reactors, shape of particles can influence bed permeability, gas flow distribution, diffusion of mass and heat and reaction rates.

The most popular empirical factor to describe non-spherical shapes of particles is sphericity. In this study sphericity of Highveld coal particles in the range 4.7–106 mm and chars formed by devolatilization of this coal in the range 3.4–45 mm was determined using 3-D laser scanning technique. It was found that the relative variation in sphericity of the coal particles does not exceed 15% and, therefore, it can be possible to describe Highveld coal particles using an average value of sphericity calculated for all size classes. This average value is 0.793 (standard deviation 0.034) and it is very close to the sphericity of particles in the +37.5–53.0 mm size class (\(\phi_s = 0.798\)). In contrast to this, the sphericity of devolatalized coal particles were observed to decrease slightly with increasing particle diameter, assuming an average value of 0.749 (standard deviation 0.042)

INTRODUCTION

Most solid particles of practical interest (natural or man-made) are irregular in shape. In fixed (or packed) bed reactors, shape of particles and particle size distribution influence the bed permeability (voidage) which can affect the pressure drop, gas flow distribution and heat transfer inside the reactor. In fluidized bed reactors, some important design parameters such as the superficial gas velocity at minimum fluidizing conditions, \(U_{mfp}\), and the terminal velocity of a falling particle, \(U_t\), depend on the shape of solids used in the process. Changes in shape and area-to-volume ratio affect the diffusion of heat and mass and may, thereby, control reaction rates.

A variety of empirical factors have been proposed to describe non-spherical shapes of particles. These empirical descriptions are usually provided by identifying some characteristic parameters such as volume of the particle, external surface area of the particle, projected area of the particle and projected perimeter of the particle.

All, proposed to date, shape factors are open to criticism because a range of bodies with different shape may have the same shape factor. This is really inevitable if complex shapes are to be described only by a single parameter.

The most popular empirical factor used to describe non-spherical shapes of particles is the “degree of true sphericity” proposed by Wadell. It is defined as:

\[
\phi_s = \left(\frac{\text{surface area of sphere}}{\text{surface area of particle}}\right)_{\text{same volume}}
\]

With this definition \(\phi_s = 1\) for spheres and \(0 < \phi_s < 1\) for all other particle shapes. Exemplary values of the sphericity for some regular and irregular particles are shown in Table 1.
Table 1. Sphericity of regular and irregular particles

<table>
<thead>
<tr>
<th>Type of particle</th>
<th>Sphericity</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sphere</td>
<td>1.00</td>
</tr>
<tr>
<td>Cube</td>
<td>0.81</td>
</tr>
<tr>
<td>Cylinders</td>
<td></td>
</tr>
<tr>
<td>$h = d$</td>
<td>0.87</td>
</tr>
<tr>
<td>$h = 5d$</td>
<td>0.70</td>
</tr>
<tr>
<td>$h = 10d$</td>
<td>0.58</td>
</tr>
<tr>
<td>Disks</td>
<td></td>
</tr>
<tr>
<td>$h = d/3$</td>
<td>0.76</td>
</tr>
<tr>
<td>$h = d/6$</td>
<td>0.60</td>
</tr>
<tr>
<td>$h = d/10$</td>
<td>0.47</td>
</tr>
<tr>
<td>Activated carbon and silica gels</td>
<td>0.70—0.90</td>
</tr>
<tr>
<td>Coal</td>
<td></td>
</tr>
<tr>
<td>anthracite</td>
<td>0.63</td>
</tr>
<tr>
<td>bituminous</td>
<td>0.63</td>
</tr>
<tr>
<td>natural dust</td>
<td>0.65</td>
</tr>
<tr>
<td>pulverized</td>
<td>0.73</td>
</tr>
<tr>
<td>Magnetite, Fischer-Tropsch catalyst</td>
<td>0.58</td>
</tr>
<tr>
<td>Mica flakes</td>
<td>0.28</td>
</tr>
<tr>
<td>Sand</td>
<td></td>
</tr>
<tr>
<td>round</td>
<td>0.86</td>
</tr>
<tr>
<td>sharp</td>
<td>0.66</td>
</tr>
<tr>
<td>Tungsten powder</td>
<td>0.89</td>
</tr>
</tbody>
</table>

The drawback of the sphericity, $\phi_s$, is that it is difficult to obtain the surface of an irregular particle and thus it is difficult to determine $\phi_s$ directly. There are only two classical techniques that can be used to estimate $\phi_s$: image analysis (IA) methods, and permeation methods. In the IA method, the sphericity is calculated using 2-D projected area and projected perimeter of a particle. The $\phi_s$ is defined as

$$
\phi_s = \frac{4\pi A_p}{P^2}
$$

The relationship in eq. 2 assumes that the measurements in two dimensions can be translated to a quantity $\phi_s$ in three dimensions. It is suspected that the IA method estimates a value of $\phi_s$ that is lower than the true value.\(^6\)

In permeation methods, $\phi_s$ is derived from pressure drop measurements across the fixed bed of particles. Usually, the Ergun equation is used to obtain the relationship between pressure drop and $\phi_s$.\(^7\)

Recently, problems with the estimation of volume and surface area of irregular particles have been greatly alleviated by the introduction of computed tomography and 3-D laser scanners.\(^8\)–\(^14\) Both techniques offer true 3-D approximations via numerical “reconstruction” of the body.

According to data available in the open literature,\(^1,\)\(^4,\)\(^15,\)\(^16\) the sphericity of pulverized coal particles and small particles of crushed coal lies in the range from 0.59 to 0.83. To the authors’ best knowledge no data are available on sphericities of large coal particles (greater than 5 mm) used in fluidized-bed boilers, fixed-bed gasifiers, coke ovens and metallurgical furnaces.

In this study, the influence of the particle sphericity on the characteristics of fixed beds and fluidized beds is discussed first. Then the results of an investigation undertaken to estimate sphericities of large coal and char particles (coal: 4.7–106 mm, char: 3.4–53 mm) are presented. The particles were divided into several narrow size fractions and scanned using a 3-D laser scanner. The sphericity for each size fraction was then calculated from the volume and surface area data obtained via numerical reconstruction of the particle.
INFLUENCE OF SPHERICITY ON THE CHARACTERISTICS OF FIXED AND FLUIDIZED BEDS

Void fraction

A great deal of experimental and modelling work has been done to relate mean void fraction (or voidage) to the properties of individual particles. These studies have shown that the voidage of a fixed bed, \( \varepsilon \), depends on particle size, particle size distribution, particle sphericity, surface roughness, the method of packing, and the size of the vessel relative to the particle diameter. Particle sphericity is an important variable in voidage determination. For fixed beds of uniformly sized particles, voidage increases with decreasing sphericity. Hartman et al. obtained the following correlation by fitting the experimental data from the literature:

\[
\varepsilon = 1.0 - 0.8648\phi_S + 0.2745\phi_S^3
\]  

This correlation is valid for fixed beds of granular materials with voidages in the range from 0.4 to 1.0. In Figure 1, experimental data of Brown et al. are compared with those predicted by eq. 3.

Frictional pressure drop in a fixed bed

The frictional pressure drop, \( \Delta p \), during one-dimensional flow of gas through a fixed bed of granular material is given by the sum of two terms: a viscous energy loss term proportional to the gas velocity, \( U \), and inertial loss (kinetic energy) term proportional to velocity squared, i.e.:

\[
\frac{\Delta p}{L} = AU + BU^2
\]  

where \( A \) and \( B \) are empirical parameters. One form of eq. 4, widely used in engineering practice, was proposed by Ergun:

\[
\frac{\Delta p}{L} = 150 \left( \frac{1 - \varepsilon}{\varepsilon^3} \right)^2 \frac{\mu U}{(\phi_S d_p)^2} + 1.75 \frac{1 - \varepsilon}{\varepsilon^3} \frac{\rho_g U^2}{\phi_S d_p}
\]  

The Ergun equation, eq. 5, is based on the capillary model that approximates the bed of particles as a bundle of tangled tubes in which the gas flows.

Figure 2 shows the influence of sphericity on the frictional pressure drop in a fixed bed (\( \varepsilon = 0.45 \)) at \( U = 0.25 \) m/s. For 5-mm particles with \( \phi_S = 0.5 \) the \( \Delta p \) calculated from eq. 5 is ~3.7 times greater than that for spherical particles and for 90-mm particles ~2.5 times greater than that for spherical particles.

Superficial gas velocity at minimum fluidizing conditions

According to Kunii and Levenspiel, the superficial gas velocity at minimum fluidizing conditions, \( U_{mf} \), is a function of particle sphericity and for isotropic-shaped solids is given by:

\[
\frac{1.75}{\varepsilon_{mf}^3} Re^{3}_{p, mf} + \frac{150(1 - \varepsilon_{mf})}{\varepsilon_{mf}^3 \phi_S} Re_{p, mf} = Ar
\]  

where: \( Re_{p, mf} = \frac{U_{mf} d_p \rho_g}{\mu} \), and \( Ar = \frac{d_p^3 \rho_g (\rho - \rho_g) g}{\mu^2} \).

Figure 3 shows the influence of particle sphericity on \( U_{mf} \) (calculated from eq. 6) for particles with \( \rho = 1600 \) kg/m\(^3\) fluidized with nitrogen at 850°C and 100 kPa. The \( U_{mf} \) decreases with decreasing \( \phi_S \). For 0.5-mm particles, the \( U_{mf} \) for non-spherical particles with \( \phi_S = 0.5 \) is equal.
~25% of that for spherical particles. In the case of 9-mm particles, \( U_{\text{mf}} \) for non-spherical particles is equal ~62% of that calculated for spherical particles.

**Terminal velocity of a falling particle**

According to Haider and Levenspiel\(^2\), the terminal velocity, \( U_t \), for a free-falling particle can be calculated from:

\[
U_t = \left[ \frac{U^*}{\rho g^2} \right]^{1/3} \left[ \frac{\mu (\rho - \rho_g)}{g} \right]^{-1}
\]

where: \( U^* = \left[ \frac{18}{(d_p^*)^2} + \frac{2.335 - 1.744 \phi_S}{(d_p^*)^{1/2}} \right] \), and \( d_p^* = Ar^{1/3} \).

Similarly like in the case of \( U_{\text{mf}} \), the terminal velocity, \( U_t \), decreases with decreasing particle sphericity. For non-spherical particles with \( \phi_S = 0.5 \), the terminal velocity is ~35% lower for 0.5-mm particles and ~59% lower for 9-mm particles compared to the \( U_t \) values for their spherical counterparts. The relative difference between terminal velocities for spherical and non-spherical particles increases with increasing particle diameter. This is an opposite trend to that observed for \( U_{\text{mf}} \).
EXPERIMENTAL PROCEDURE

A typical sample of Highveld coal was split, through sieving, into nine size classes (see Table 2). The preparation of the char was done by devolatilizing the Highveld coal under a nitrogen atmosphere (atmospheric pressure) at 600°C for one hour, cooling and then sieving into six size classes (see Table 3). The reason for the lesser amount of size classes and smaller char particles is due to thermal fragmentation of the larger coal particles during charring. Five particles were selected from each size class coal and char. Their density was estimated using the water displacement technique. External surface area and volume of each particle were determined from 3-D models obtained through laser scanning. The sphericity of each particle was then calculated according to the definition eq. (1).

The experimental procedure included the following steps:

- Each raw particle was dusted to remove debris
- The particle was coated with white spray paint to improve scan results
- After drying, the particle was placed and secured inside the Roland LPX-1200 scanner
- Scanning settings were configured via the scanner interface and the scanning process was initiated (the maximum and minimum scanning resolutions were 0.1 and 0.4 mm respectively)
- A raw point cloud was obtained
- The raw point cloud was cleaned via filters to reduce noise and to remove points that were not part of the scanned particle
- A water-tight mesh was generated from the point cloud and checked for anomalies such as non-manifold edges, self intersections, highly creased edges, spikes and holes
- The mesh was compared to the point cloud to ensure that it was a perfect fit
- The external surface area and volume of the particle were calculated using the final mesh data

Figure 5 shows the point cloud (a) and mesh (b) generated for the particle 7A (+37.5–53 mm). Figure 6 shows the 3-D model of the 7A particle and corresponding data on the calculated external surface area, volume, sphericity and scanning accuracy.

Figure 5. Point cloud (a) and water-tight mesh (b) for particle 7A (+37.5–53 mm)
RESULTS AND DISCUSSION

Particle densities and average sphericities for coal particles tested are presented in Table 2. Figure 7 shows the relationship between the sphericity and particle size for the coal particles.

Measurements of particle density show little scatter and no clear trend. Tested coal particles can be described using the average particle density of 1600 kg/m³ and standard deviation of 60 kg/m³.

Table 2. Particle density and average sphericity for tested coal particles

<table>
<thead>
<tr>
<th>Particle size, mm</th>
<th>Particle density kg/m³</th>
<th>Average sphericity</th>
<th>Standard deviation</th>
</tr>
</thead>
<tbody>
<tr>
<td>+4.7–6.7</td>
<td>–</td>
<td>0.731</td>
<td>0.026</td>
</tr>
<tr>
<td>+6.7–9.5</td>
<td>1590</td>
<td>0.775</td>
<td>0.016</td>
</tr>
<tr>
<td>+9.5–13.2</td>
<td>1700</td>
<td>0.786</td>
<td>0.019</td>
</tr>
<tr>
<td>+13.2–19.0</td>
<td>1620</td>
<td>0.777</td>
<td>0.041</td>
</tr>
<tr>
<td>+19.0–26.5</td>
<td>1530</td>
<td>0.773</td>
<td>0.011</td>
</tr>
<tr>
<td>+26.5–37.5</td>
<td>1570</td>
<td>0.825</td>
<td>0.045</td>
</tr>
<tr>
<td>+37.5–53.0</td>
<td>1560</td>
<td>0.798</td>
<td>0.031</td>
</tr>
<tr>
<td>+53.0–75.0</td>
<td>–</td>
<td>0.829</td>
<td>0.009</td>
</tr>
<tr>
<td>+75.0–106.0</td>
<td>–</td>
<td>0.841</td>
<td>0.013</td>
</tr>
</tbody>
</table>
Figure 7. Sphericity of coal particles as a function of particle diameter

Sphericities of tested coal particles fall into the relatively narrow range from 0.731 (for the smallest particles) to 0.841 (for the largest particles). The sphericity, $\phi_s$, increases with increasing particle diameter but the relationship between these two parameters is rather weak. The trend line in Figure 7 shows that $\phi_s$ is proportional to $d_p^{0.03}$. Because values of $\phi_s$ are scattered, the correlation coefficient for this trend line is only 0.80.

In principle, the tested coal particles can be divided into three groups according to their sphericity: small particles (below 6.7 mm) with $\phi_s = 0.730$; middle size particles (6.7–26.5 mm) with average $\phi_s = 0.778$ (standard deviation 0.006), and large particles (26.5–106 mm) with average $\phi_s = 0.823$ (standard deviation 0.018). However, because the relative variation in sphericity does not exceed 15%, it can be possible to describe Highveld coal particles using an average value of sphericity calculated for all size classes. This average value is 0.793 (standard deviation 0.034) and it is very close to the sphericity of particles in the +37.5–53.0 mm size class ($\phi_s = 0.798$).

Particle density and average sphericity for the char particles evaluated are shown in Table 3. Figure 8 shows the variation of sphericity with particle size for the char particles.

Table 3. Particle density and average sphericity for tested char particles

<table>
<thead>
<tr>
<th>Particle size, mm</th>
<th>Particle density $\text{kg/m}^3$</th>
<th>Average sphericity</th>
<th>Standard deviation</th>
</tr>
</thead>
<tbody>
<tr>
<td>+2.4–3.4</td>
<td>1211</td>
<td>0.767</td>
<td>0.058</td>
</tr>
<tr>
<td>+3.4–4.7</td>
<td>1269</td>
<td>0.790</td>
<td>0.014</td>
</tr>
<tr>
<td>+6.7–9.5</td>
<td>1230</td>
<td>0.746</td>
<td>0.047</td>
</tr>
<tr>
<td>+13.2–19.0</td>
<td>1181</td>
<td>0.760</td>
<td>0.035</td>
</tr>
<tr>
<td>+26.5–37.5</td>
<td>1235</td>
<td>0.707</td>
<td>0.046</td>
</tr>
<tr>
<td>+37.5–53.0</td>
<td>1295</td>
<td>0.728</td>
<td>0.051</td>
</tr>
</tbody>
</table>
The char particles evaluated display a slight linear trend of decreasing sphericity with increasing particle size (slope = 0.0014). As result of the scatter in the data, the correlation coefficient is 0.62. It is proposed that the decreasing trend is bought about by the thermal fragmentation of larger particles during the devolatilization process. To simplify complex simulations, it can be possible to assume that the sphericity of char derived from Highveld coal heated to 600°C is 0.749. This is lower than the average sphericity of coal particles (Figure 7).

In addition to the differences in sphericity, it can clearly be observed that the char particles have a lower density compared to the coal particles (1237 kg/m$^3$ vs 1595 kg/m$^3$). This is in agreement with published results.$^{23,24}$

**CONCLUSIONS**

Sphericity is an important parameter that describes the shape of irregular particles. In fixed-bed reactors, shape of particles can significantly influence the bed permeability, gas flow distribution and pressure drop across the bed. In fluidized-bed reactors, some important design parameters such as $U_{mf}$ and $U_t$ depend strongly on size and sphericity of solids. The drawback of sphericity is that it is difficult to determine $\phi_s$ directly. However, recently introduced techniques such as computed tomography and 3-D laser scanning allow $\phi_s$ to be estimated with an accuracy that sufficient for most practical applications.

Sphericities of Highveld coal particles in the range from 4.7 to 106 mm and char particles in the range 3.4 to 53 mm were estimated using the 3-D laser scanning technique. It was found that sphericities of the coal particles are higher than those reported in the open literature for pulverized coal and small crushed coal particles. Because the relative variation of sphericity with particle size is small (~15%), it is possible to use an average value, calculated for the entire size range, to describe the sphericity of the coal particles. This value is 0.793 and it is very close to the sphericity of particles in the +37.5–53.0 mm size class. Similarly, the sphericity of char particles was found to decrease slightly with increasing particles size and range from 0.707 to 0.790. The small variation in sphericity with particle diameter allows one to approximate the char particle sphericity by the average value of the range, being 0.749.
**NOTATION**

- $A_p$: projected surface area, m$^2$
- $Ar$: Archimedes number
- $d_p$: particle diameter based on screen analysis, m
- $d'_p$: dimensionless measure of particle diameter
- $L$: height of fixed bed, m
- $p$: pressure, Pa
- $P$: projected perimeter, m
- $Re'_p$: modified Reynolds number
- $Re_{pf}$: particle Reynolds number at minimum fluidizing conditions
- $U$: superficial gas velocity, m/s
- $U_{mf}$: superficial gas velocity at minimum fluidizing conditions, m/s
- $Ut$: terminal velocity of a falling particle, m/s
- $U^*_t$: dimensionless measure of terminal velocity of a falling particle

**Greek letters**

- $\Delta p$: pressure drop across the bed, Pa
- $\varepsilon$: void fraction (voidage) in a fixed bed
- $\varepsilon_{mf}$: void fraction at minimum fluidizing conditions
- $\mu$: viscosity of gas, kg/m s
- $\rho$: density of solids, kg/m$^3$
- $\rho_g$: gas density, kg/m$^3$
- $\phi_s$: sphericity of a particle

**REFERENCES**


