

Fluid and Particle Mechanics
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Lecture – 38

Tutorial - 05

So, hello everyone, now we will look at the problem of calculating sphericity of the particles. So, in the question in the question it is given that the figure shows the scanning electron microscopy images of hematite ellipsoids synthesized by method called forced hydrolysis. And the average dimensions and average aspect ratio of the particles are given. And we are supposed to calculate the calculate and plot the sphericity of the particles as a function of aspect ratio.

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Handwritten notes on a Windows Journal window showing the formula for sphericity and calculations for an ellipsoid.

$$\text{Sphericity} = \left(\frac{\text{Surface Area of a sphere}}{\text{volume of sphere}} \right) \div \left(\frac{\text{Surface area of particle}}{\text{volume of particle}} \right)$$

where volume of sphere = volume of particle

i) length = 57 nm ; Diameter = 42 nm. $\Rightarrow \alpha = L/d = 1.3$

Volume of ellipsoid = $\frac{4\pi}{3} (abc)$

Surface Area of ellipsoid = $4\pi \left(\frac{(ab)^{1.6} + (bc)^{1.6} + (ca)^{1.6}}{3} \right)^{1/1.6}$

So, first we will see what is sphericity? So, sphericity is defined as surface area of a sphere to volume of sphere, divided by surface area of particle by volume of particle; where volume of sphere equal to volume of particle. So, its actually surface area of sphere by surface area of the particle in which the volume of the sphere and volume of the particle are same.

So, here we were given the hematite ellipsoids. And its given that let us look at the first case where length equal to 57 nanometers and diameter equal to 42 nanometers. So, that

alpha is L by d which is 1.3 ok. So, volume of ellipsoid is to calculate sphericity we need surface area of sphere.

As well as surface area of the sphere, which has the same volume as volume of the particle and surface area of the particle. So, first we will look at the expressions which will give us the surface area of the ellipsoids. So, even before that we will look at volume of ellipsoid. So, the volume of ellipsoid is given by $\frac{4}{3} \pi abc$ where a b and c are the dimensions that we get from the ok.

Let us say that this is an ellipsoid and this is the major axis. So, half of it is a; half of it is taken as a and half of it will be taken as b and in this direction we have c. So, these are the a b and c and if you see when a b and c are same we will end up with $\frac{4}{3} \pi a^3$ or $\frac{4}{3} \pi b^3$ or $\frac{4}{3} \pi c^3$ which means $\frac{4}{3} \pi r^3$ which is a volume of a sphere.

Similarly surface area of ellipsoid equal to $4 \pi a^{1.6} b^{1.6} c^{1.6}$ divided by 3 whole to the power of 1 divided by 1.6. And again if here if we see when a equal to b equal to c, we will end up with the equation very similar to the surface area of a sphere ok. So, now we have the expressions for volume of the ellipsoid surface area of the ellipsoid and we know the dimensions.

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The image shows a handwritten derivation for the sphericity of an ellipsoid, written in a Notepad window. The derivation starts with the volume of an ellipsoid, $\frac{4}{3} \pi abc$, and equates it to the volume of a sphere, $\frac{4}{3} \pi r^3$, to find the equivalent radius $r = (abc)^{1/3}$. Then, the surface area of the sphere, $4 \pi r^2$, is expressed as $4 \pi (abc)^{2/3}$. The sphericity ϕ_s is defined as the ratio of the surface area of the sphere to the surface area of the ellipsoid. The surface area of the ellipsoid is given as $4 \pi \left(\frac{a^{1.6} b^{1.6} c^{1.6}}{3} \right)^{1/1.6}$. The final formula for sphericity is derived as:

$$\phi_s = \frac{4 \pi (abc)^{2/3}}{4 \pi \left(\frac{a^{1.6} b^{1.6} c^{1.6}}{3} \right)^{1/1.6}} = \frac{(3)^{1/1.6} (abc)^{2/3}}{(a^{1.6} + b^{1.6} + c^{1.6})^{1/1.6}}$$

And now first we will calculate those. So, even before that let us look at this case, so we have we know that the volume of the ellipsoid is $\frac{4}{3} \pi abc$. And to calculate the sphericity, the volume of the particle should be equal to the volume of the sphere should be equal to the volume of the particle.

So, $\frac{4}{3} \pi abc$ will give us the volume of the particle. It will be equal to a sphere, which has a volume of $\frac{4}{3} \pi r^3$ from this we will get that r equal to abc to the power of $\frac{1}{3}$. So, now we will calculate the surface area of a sphere with a radius of r that is abc to the power of $\frac{1}{3}$. So, surface area of the sphere we will be $4 \pi r^2$ which is $4 \pi abc^{\frac{2}{3}}$ we know it as abc to the power of $\frac{1}{3}$.

So, r^2 will be to the $4 \pi abc$ to the power of $\frac{2}{3}$. So, this is the surface area of this sphere. So, now, if we write the expression for sphericity, sphericity is usually expressed with an ϕ_s . So, it will be surface area of this sphere $4 \pi abc^{\frac{2}{3}}$ divided by volume of the sphere which is $\frac{4}{3} \pi r^3$ actually its $\frac{4}{3} \pi abc$.

But we know that its a same as the ellipsoid and we will use the volume of the ellipsoid which is $\frac{4}{3} \pi abc$. So, this is the now the numerator this whole term will be surface to the volume ratio of ellipsoids sphere. And now if you write for the particle we know that its $\frac{4 \pi a^2 b^2 c^2}{3}$ plus bc to the power of $\frac{1}{3}$ plus ca to the power of $\frac{1}{3}$ divided by 3 whole to the power of $\frac{1}{3}$.

This is the surface area and we need the volume is $\frac{4}{3} \pi abc$. So, this and this will cancel out 4π will go and we will end up with 3 to the power of $\frac{1}{3}$ times abc to the power of $\frac{2}{3}$ divided by $a^{\frac{1}{3}} b^{\frac{1}{3}} c^{\frac{1}{3}}$ plus $bc^{\frac{1}{3}}$ plus $ca^{\frac{1}{3}}$ whole to the power of $\frac{1}{3}$. So, this is the expression we have for calculating the sphericity of an ellipsoid.

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$$i) L = 57 \text{ nm}; D = 42 \text{ nm}$$

$$\phi_s = \frac{(3^{1/6}) \left(28.5 \times 10^{-9} \times 21 \times 10^{-9} \times 21 \times 10^{-9} \right)^{2/3}}{\left((28.5 \times 21 \times 10^{-18})^{1/6} + (21 \times 21 \times 10^{-18})^{1/6} + (28.5 \times 21 \times 10^{-18})^{1/6} \right)^{1/6}}$$

$$= 0.9845$$

$$ii) \phi_s = 0.9397$$

$$iii) \phi_s = 0.9179$$

$$iv) \phi_s = 0.8714$$

$$v) \phi_s = 0.7672$$

And now we will just substitute those values. So, for the first case we have we were given that the length is 57. And diameter is given as 42 sorry its a nanometers. And we have seen that in the ellipsoid a will be L by 2 and we considered that its symmetric in both the direction. So, b and c are same. So, b will b equal to c equal to D by 2. With that we will calculate the sphericity.

So, phi s sphericity will be 3 to the power of 1 by 1.6 times 28.5 which is half of 57 nanometers to 10 to the power of minus 9 times 42 by 2 is 21. So, 21 into 10 to the power of minus 9 into 21 into 10 to the power of minus 9 whole to the power of 2 by 3 divided by 28.5 into 21 into 10 to the power of minus 18 to the power of 1.6. Plus 21 times 21 times 10 to the power of minus 18 whole to the power of 1.6, plus 28.5 times 21 times 10 to the power of minus 18 whole to the power of 1.6 and whole to the power of 1 by 1.6.

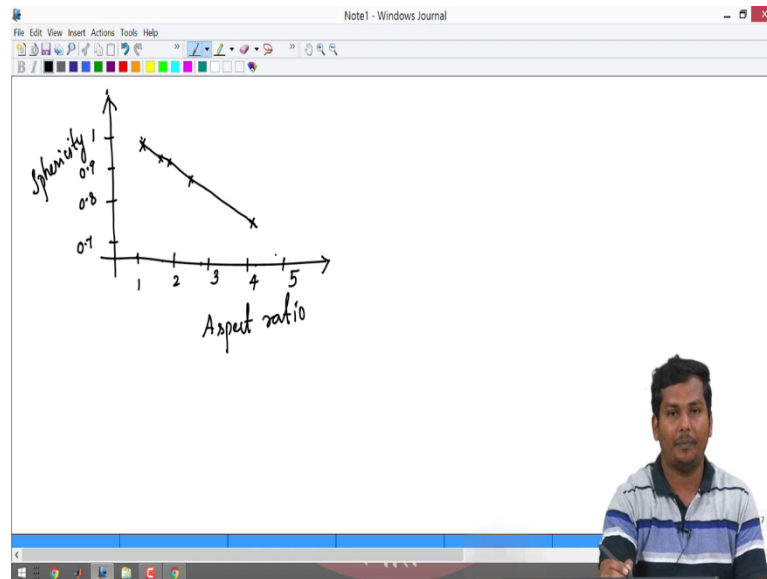
So, this is the phi s and if you if we do these calculations we will get 0.9845. So, when sphericity is a comes out to be equal to 1; that means, we have an exact spherical particle. And here we are getting a value of 0.9845 which is very nearer to 1. And if we see the images in if you see the images of a first one where alpha equal to 1.3 they look very similar to spherical particles.

They deviate from they deviate a bit form sphericity. So, that is why we see this deviation from 1 and we did not get the exact value of 1. So, phi s is 0.9845 for the first case and similarly if we calculate for the second case phi s will be; phi s will be 0.9397. And for the

third case ϕ_s will be 0.9179 for the fourth case ϕ_s comes out to be 0.8714. Whereas, for the fifth case we come to it comes out to be 0.7672.

So, these are the different sphericity values for a different aspect ratio of the particles. And we see that when aspect ratio is being increased we see and decrease in the sphericity.

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So, that is a last part of the problem. We are supposed to plot sphericity versus aspect ratio. So, its 0, so its 1, 2, 3, 4, 5 and the y axis we will the values that we have thought ordering is in the range of 0.7622, 0.9845 then we will take from 0.7. Let us say this is 0.7 and this is 0.8, 0.9 and 1.

So, in x axis we have a aspect ratio and y axis we have sphericity. And for the first one the aspect ratio was 1.3 and comes out to be here 1.3 for that the sphericity is around 1 which is 0.9845 some something wrong there and the next one we have the aspect ratio 1.7. So, there 1.7 and the value is 0.9397 we can take it as 0.94.

So, just around there and then for the aspect ratio of 2.1 we have got the sphericity to be 0.9179, which is 0.92 which is around there. And then point a 2.7 for the aspect ratio of 2.7 we have got the value to be 0.8714 something like that.

And the final one the aspect ratio is 4.2. And we got the sphericity to be 0.7672 which is around; which is around that. So, the line looks something like that. So, this is the plot of

it need not to be a straight line, but if you plot this sphericity versus aspect ratio for different part different shapes of particles this is how we have time.

Thank you.