The Determination of Topological Properties in Polydispersed Mixtures on the Results of Sieve Laser and Particle Size Analysis

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Abstract: In this article the theory and method of obtaining of additional information about the topological properties of polydispersed mixtures and the consisting factions according to data of the curves of the sieve and laser analysis of their particle-size distribution is presented. The proposed method and the based topological properties can be used to optimize the composition of polydispersed of grinding products of mineral raw materials in order to reduce the consumption of mineral binder or polymer binder when production of highly filled composites and non hydration hardened geopolymer binders.

Key words: Polydispersed mixture · Particle-size distribution · Particle packing density

INTRODUCTION

Industrial dust or powders are widely used as fillers in polymers [1] when production of parts and products based on polymers and cementitious composites as catalysts and active admixture in the production of mineral binders [2-6]. Differential and Integral particle size distribution curves does not provide enough information about the topological properties for narrow fractions and polydispersed mixtures. Therefore particle packing density ($\eta = \gamma/\rho$ where γ is particle bulk density of granulated and dispersed material compacted by wetting or bumping-down process) and the coordination number are directly used in the calculation of composition formulation and consumption of mineral or polymer binder in.

Main Part: Graphic data of particle size distribution obtained by a laser particle size analyzer and polydispersed mixtures and by sieving of polydispersed granulated mixtures for fractions allow determination the particle packing density without an experimental process. For simple polydispersed mixtures sloping stretches from the top of one of the largest peak are typical. The mixtures (Fig. 1, Fig. 2-1) are not high-density compositions.

Complex polydisperse mixtures have a number of maxima on curve of particles content dependence on their size (Fig. 2-2) and are approached to high density compositions according to the number and height of the smaller peaks. As the test with laser particle size analyzer is carry out in an aqueous medium, the particles form jointly with an interfacial layer at the surface is spherical, it should be expected not only the highest density value of a random particle packing in each narrow fractions, where $\eta 1 \leq 0{,}64029\ 0.64976$ [7,8], but the highest deposition density similar atoms or ions in the crystal metal lattice with packing density $\eta_1' = \pi/3\sqrt{2} = 0{,}7405$.

If we take the ratio of average particle size of the maxima in the average size of particles of the coarse fraction according to data of the curve of particle size distribution of a complex polydispersed mixture we can set a class of the particle size distribution due to the their relative sizes according to law of particle distribution in high-density packed mixture as following [8]:

$$d_n/d_1 = \left(\frac{2{,}549}{10\eta_1}\right)^{mn/3} \qquad (1)$$

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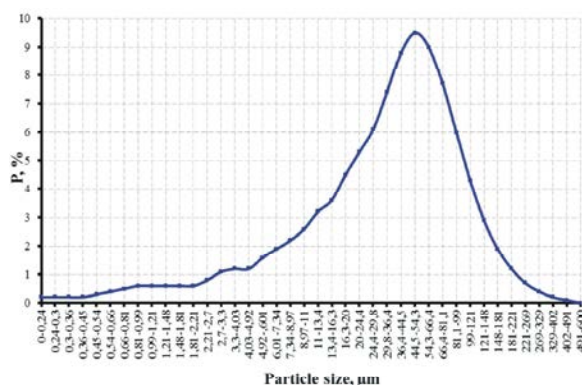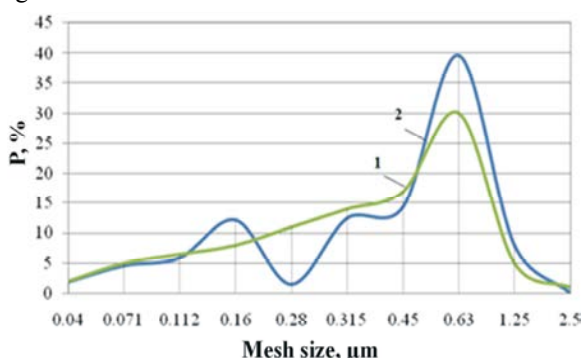
Fig. 1: Particle size distribution for Portland cement

Fig. 2: Particle size distribution for polydispersed aggregates:1 - expanded perlite sand, 2 - polydispersed aggregate on the basis of expanded perlite sand and perlite dust

where in m is particle class in the mixture distribution systems for high-density packaging, m = 0-12...; η_1 is random particles packing density for larger fraction (basic), n is number of the next selected fractions in the mixture from a of basic one, n = 1 2, 3.

Thus, when η_1 = 0,64976, m = 1 and n = 0, 1, 2, 3... from the equation (1) we can obtain the relative particle sizes of the common distribution system of following class m = 1: 1, 0.732, 0.536: 0.392, 0.287, 0.210, 0.154, 0.113, 0.082, 0.060, 0.044, 0.032, 0.024.... These dimensions correspond to the second fraction of systems (subsystems) of class m+1. Thus, when m = 2 and n = 1, 2, 3,... we receive the distribution system for particles of the second class: 1, 0.536, 0.287, 0.154, 0.082, 0.044, 0.024.... Finally, we get the particle distribution system at high density packaging in the mixture for each class m. Feature of system of m=12 class the particle packing density in their two-fractioned compositions is maximum. Thus, when $\eta_1 \leq$ 0,64976 and $\eta_1 = \eta_2 = \eta_3 = \eta_i = \gamma_i$, ρ_i, where γ_i, ρ_i, is bulk density of compacted material in this medium and the particle density of, we have:

0.64976 + (1 0.64976) 0.64976 = 0.8773,
0.64029 + (1 0.64029) 0.64029 = 0.8706.

Presence of intermediate fractions in such fine tow-fractioned formulations leads to a slight increasing in particle packing density in polydispersed mixtures. This is due to the formation of a charge on their surface when dry mechanical grinding of granulated raw as well as the demonstration of electrostatic repulsion forces as loosening the particulate layer. Partial shielding the particle surface charge with interface (adsorption) layer during the wet grinding of mineral raw leads to the particle compaction. However, the smaller the particle size, the greater the thickness of the adsorption layer on the particle surface. Hence typically for fine-dispersed mineral powders and based mixtures is a particles packing density in polydispersed mixtures slightly higher the same packing density for two-fractioned compositions, obtained from the finnest and largest particle fractions, i.e. $\sigma_n \cong \sigma_{12}$ Therefore, the particles packing density in polydispersed mixtures can be calculated from the particles packing density for two-fractioned compositions consisting of finnest and largest particle fractions, particularly when m = 2, with the following equation:

$$\sigma_n = \sigma_{1n} = \eta_1 + (1-\eta_1)\psi_i^{(m)} = \eta_1 + (1-\eta_1)(1-\eta_n)^2 \eta_n^2,$$

where $\psi_i^{(m)}$ _ the filling degree of free volume in the coarse fraction (basic) with fine particles fraction (Table 1 and Table. 6.1 page 49 [9]) depending on the system class m of the particle distribution in the mixture, for a class m = 2, which is typical for sieve and laser analysis of fine dispersed mixtures $\psi_i^{(2)} = (1-\eta_2)^2 \eta_2^2$

This rule does not work in natural polydispersed granulated mixtures of natural and in artificial grain compositions. It is shown below that the particle packing density for some fraction of a polydispersed mixture is readily determined without resorting to the experimental process, but on the basis of the results of the sieve or a laser particle size analysis.

The particles packing density for each fraction of some obtained system is calculated as a separate subsystem class m (according to curves of the size distribution) from the formula derived from the expression (1):

Table 1: Degree of filling of the free volume in a layer of large particles in the bimodal fines particle packing depending on the m-class and the relative particle size

Class of system, m	< 1	1	2	3	4	4,5	5
$\psi_i^{(m)}$	$\varepsilon_i^3 \eta_i^3$	$\varepsilon_i^2 \eta_i^3$	$e_i^2 \eta_i^2$	$\varepsilon_i^2 \eta_i$	ε_i^2	$\varepsilon_i \eta_i^2$	$\varepsilon_i^2 \eta_i$
$\psi_i^{(m)}$	0,012	0,033	0,052	0,080	0,123	0,148	0,189
d_n/d_1	$\leq 0,73$	0,73	0,54	0,39	0,29	0,25	0,21
Class of system, m	6	7	8	9	10	11	12
$\psi_i^{(m)}$	$\varepsilon_i \eta_i$	$\varepsilon_i \eta_i^{3/2}$	ε_i	η_i^2	$\eta_i^{3/2}$	$1 - \eta_i^2$	η_i
$\psi_i^{(m)}$	0,297	0,290	0,35	0,422	0,524	0,578	0,65
d_n/d_1	0,15	0,11	0,08	0,06	0,04	0,03	0,02

Table 2: Particle size distribution of expanded perlite sand according to the results of sieve analysis

Grain size, mm	Average grain size, d_{cpi}, mm	Relative grain size, d_{cpi}/d_{cp1} / di/d_1	Content φ_i, %	$d_{cpi}\varphi_i$
2,50 - 1,25	1,7678		7,9	13,9656
1,25 - 0,63*	0,8874	1,0	39,6	35,1410
0,63 - 0,45	0,5324		14,3	7,6140
0,45 - 0,315	0,3765	0,4243/0,500	12,4	4,6686
0,315 - 0,28	0,2970		1,4	0,4160
0,28 - 0,16	0,2117	0,2386/0,254	12,1	2,5611
0,160 - 0,112	0,1339		2,8	0,7764
0,112 - 0,071	0,0892	0,100/0,1127	4,5	0,4052
0,071 - 0,004	0,0533		1,8	0,0959
			99,8	Total: 65,64

* Bolds are particle size, typical for class $m = 2$.

$$\eta_1 \left[\frac{2,549}{(d_n/d_1)^{3/nm}} \right] \quad (2)$$

Equating equation (1) to any relative size of the systems, such as, when $m = 2$ and $d_2/d_1 = 0.536$ we can define η_1 according to (2):

$$\left(\frac{2,549}{10\eta_1} \right)^{(2n/3)(3/2n)} = 0,536^{3/2n}$$

hence for $n = 1$ is $\eta_1 = \left(\frac{2,549}{10 \cdot 0,536^{3/2n}} \right) = 0,64976$ Using this method for the calculation of η_1 in polydispersed granulated mixture of expanded perlite sand the particle size distribution is shown in Fig. 1 and Table 2.

The average grain size of polydispersed perlite sand is defined by the mass fraction of each fraction in the mixture, where $\rho_1 = \rho_2 = \rho_3 \dots \rho_i$, ρ_i is grain density:

$$d_{1cp} = \frac{\sum d_{cpi} \cdot \varphi_i}{99,8} = \frac{65,64 \;??}{99,8} = 0,6577??$$

On the curve in Fig. 1 the perlite sand sieving into fractions is presented where we can see the highest concentration of grains in the mixture with the size $d_{1max} = 0.63$ mm (the first basic peak). Next one is the size fraction of 0.315, 0.16, 0.071 mm, i.e. we have a system class of the grain size distribution of $m = 2$, which is defined as the ratio of fractions averaging or topological value, respectively :

$$d_2/d_1 = \frac{0,315}{0,63} = 0,5 \; m = 2 \; ? \; d_2/d_1 = \frac{0,3765}{0,8874} = 0,4243,$$
$$m = 1/0,4243 = 2,36$$

From the general law (1) for grain size distribution [8, 9] taking and converting the class of $m = 2$ and we can obtain an equation for η_1 basics:

$$\left(\frac{2,549}{10\eta_1} \right)^{(2n/3)(3/2n)} = 0,5^{3/2n}$$

Hence, for $n = 1$, we obtain following:

$$\eta_1' = \left(\frac{2,549}{10 \cdot 0,5^{3/2n}} \right) = 0,721$$

The checking: $d_2/d_1 = \left(\dfrac{2,549}{10.0,721}\right)^{2/3} = 0,5$ confirms the equality holds.

Since the obtained value $\eta_1' = \geq 0,64976$, then this relative size of grains provides the closest packing density of their systematic (according to the face-centered cubic or hexagonal packing type, where $\eta_1' \leq \pi/(3\sqrt{2}) \leq 0,7405$). The average thickness of the water layer between the grains in a compact dispersed layer of coarse fraction is equal to:

$$\delta = \left[(0,74048005/0,7209769)^{1/3} - 1 \right] d/2^{0,00894.0,8874/}$$

2,F = 2,64 μm,

where F is the coefficient of grain shape, F = 1.2... 1.5 [9].

As $\eta_1' \geq 0,64976$ the density of the random grain packing for coarse fraction (basic) in this case (n = 1) is equal to: $\eta_1 = \left(\dfrac{2,549}{10 \cdot 0,5^{3/(2n+1)}}\right)^{3/2(n+1)} = \left(\dfrac{2,549}{10 \cdot 0,5}\right)^{3/4} = 0,5098^{3/4} = 0,6033,$

where the value of 2 in the exponent is system class. The density of the random grain packing for second perlite fraction (n=2, m=2) at $d_2/d_1 < 0,536$, is equal to :

$$\eta_2 = \left(\frac{2,549}{10 \cdot 0,5^{3/2(n-1)}}\right)^{3/2(n-1)} = 0,721^{3/2} = 0,6122.$$

Random grains packing density in the mixture consisting of the first two (n = 2) adjacent fractions (Table 1) are:

$$\sigma_2 = \left(\frac{2,549}{10 \cdot 0,5^{3/(2n+1)}}\right)^{3/2(n+1)} = 0,3864^{1/2} = 0,6216,$$

If the packing density of large grains for the first fraction was initially random and $0,6038 \leq \eta_1 \leq 0,64976$ then the value σ_2 would reach a maximum value. In this case we have following:

$$\sigma_2 \leq \left(\frac{2,549}{10 \cdot 0,5^{3/2n}}\right)^{3/2(n+1)} \leq 0,4287^{1/2} \leq 0,65475.$$

Further, the individual indexes in equations besides the obvious ones, are specified on the packing density of various compositions, according to methods of calculation given in the work [9]. The denominator in these equations must be greater than 2.549. The grains packing density of perlite in a polydispersed mixture of class m = 2 (Fig. 1), consisting of three fractions with particle sizes $d_1 = 0,63$ (0,8874), $d_2 = 0,315$ (0,3765) and $d_3 = 0,16$ (0,2117) mm, for those the maximums of their content in the mixture on the curve of particle size sieve analysis are typical, we can define by the value of the d_3/d_1 ratio.

$$d_3/d_1 = 0,16(0,2117) / 0,63(0,8874) = 0,254(0,2386).$$

From Table 1 [9] for $d_3/d_1 = 0,254$ (0,2386) it is possible to determine the class of subsystem of fraction distribution in bimodal package, m = 4,5. For subclass m = 3 the following equation corresponds (1):

$$\left(\frac{2,549}{10\eta_3}\right)^{(4,5n/3)(3/4,5n)} = 0,254^{3/4,5n}.$$

Thus packing density for third fraction (n = 1, n = 3) and for distribution system class (n' = 2) is:

$$\eta_3 = \left(\frac{2,549}{10 \cdot 0,254^{3/4,5}}\right) = \left(\frac{2,549}{10 \cdot 0,254^{3/4,5(n-2)}}\right) = \left(\frac{2,549}{10 \cdot 0,254^{3/4,5(n-1)}}\right) = 0,6356$$

The particle packing density in polydispersed mixture of quartz sand consisting of the first three fractions (n = 3, m = 2) is equal to:

$$\sigma_3 = \left(\frac{2,549}{10 \cdot (0,254...0,2386)^{3/(2n-1)}}\right)^{3/2(n-1)}$$
$$= (0,5800...0,6022)^{3/4} = 0,6647...0,6836.$$

Whereas the grain packing density of two-fractioned granulated mixture consisting of the first coarse fraction as well as third fraction of subsystem of m = 4,5 class (Table 1) and n = 2 class, is:

$$\sigma_{13} = \left(\frac{2,549}{10 \cdot (0,254...0,2386)^{3/(4,5n+1)}}\right)^{3/4,5n-2}$$
$$= (0,3845...0,3918)^{3/7} = 0,6639...0,6693.$$

The particles packing density the according for fourth fraction according to (2), wherein $d_4/d_1 = 0,071/0,63 = 0,1127$, n=4 and subsystem of m=7 class (Table 1) is:

$$\eta_4 = \left[\frac{2,549}{0,1127^{3/7(n-3)}}\right] = 0,64967$$

The particles packing density in polydispersed mixtures consisting of four fractions of expanded perlite sand with a sufficient content of the fourth fraction where $d_4/d_1 = 0,071/0,63 = 0,1127$, n=4 and m=2 in this case will be equal:

$$\sigma_4 = \left(\frac{2,549}{10 \cdot 0,1127^{3/(2n-1)}}\right)^{3/2(n-2)} = \left(\frac{2,549}{10.0,1127^{3/7}}\right)^{3/4} = 0,64967^{3/4} = 0,7236$$

Whereas the particle packing density in two-fractioned mixture consisting of a first coarse fraction and a fine the fourth fraction (n=2, m=7) will be equal:

$$\sigma_{14} = \left(\frac{2,549}{10.1127^{3/(7n-2)}}\right)^{3/7(n-1)} = 0,43994^{3/7} = 0,7033$$

However, from Table 2 it is seen the contents of the fourth fraction in the mixture (4.5 %) is insufficient to obtain high-density packing of grains therein, so the mixture must content additional amount of fourth fraction. The calculation of the required content of fourth fraction and thus increasing of the grains packing density in the mixture is shown bellow. According to the analysis of particle size distribution of a polydispersed mixture of fine polydispersed perlite dust $d_{2everage} = (0,036\ 0,044)\ 1/2 = 0.0398$ mm. We find the ratio of $d_{2everage}/d_{1everage} = 0.06$. In this subsystem class of particle distribution for large and small polydispersed mixtures equals: m=9 and $\psi_i^{(9)} = \eta_n^2$

(Table 1) and it is possible to determine the requirement of fine fraction:

$$G_2 = G_1(1 - \sigma) \cdot (\eta_5/\sigma_4) \cdot \beta_5$$

where β_2 is a coefficient of the grain separation of coarse fraction mixture by dust particles.

The unknown parameter in this expression is η_5. It is the packing density of the dust particles, which is in the quasi-solid state, where $\eta_5 < 0,545$ [9]. According to well-known equation [9] we can specify the value of the packing density of η_5 according to

$\eta_1 = 0,6122$:

$$\eta_5 = 0,6122\left[1 - \frac{1}{3\ln\left(120,754 \cdot 0,6122^5\right)}\right] = 0,525,$$

Then the requirement of fine polydispersed mixture (dust) when introduction into coarse polydisperses mixture of expanded perlite sand, taking its quaitity of $G_1 = 100$ parts (parts by weight) and assuming that $\beta_2 = \sigma_4 / \eta_5$ and β_5=1 will be equal :

with $\beta_5 = \sigma_4 / \eta_5$

$G_2 = G_1 \cdot \ (1-\sigma_4)\dfrac{\eta_5}{\sigma_4} \cdot \beta_5 \cdot \dfrac{\rho_5}{\rho_1} = \ 100$ wt. part (1-0,7236)2200/2650 = 22.9 wt. part,

where ρ_1, ρ_5 is grain density of expanded perlite sand and perlite dust particle density respectively;
when β_5 =1

$G_2 = G_1(1-s_4)\dfrac{?_s}{s_4} \cdot \dfrac{?_s}{?_1} = 100$wt. part (1-0,700) 2200/2650=16.7 wt. part

In terms of 100 % by weight of mixture that is:

$G_2 = 22,9/122,9 = 18,6$ % (при $\beta_5 = \sigma_4/\eta_5$),
$G_2 = 16,7/116,7 = 14,3$ % (при $\beta_5 = 1$).

Missing number of the fourth fraction, filled with

perlite dust introduced into a mixture is from 14.1% (18.6%-4.5%) to 9.8% (14.3%-4.5%).

Taking into account the presence of a very fine fractions in coarse polydispersed mixture fine fraction consumption can be reduced by the amount of (1.8 + 0.2) = 2%, then

$G_{2max} = 14,1 - 2 = 12,1$ %, $G_{2min} = 9,8 - 0,2 = 9,6$ %.

The particles packing density in binary polydispersed a mixture is equal:

$$s_n = s_{n1} + \left(1 - s_{n1}\right)?_5^2 = 0,7236 + (1-0,7236) \cdot 0,525^2 = 0,800.$$

Thus, for preparation of high-density binary mixture, a second fine polydisperse mixture (dust) is required of 12... 10%. Consumption of mineral binder or polymer binder in volume fractions thus is: $\varphi = (1-0,80)\ \alpha^3 = 0,20\ \alpha^3$ where $\alpha_3\ \alpha^3 = 1,05...\ 1,1$.

Here is an example of calculation of the topological properties of the product of joint grinding of materials with following composition: clinker cement

Table 3: Size distribution of the milled Portland with additives according to data of sieve analysis

Particle size, μm	Average particle size $d_{average i}, \mu m$	Relative particle size $d_{average i}\, d_{average1}, \mu m$	φ_i content, wt.part	φ_i content,wt.part (calculated)
13,4 - 11	12,14	1,0	6,5	6,5
8,97 - 7,34	6,64	0,547	5,4	2,4
4,03 - 3,30	3,65	0,300	4,0	3,2
1,48 - 1,21	1,34	0,164	4,4	4,3
$\leq 1,21$	$\leq 1,21$	0,0895	0,7	3,6

(Belgorod plant) is 70%, gypsum dihydrate is 5%, superplastisizer is 1%, crushing screenings of quartzitic sandstone (Lebedinsk mining and concentrating company) is 30% (Table 3) [10].

As can be seen from Table 3, the particle size composition of the mixture corresponds to the particle size distribution of class $m = 2$. For this class of particle distribution according to (1) we have:

$$d_n / d_1 = \left(\frac{2,549}{10?_1}\right)^{(2n/3)(3/2n)} = 0,547^{3/2n}$$

When the random particle packing density for coarse fraction ($n = 1$), according to (2) will be equal:

$$d_n / d_n = \left(\frac{2,549}{10\eta_1}\right)^{(2n/3)(3/2n)} = 0,547^{3/2}$$

The particle size distribution is following (with $m = 2$ and $n = 0, 1, 2, 3...$):

$$d_n / d_1 = \left(\frac{2,549}{10 \cdot 0,6301}\right)^{2n/3} = 1,0;\ 0,5470;\ 0,2992;\ 0,1637;\ 0,0895...$$

Here, all values of the particles relative sizes have a good convergence with the real distribution in the milling product (Table 2).

Therefore, the particles packing density for all the fractions by (2) will be equal to: $\eta_1 = \eta_2 = \eta_3 = \eta_4 = \eta_5 = 0,6301$, so for $m=2$:

$$?_n = \left(\frac{2,549}{10 \cdot 0,547^{3/2(n-1)}}\right) =$$

$$= \left(\frac{2,549}{10 \cdot 0,547^{3/2}}\right) = \left(\frac{2,549}{10 \cdot 0,2992^{3/2^2}}\right) = \left(\frac{2,549}{10 \cdot 0,1637^{3/2^3}}\right) = \left(\frac{2,549}{10 \cdot 0,0895^{3/2^4}}\right) = 0,6301$$

As $\eta_1 = 0,65$, the particles random packing in the mixture with first two adjacent fractions ($n = 2$) is equal to :

$$s_2 = \left(\frac{2,549}{10 \cdot 0,547^{3/(2n+1)}}\right)^{3/(2n^2-1)} = 0,36609^{3/7} = 0,6501.$$

The particles packing density in the mixture consisting of the first three fractions ($n=3$) will be:

$$s_3 = \left(\frac{2,549}{10 \cdot 0,3^{3/2(n+1)}}\right)^{3/(2n+1)} = 0,4008^{3/7} = 0,6758.$$

As $d_3/d_1 = 3,65/12,14 = 0,30$ and the class of subsystems with $m=4$ (Table 1), the packing density of the mixture consisting of the first and third fractions (n=2) is equal to:

$$s_{13} = \left(\frac{2,549}{10 \cdot 0,3^{3/4n}}\right)^{3/(4n-1)} = 0,4008^{3/7} = 0,6758.$$

The particles packing density in the mixture consisting of the first four fractions ($n=4$, $m=2$) is equal to:

$$s_4 = \left(\frac{2,549}{10 \cdot 0,16367^{3/2n}}\right)^{3/2(n-1)} = 0,5025^{1/2} = 0,7089.$$

Then, as the particles packing density in the mixture consisting of the first and fourth fractions ($m = 6$, Tab. 1 and $n = 2$) is equal to :

$$s_{14} = \left(\frac{2,549}{10 \cdot 0,16367^{3/6n}}\right)^{3/2(n+2)} = 0,4008^{3/8} = 0,7097,$$

and packing density of the mixture when introducing the fifth fraction ($n = 5$, $m = 2$) could be equal to :

$$s_5 = \left(\frac{2,549}{10 \cdot 0,0895^{3/(2n-1)}}\right)^{3/2(n-2)} = 0,56986^{1/2} = 0,7549.$$

The particles packing density in the mixture with the largest and the finest fractions (n=2, $m=8$, Table 1) will equal to:

$$\sigma_{15} = \left(\frac{2,549}{10 \cdot 0,0895^{3/(8n-4)}}\right)^{3/(8n-1)} = 0,4660^{3/8} = 0,7510.$$

CONCLUSION

This method is recommended to calculate the particle packing density for the largest fractions in η_1 polydispersed mixtures (in quartz sand, in crushing and screening products of pulverizing mineral rocks) in each subsequent η_n fraction and the overall particle packing density in mixtures - η_n according to the analysis of particle size distribution.

Summary: Theory and method for more information receiving on the topological properties of polydispersed mixtures and fractions within them, basing of the curves of the sieve and laser particle size analysis needs in order to optimize polydispersed formulations of crushing products of mineral raw materials in order to reduce the consumption of mineral binders or polymer binders in the production of highly-filled composites and non-hydration geopolymer mineral binders.

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