Dependencies between grain shapes, grain composition and size of specific surface

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ABSTRACT: The grained materials are very common in many production branches. However, it is very hard to precise their chemical and physical features as shape, specific surface, porosity etc. The paper presents the comparison of the grain surfaces of three materials (diabase, sandstone and magnesite) given in base of various shape coefficients, as well specific surfaces determined by Blaine's and BET methods. These analyses were made for grain compositions obtained by laser particle sizer Analysette 22 and Infrared Particle Sizer IPS. It seems to be possible to search the functional formulae of changing the grain surfaces dependably on shape coefficients for both devices. The proposal of such functions has been made in the paper.

1 INTRODUCTION

In every branches of production transforming mineral raw materials, the grained materials are being used. They are groups of grains, featured by various shapes, sizes and mineral and chemical composition. The whole characteristics of fine grained material includes the indication and quantitative identification of mineral and chemical composition, as well its granulation. Apart from knowledge of powdery material grain composition, it is necessary also to know its specific surface because this value determines many features of certain material.

The results of grain composition or specific surface measurement of the same material, obtained by application of various methods are not identical. These differences occurred not only because of typical errors for these methods, but also because of differences in interpretation of basic conceptions, as grain size, its shape or surface, which are accepted as the model ones in certain method. Considering the variety of measurement methods, it seems to be right to search unequivocal, miscellaneously conditioned and justifiable quantitative dependencies between grain size, its shape and specific surface. The searching for these dependencies is the purpose of this article. To their determination the distinctive considerations were carried out, as well the number of experiments and calculations. The researches were conducted for comminuted materials (diabase, sandstone) and their narrow classes. The precise granulometric analyses were done by laser particle sizer Analysette 22 (laser diffract meter), particle sizer IPS (Infrared Particle Sizer) and Coulter sizer (method of sensitive zone C-C). In purpose to estimate and determine the shape coefficient, the researches on scanning microscope were carried out. The specific surface was determined by Blaine's flow and BET methods. The results of analyses could be the base to search the functional formulae to unify the description of dependencies between the results of various types of analyses. The proposal of such functions are presented in the paper. The preciseness and recurrence of applying these equations should be verified by statistical methods. It seems to be possible also to apply the theory of complex distribution functions and fuzzy functions.

2 EXPERIMENTAL WORKS DESCRIPTION

In purpose to prove the correlations mentioned in introduction, three materials were selected: diabase, sandstone and magnesite. These materials have pores from range of micropores, through mezopores till macropores.

The selected materials were comminuted in jaw crusher, then milled in laboratory ball grinder till the grain composition below 0,315 mm. Then, so prepared material was classified into narrow grain classes by using sieves. The classes 40 – 63, 63 – 71, 71 – 80, 80 – 100 and 100 – 160 μm were selected to the researches. For all of these classes the precise granulometric analyses were conducted by granulometric laser particle sizer Analysette 22 (laser diffract meter) and particle sizer IPS (Infrared Particle Sizer). In purpose to evaluate and determine the shape coefficients, the researches were conducted on scanning microscope. The pictures of various grey level and 50-, 100- and 200-times magnifications were obtained, which were saved in JPEG format. They were the source of information for picture analysis computer programs. The determination of basic factors were done by using the Aphelion program. This is an universal and elastic tool for image working and analysis, which can be used in many scientific branches. Apart from the standard arithmetic, logic and morphologic operation set, Aphelion has also the possibilities of applying the Fourier transform, color pictures analysis and 3-D pictures analysis.

The image analysis is the process, which bases on selection from the whole data this part, which is significant from the process point of view. The results are both the qualitative and quantitative ones, describing certain picture or group of pictures features (Serra, 1982; Tadeusiewicz & Korohoda, 1997).

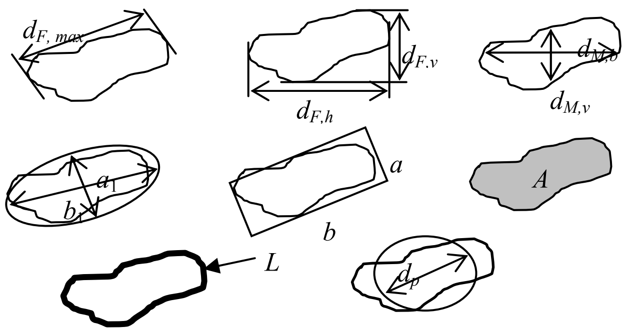

Figure 1. Various shape coefficients interpretation

where: $d_{F,max}$ – maximum Feret diameter; $d_{F,h}$ – horizontal Feret diameter; $d_{F,v}$ – vertical Feret diameter; $d_{M,h}$ – horizontal Martin diameter; $d_{M,v}$ – vertical Martin diameter; a_1 – length of longer ellipse axis featured on object; b_1 – length of shorter ellipse axis featured on object; a – height of rectangle featured on object; b – width of rectangle featured on object; A – surface field of object, μm^2; L – perimeter length, number of pixels in object, which neighbour pixel not belongs to object (Xu & di Guida, 2003).

Table 1 contains the most often applied shape coefficients. There are many formulas of grain shape coefficients in literature (Allen, 1997; Feda, 1982; Russ, 1986; Wadell, 1933; Wojnar et al, 2002). Mainly, they are based on similarities of grains or their projections to certain geometric shape in many dimensions.

Figure 1 presents the basic geometric parameters, which were obtained by the image analysis.

In base of these geometric values, the projective diameter d_p was calculated, as well the mean values of shape coefficients. Also for these grain classes, the specific surface was measured by flow Blaine's method and by BET method and then the shape coefficients for both methods were calculated from the formulae:

$$\Phi = \frac{6}{S\rho d_p} \tag{1}$$

where: S – specific surface measured by certain method in narrow class of researched material [m^2/kg], ρ - specific density [kg/m^3], d_p – grain projective diameter [m].

3 RESULTS AND DISCUSSION

The obtained results of narrow classes grain composition of diabase, sandstone and magnesite were researched over the conformity with classical parameter distribution functions as Weibull, Gaudin-Schuhmann-Andreyev (GSA) and log-norm. As the criterion of fitting the rest deviation was accepted, which is determined by the following equation:

$$s_r = \sqrt{\frac{\left(F(d) - \hat{F}(d)\right)^2}{n-2}} \tag{2}$$

where: n – grain classes number; $F(d)$ – values of empirical distribution function; $\hat{F}(d)$ - values of theoretical distribution function.

Table 2 shows the results of these approximations. The results for diabase also featured by high values of error. They were published in work (Gniadek et al, 2005). As we can see, none of the considered distribution functions approximate sufficiently well the empirical analyses results changeability. It may be said then that it is not recommended to approximate the fine grained classes grain composition functions of such materials as diabase, sandstone and magnesite by these functions. Relatively, the best effects are given by Weibull distribution function, but also in this case the values of residual deviations are too high.

For every of these materials, the basic parameters describing grain were determined. The mean values of every typical shape coefficients were given. For diabase and sandstone, the measurements for 5 classes were done and for magnesite for 4. They are presented in tables 3, 4 and 5.

Table 1. Typical shape coefficients.

Shape coefficient	Description	Formulae
projective diameter d_p	diameter of circle of the same surface as grain	$d_p = \sqrt{\frac{4A}{\pi}}$
coefficient of sphericity K_{C1}	sphericity of object, maximally is equal to 1 for circular objects	$K_{C1} = \frac{4\pi A}{Cr^2}$
Wadell's coefficient of sphericity K_W	ratio of grain perimeter to circle perimeter of surface equal to grain surface	$K_W = \frac{L}{L'}$
filling coefficient K_1	number of pixels of area divided by product of grain height and width. This parameter is equal to 1 for ideal rectangle and achieves values near 0 for the very simple structures	$K_1 = \frac{n}{x \cdot y}$
convexity parameter K_2	parameter is equal to 1 for convex areas and higher for areas containing concave ones	$K_2 = \frac{L}{2y + 2x}$
elongation (in ratio to ellipse) K_E	an ellipse is featured on grain, which has axes a_1 (longer one) and b_1 (shorter). With growth of value of this parameter, the elongation of grain becomes higher. This coefficient achieves values below 1	$K_E = \frac{a_1 - b_1}{a_1 + b_1}$
elongation (in ratio to circle) α	ratio of width to height of rectangle featured on grain ($b > a$). The coefficient achieves the minimal value equal to 1 for circle or rectangle and is higher for elongated shapes	$\alpha = \frac{b}{a}$
grain surface corrugation coefficient β	coefficient is very sensitive to irregularity of grain shape and at the same time very little sensitive to elongation. Its minimal value is equal to 1 for circle and achieves higher values for every other shapes	$\beta = \frac{L^2}{4\pi A}$
conciseness coefficient K_Z	this parameter is equal to 1 for square and smaller for shapes of not so regular boundaries	$K_Z = \frac{16n}{L^2}$
symmetrical measure of grain elongation K_s	logarithm from quotient of grain height and width	$K_S = \log_{10}\left(\frac{y}{x}\right)$

Where: x– area width, difference between highest and lowest co-ordinate X of the area or horizontal Feret diameter - $d_{F,h}$; y – area height, difference between highest and lowest co-ordinate Y of the area or vertical Feret diameter; n – number of pixels; L – perimeter of object; A – surface field of object; Cr – Crotton perimeter; L' – circle perimeter of surface equal to grain surface; a_1 – length of longer ellipse axis featured on object; b_1 – length of shorter ellipse axis featured on object.

Crotton perimeter – mean intersection length in direction 0, 45, 90 i 135°. Lengths of intersections in directions 45 i 135° are being revised (normalized) by coefficient $\sqrt{2}/2$;

Table 2. Approximation of grain composition curves by various parametric distribution functions.

Laser particle sizer – sandstone								
Distribution type	0-32	32-40	40-63	63-71	71-80	80-100	100-160	+160
GSA	17,86	13,92	13,93	10,13	7,79	8,96	9,06	12,57
Log-norm	8,09	12,49	13,54	14,29	16,98	18,42	16,33	15,25
Weibull	2,55	6,55	8,11	7,70	8,33	9,34	11,78	15,04
Laser particle sizer – magnesite								
GSA	17,11	18,32	19,94	10,82	15,47	18,55	11,63	12,66
Log-norm	3,48	14,32	15,38	21,94	14,06	14,17	14,45	17,05
Weibull	5,17	7,51	8,15	8,31	9,23	11,42	10,27	7,95
IPS – sandstone								
GSA	22,52	15,72	23,47	21,65	18,79	21,85	18,65	19,95
Log-norm	6,79	4,26	5,67	8,60	10,05	12,30	10,49	8,16
Weibull	8,41	13,96	15,73	19,63	19,05	10,60	15,17	11,38
IPS – magnesite								
GSA	3,92	16,69	28,11	17,63	17,74	16,13	20,13	17,69
Log-norm	9,19	7,13	11,42	10,58	12,42	14,35	9,67	10,61
Weibull	4,02	15	13,05	11,79	11,11	7,76	10,59	4,43

Because these coefficients were calculated as arithmetic mean values of individual measurements, it is advisable to calculate the variation factors v for these values to see which ones are relatively the most stable. As the variation factor we understand the value determined by formulae (3).

$$v = \frac{s}{\bar{x}} \cdot 100\% \qquad (3)$$

where: s – standard deviation of measurements; $\bar{x}$ - mean value of measurements.

Table 3. Shape coefficients for diabase (specific gravity =2,69 kg/m^3).

Diabase					
Class [μm]	**40-63**	**63-71**	**71-80**	**80-100**	**100-160**
d_p **[μm]**	62,76	71,05	87,46	96,20	113,71
K_{C1}	0,75	0,75	0,80	0,77	0,79
K_W	1,50	1,48	1,43	1,48	1,45
K_1	0,63	0,64	0,68	0,66	0,67
K_2	1,04	1,04	1,03	1,04	1,03
K_F	1,13	1,08	1,16	1,13	1,12
K_E	0,38	0,37	0,36	0,35	0,39
α	1,48	1,37	1,40	1,37	1,41
β	2,25	2,20	2,04	2,18	2,10
K_S	-0,04	-0,02	-0,05	-0,04	-0,02
K_Z	0,57	0,58	0,63	0,59	0,61
Blaine's spec. surface [cm^2/g]	794,3	718,0	646,0	573,3	472,0
Φ Blaine	0,447	0,437	0,395	0,404	0,416
BET surface [m^2/g]	3,209	3,293	2,819	1,872	2,483
Φ BET	0,011	0,01	0,009	0,012	0,008

Table 4. Shape coefficients for sandstone (specific gravity=2,7269 kg/m^3.

Sandstone					
Class [μm]	**40-63**	**63-71**	**71-80**	**80-100**	**100-160**
d_p **[μm]**	60,91	77,44	91,07	102,19	168,21
K_{C1}	0,81	0,77	0,81	0,79	0,81
K_W	1,42	1,46	1,43	1,47	1,43
K_1	0,68	0,66	0,67	0,65	0,67
K_2	1,03	1,04	1,02	1,03	1,03
K_F	1,16	0,95	1,18	1,19	1,01
K_E	0,37	0,31	0,32	0,36	0,32
α	1,42	1,32	1,34	1,41	1,31
β	2,03	2,13	2,05	2,18	2,03
K_S	-0,05	0,04	-0,05	-0,05	0,003
K_Z	0,64	0,61	0,63	0,61	0,63
Blaine's spec. surface [cm^2/g]	947,0	831,7	745,0	654,3	614,7
Φ Blaine	0,381	0,341	0,324	0,329	0,213
BET surface [m^2/g]	2,415	1,759	2,093	1,708	1,77
Φ BET	0,015	0,016	0,012	0,013	0,007

Table 5. Shape coefficients for magnesite (specific gravity = 3,01 kg/m^3).

Magnesite				
Class [μm]	**32-40**	**40-63**	**63-71**	**71-80**
d_p **[μm]**	46,86	62,22	74,80	92,56
K_{C1}	0,76	0,80	0,79	0,82
K_W	1,47	1,43	1,44	1,41
K_1	0,66	0,67	0,66	0,67
K_2	1,03	1,01	1,01	1,01
K_F	1,12	1,07	1,11	1,04
K_E	0,39	0,41	0,41	0,39
α	1,47	1,50	1,52	1,48
β	2,16	2,05	2,08	1,99
K_S	-0,03	-0,01	-0,02	0,01
K_Z	0,60	0,63	0,62	0,65
Blaine's spec. surface [cm^2/g]	1746	1730	1094	1021
Φ Blaine	0,244	0,185	0,244	0,211
BET surface [m^2/g]	8,59	7,758	6,683	6,38
Φ BET	0,005	0,004	0,004	0,003

Tables 6, 7 and 8 present the calculated variation factors for all three researched materials. For further researches, the first four coefficients were selected in base of calculated variation factors.

Table 6. Variation factors for diabase.

Diabase – variation factors					
Class [μm]	**40-63**	**63-71**	**71-80**	**80-100**	**100-160**
d_p **[μm]**	20,62	24,90	24,42	52,86	67,08
K_{C1}	10,13	9,66	9,86	9,81	12,69
K_W	5,62	4,40	5,67	5,66	5,99
K_1	8,50	7,74	9,15	10,23	8,77
K_2	3,50	2,59	2,37	4,25	3,20
K_F	27,87	24,09	31,74	28,51	37,89
K_E	50,83	42,68	48,02	52,27	44,57
α	24,16	19,64	24,19	22,76	23,88
β	11,56	8,85	11,80	11,23	12,10
K_S	-347,62	-597,86	-297,18	-351,12	-754,70
K_Z	10,41	8,70	10,29	11,99	11,57

Table 7. Variation factors for sandstone.

Sandstone – variation factors					
Class [μm]	**40-63**	**63-71**	**71-80**	**80-100**	**100-160**
d_p **[μm]**	19,07	10,03	17,01	45,37	12,07
K_{C1}	10,29	10,44	10,93	17,95	5,40
K_W	5,98	6,12	5,85	11,52	3,18
K_1	9,75	8,01	9,87	14,27	6,85
K_2	2,66	2,33	2,82	2,59	1,52
K_F	28,97	22,22	31,83	45,39	19,02
K_E	48,43	47,79	52,44	59,02	48,16
α	23,85	25,23	24,47	38,22	21,78
β	12,18	12,70	11,85	25,48	6,39
K_S	-266,33	309,12	-227,20	-270,41	3342,83
K_Z	11,51	11,18	11,34	18,86	6,23

Table 8. Variation factors for magnesite.

Magnesite – variation factors				
Class [μm]	**32-40**	**40-63**	**63-71**	**71-80**
d_p **[μm]**	19,78	20,42	19,80	20,35
K_{C1}	11,81	11,87	11,51	9,23
K_W	6,67	7,44	6,81	5,58
K_1	11,43	12,12	11,08	11,07
K_2	2,69	1,79	1,93	0,99
K_F	33,44	33,55	32,02	35,54
K_E	48,01	43,70	46,92	50,70
α	25,13	27,06	28,84	25,22
β	13,60	15,65	14,19	11,56
K_S	-515,15	-1735,66	-607,07	1589,17
K_Z	12,72	13,35	12,35	10,25

In purpose of finding correlations between grain size, its shape and surface, the following reasoning was carried out. In every grain class, the theoretical grain surface of d_p diameter was calculated, assumed as the representative grain for the class. The grain surface was calculated from the following equation:

$$S_p = \pi \frac{d_p^2}{\Phi} \tag{4}$$

Also, the coefficient Φ= 1 was assumed for grain of theoretical spherical surface. Considerations for every material were conducted by assuming the grain from certain class as the spherical one and then as the grain with the following calculated shape coefficients. As the basic parameter, the grain surface and its shape connected with size were assumed. The calculated surface values were grouped in Table 10.

The Figures 1, 2 and 3 show the changeability of grain surface dependably on specific surface measuring method and selected shape coefficients. Because of the completely other scale of results, the changeability of grain size calculated in base of specific surface determined by BET method must be compared separately. This comparison is possible only for three grain classes, for which the data were available for every material.

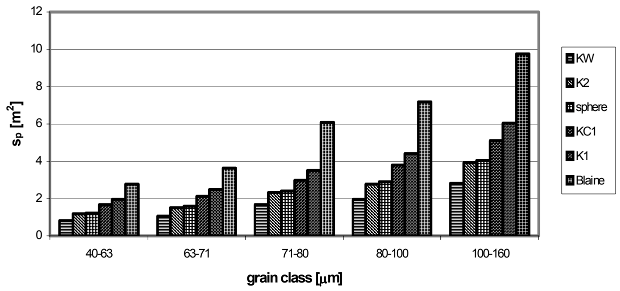

Figure 2. Various grain surfaces for diabase.

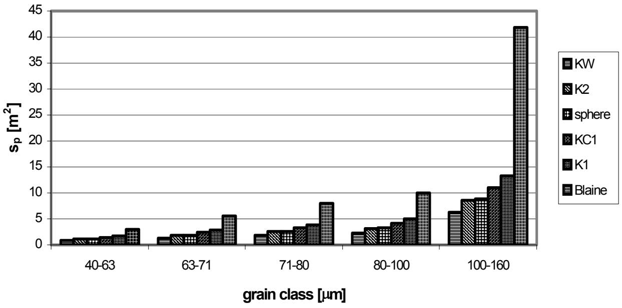

Figure 3. Various grain surfaces for sandstone.

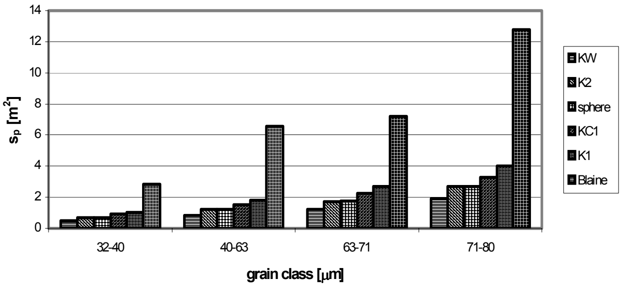

Figure 4. Various grain surfaces for magnesite.

Looking at the values of S_p determined in base of BET specific surface (Table 10) it is also clearly visible that the lower values of S_p are given for sandstone, medium ones for diabase and the highest for magnesite.

The significant growth of this surface is obvious, beginning from sandstone, which is the less porous, through diabase till magnesite, which is the porous material. In the last case, the significant porosity causes very high growth of measured surface (and similarly deceleration of calculated shape coefficients values). In case of application of shape coefficient calculated from adsorptive specific surface measuring method, the results differ significantly from the others. Inconsiderable change of grains surface with individual coefficients being applied proves their regular shape and also their porosity (Dubinin, 1975). It seems that the attempt of mathematical description of these dependencies is possible in way assuring the physical interpretation of given function. In base of figures 2, 3 and 4 it is suggested to check the fitting level of grain surface changeability to the function formulas as (Peszko & Szymanska-Czaja, 2003): second degree polynomial $y = ax^2 + bx + c$; exponential function $y = ae^{bx}$ or exponential function $y = (x+a)^{bx+c}$. Finally, it is proposed to apply the exponential function of the following equation:

$$S_p = a(x+1)^{b(x+c)} \tag{5}$$

where: a – grain surface by x=1 (for spherical grain) x=Φ - selected shape coefficient; b – factor connected with surface texture.

Table 10. Values of surfaces for various materials calculated in base of various Φ coefficients values.

Material	Class [μm]	S_p sphere	S_p K_{C1}	S_p K_W	S_p K_1	S_p K_2	S_p Blaine	S_p BET
		$\times 10^{-8}$, [m^2]						
Diabase	40-63	1,24	1,66	0,83	1,96	1,19	2,76	111,7
	63-71	1,59	2,11	1,07	2,49	1,53	3,63	166,37
	71-80	2,40	2,99	1,68	3,52	2,34	6,09	266,67
	80-100	2,91	3,79	1,97	4,42	2,78	7,19	235,62
	100-160	4,06	5,11	2,81	6,03	3,93	9,78	514,24
Sandstone	40-63	1,17	1,44	0,82	1,70	1,14	3,06	78,02
	63-71	1,88	2,44	1,29	2,84	1,82	5,52	117,48
	71-80	2,60	3,23	1,82	3,87	2,54	8,04	225,96
	80-100	3,28	4,13	2,23	5,01	3,19	9,98	260,56
	100-160	8,88	11,01	6,24	1,33	8,64	41,81	1204,12
Magnesite	32-40	0,69	0,91	0,47	1,05	0,67	2,83	139,3
	40-63	1,22	1,53	0,85	1,83	1,2	6,57	295,52
	63-71	1,76	2,23	1,22	2,67	1,73	7,22	440,8
	71-80	2,69	3,29	1,91	3,99	2,68	12,76	797,36

4 CONCLUSIONS

Summarizing, it is necessary to remember that rightness of observations and conclusions is correct only for the specified group of materials of similar surface nature. The necessary condition is to know the texture of researched material. The dependencies for solid crystal materials (isomorphic crystals) will be different from these for porous ones and for plate ones. Furthermore, it is possible to assume (Lasoń, 1988) that the specific surface has its physical sense in case of no-porous materials and macro- and mesoporous ones. For microporous materials of very expanded inner surface, the term of specific surface as the feature characterizing the comminution level of material has no longer physical sense. The inner surface being created by micropores is so large that the growth of surface e.g. in effect of comminution is only its insignificant part. Generally, the character of grain surface changeability results for researched materials indicates that it is possible to search for functional dependencies for them, which were proposed in the paper. Works and calculations are being continued and will be presented in future.

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