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A Geometrical Inclusion-Matrix Model For Concrete

I. Rasoolan¹, S. A. Sadrnejad^{2,*}, A. R. Bagheri³

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Abstract: Concrete is a heterogeneous material with a highly non linear behavior, which is mainly caused by the initiation and propagation of micro cracks within the several components of the material. The damage behavior of concrete is usually simulated on the macro scale using complex constitutive models. The direct determination of the homogenized material parameters is often difficult and sometimes impossible. Furthermore these materials models do not explicitly represent effects and bond behaviors of interfaces between the several components. So in order to predict of concrete behaviors and characteristics, it should be modeled as a three phase composite material consisting of aggregate, interfacial transition zone (ITZ) and cement paste. The size and distribution of aggregate affects concrete characteristics. Because of the random distribution and size variation of aggregate in concrete, the modeling of concrete behavior based on component in meso structure is difficult and so we must use simple assumption. In this paper with mixing design and grading curve we developed a simple method to replace real aggregate with equivalent sphere aggregate with effective diameter. So we can use simple methods instead of complex numeral and randomness or x ray methods to find effective diameter and use it to determine two arrangements with maximum and minimum aggregate volume as a repeatable basic element. As a result we can use this element to modeling the behavior of sample concrete in meso scale and three phases.

Keywords: Aggregates, Equal shape, Concrete, Interfacial zone, Grading, Specific surface area

1. Introduction

Theoretical analysis by Monteiro(1993) [1], Simeonov(1995) [2] and Lutz (2005) [3] work's has confirmed that, when the interfacial transition zone (ITZ) in concrete is ignored, the theoretical lower bound of Hashin and Shtrikman bounds for elastic modulus of concrete is higher than the measured elastic modulus of concrete. This implies that the concrete should be modeled as a three-phase composite material at a mesoscopic level, consisting of aggregates, ITZ and cement paste as shown by Ramesh (et al., 1996) [4].

The shape of the particles is a very important parameter in analysis. Modeling particular media with discs (in 2D), as it is shown in Fig. 1, or spheres (in 3D) is quite simple from a computational point of view but it has been found

by Ting(et al. 1995) that the particles tend to roll or rotate excessively. In order to reduce particle rotations to more realistic levels, many authors have used particles with more complex shapes that more closely replicate those in natural media. Walton (1982) Issa and Nelson (1992) employed arbitrary polygon-shaped elements (Fig. 1) that yield better qualitative response but have some computational disadvantages related to the contact detection scheme which may be time-consuming because of the large number of surfaces that requires monitoring. [5] Additional disadvantages arise from the treatment of the vertices that are present in polygon-shaped particles.

Furthermore, extension from 2D to 3D is much more complex in comparison to extensions using simple particle shapes. Ting (et al, 1995) developed elliptically shaped particles (Fig. 1) and established that such an idealization better replicates the resistance of particles to rotation that is observed in natural media. Also, an elliptical particle has a unique outward normal direction, and has a surface that is represented by a single function. Disadvantages with elliptical particles are that the contact detection algorithm

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is still not as efficient as those for simple circular disks and spheres. The problems arising from the choice of the particle shape have been also addressed by Jensen (et al, 1999, [5]) with using clustered particles. [5]

A certain number of circular-shape particles are combined in a semi-rigid configuration (cluster) as it is shown in Fig. 1. The semi-rigidity of the cluster is enforced by assuming a linear elastic behavior of the contact between the particles belonging to the same cluster. In this way one can simulate particles with arbitrary shape preserving the computational efficiency of the circular particles. Similar model is the Rigid-Body-Spring Model (RBSM) that developed by Kawai (1978, [6]). The RBSM subdivides the material domain in rigid elements interconnected by zero-size springs placed along their common boundary segments. This model has been used to simulate concrete fracture by nagai (et al 2004, [7]). The subdivision is random and is obtained using Voronoi Diagram.

For all these models, although the kinematics of the simulations appears very realistic, the quantitative stress-strain (averaged) response is not close enough to the actual behavior of the material. The main reason of this shortcoming is due to the fact that most of these models are bidimensional and then the three-dimensional effects are completely neglected. As far as lattice models are concerned, two different approaches can be found in literature. The classical one, which refers to the early studies by Hrennikoff (1941,[8]), replaces the actual material by a truss or frame whose geometry is not related to the actual internal geometry of the material. The element size is chosen by the user and the heterogeneity of the material is taken into account by assigning different properties at the lattice elements according to the real material structure. This kind of lattice model has developed to analyze concrete fracture by Schlangen and van Mier (1992, [9]), van Mier, (2003, [9]), Schalgen, (1994, [11]) and Lilliu (2003,[12]). This model is bidimensional and each element of the lattice is a beam element with three degrees of freedom per node (fig .4). Garboczi (2002, [13]) developed a Three-dimensional mathematical analysis of particle

shape using X-ray tomography and spherical harmonics for concrete. By Corri and Lori (2002, [14]) a model based on the moving window generalized method of cells is presented for the mechanical analysis of concrete microstructure. Also in approach Eckardt (et al, 2004,[15]) the aggregates are represented by ellipsoids that is fully described in 3D by nine parameters. By Lopez (et al, 2004,[16]) geometry of the aggregate particles has been obtained with a method based on the Voronóy/Delaunay theory of polygon or polyhedron. These polyhedrons represent the larger aggregates, which are in turn embedded in a matrix representing mortar plus smaller aggregate.

From the studying of the mentioned references it is defined that most of the geometrical models have been two-dimensional, two-phases and limited and the gradation effects have not seen on them. Concerning to the failures and Complexities of mentioned models, this article is

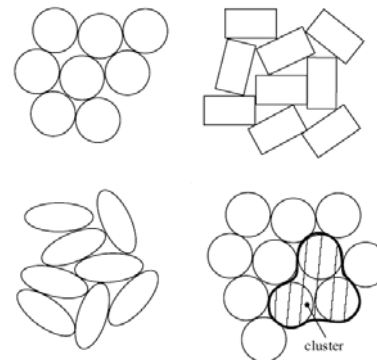


Fig. 1 Discrete element method. a) Circle particle package. b) Polygon particle package. c) Ellipse particle package. d) Cluster approach.

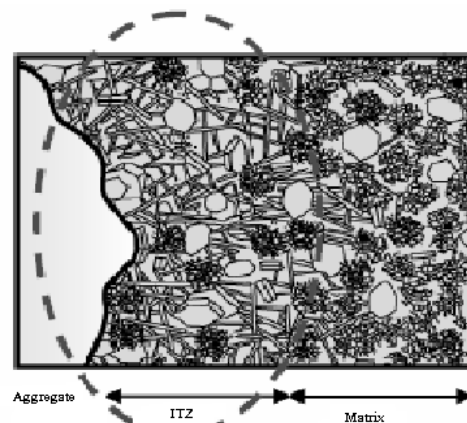


Fig. 2 component of concrete [3]

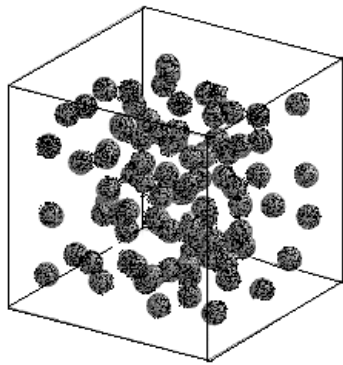


Fig. 3 aggregates Random distribution

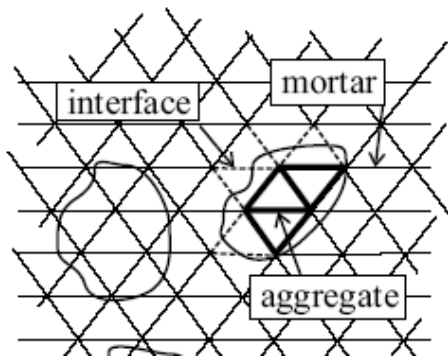


Fig. 4 Lattice models. a) Schlangen and van Mier's Regular triangular Lattice. [5]

stating a method that with aggregate gradation curve for a concrete sample. It can present simplicity, three dimensional and three -phase's model through defining all of its components and the model can use as base element in studying the fracture behavior of concrete sample.

2. Microstructure concrete

Concrete is an artificial heterogeneous composite material which consists of aggregates which are bonded together by cement paste. The influence of the material structure on the macroscopic material behaviors can be analyzed using mesoscale models. At the mesoscale, Concrete is separated into three main components: the homogenous mortar matrix, the aggregates and the interfacial zone between them. The mortar matrix is mainly composed of cement paste and aggregates with a diameter less than 2.0 mm .Fig (2). Porosities within the matrix are disregarded at this length scale. The interfacial transition zone (ITZ), which

represents the interfacial region between the particles of coarse aggregate and the hydrated cement paste, is a thin shell around the aggregate and is generally weaker than either of the two components of concrete. In Mindess (1989) works it was found that the thickness of interfacial transition zone (ITZ), is around 20 - 100 μm . (S.Mindess, 1989, [17]).

2.1. Aggregates

Aggregates takes up 60 -90 % of total volume of concrete, therefore the aggregates have been the most important and extreme component of forming the concrete, so the shape of aggregates are the most important on modeling. The aggregates have elliptical, spherical, broken shapes. Therefore the shape and distribution of aggregate and related regards for each shape must be considered on modeling.

Determining the attributes and the mathematical specifications of aggregates shapes could able us to sort the different aggregate and also present quantitatively the joint between the three-dimensional shape of aggregate attributes to the presented properties, so there are important matters.

The composites attributes consisted of particles that located on one matrix , frequently have controlled through the particles shape and size .Mathematically the determining the particle shape attributes on three-dimensional statue specially when the particle for some reasons could not seen , is not a simple work .Even if we can distinguish particles, such as the used particles on concrete ,it's mathematical process finding (determining the attributes) will be difficult with regard to random of three-dimensional particles. With accessing to the digital processing technique of image and helping the x ray, radiography, laser cutting and photogrammetry, the researchers are exerting to automatically determining the aggregates shape attributes. By using these techniques, more specifications of aggregates included area, cross section, direction, perimeter, size distribution and volume parameters of mixed could be measured. Outus and Garboczi have experiences in this field [18].

2.2.1. Aggregates Shape

The random structural of concrete with regard to ITZ and also the expand compass of aggregates size, have elaborated its modeling. So to model of that, the simple hypothesizes should be considered. The first hypothesis is sorting the aggregates and considering of definite bound for aggregates size. In this regard, those smaller particles than one special size for instance 5 mm could be considered as a sample on cement paste. The second hypothesis is considering the suitable geometrical shape for aggregates. In the modeling, it is considered spherical and elliptical of the aggregates generally. It is mentioned that most of the aggregates have not spherical shape certainly, so the non spherical of real aggregates and the difference between non spherical of them should be shown. In this regard using of the relationship between area and volume of particles instead of the sphere substitute could be utilized, like Garboczi (2002, [18]) studies.

In the three dimensional statuses through the using spherical harmonic function, Fourier series and a general formulation of the basic ellipsoid function by varying the exponent (Stefan et al, 2003,[19]), some of the aggregates attributes can be acquired.

2.2.2. Equivalent shape

The very definition of a regular body means that it can be specified by a few geometrical parameters related to size; e.g., the diameter of a sphere or the side length of a cube (one dimension), the aspect ratio and the length of one axis of a prolate or oblate spheroid (two dimensions), or the semi-axis lengths of a tri-axial ellipsoid (three dimensions). Other, more complicated shapes could require more dimensions. One of the ways that the notion of their regular shape is quantified is from the analytically simple relations between their dimensions and their geometrical properties like volume and surface area. For irregular bodies, a very great number of parameters have been proposed that purport to relate dimensions and geometry. This attempt is to have a convenient single number with which to refer to an irregular shape.

The aggregates could be sorted and the proportional amount of aggregate with any size of diameter can be acquired through the concrete technology relations and grading curve. In this article instead of using the digital images and harmonic mathematical equations the simple method as follows has been used.

2.2.3. Distribution and Aggregates Shape Criterion

There are several alternatives of distributing the aggregates. The first alternative is the regular distribution of aggregates and the second is usage of non-regular distribution and the third is the usage of uncertain distribution of functions and the forth is radiography which used the most real distribution after analyzing and studying the current sample. In this paper we use the first method. In Random distribution in sample one uncertain uniform distribution for each aggregate position is assumed. After selecting a sample, through definite amount and size of aggregate, The position coordinates of each grade center could be determined by a computer random number producer. For each new position they are checked that not to be overlapped with previous position and sample frontier. If they appear overlapped, they turn and the new position will be determined. The aggregate are entered according to large size. This process is continuing. Therefore all of the aggregates have entered randomly and the sample including the one base complex element has been completely filled of aggregates Fig (3). This process has been done by author through Rand3D computer code Fig (3). Also in this method, the over lapping matter has been controlled. After assigning the aggregates, the rest of the volume involves the cement paste and ITZ has included aggregates surrounding.

3. The geometrical modeling method

3.1. Grading curve

The grading of aggregates have determined through the relation between the size of standard sieve X_i and the total amount passing through this sieve $Y_i(x_i)$. This relation can be reflected by formulas, tables or graphic. There are different types of ideal curves that have been referred to

Fuller's, Garf's, Bolomey's, Rissel's curves.

If in a curve, the largest grade of aggregates size are D_{\max} , its passing or remained percent are ρ_N , the smallest size of aggregates is D_{\min} and it's passing or remained percentage is ρ_1 , approximately the grading curve with linear relation will show as follows, Fig(5):

$$\rho_1 = f(D, D_{\max}, D_{\min}, \rho_{\min}, \rho_{\max}) \quad (1)$$

With regard to the modeling problems and complexities and the variety of aggregates size for considering all of the aggregates in three-dimensional state, the following simple technique could be considered: Instead of all aggregate with different amount and size, a diameter size equal D_{50} could be used and the considered sample has been attended to aggregates with this substitute diameter. Also the equation between percent and volume of each aggregates with percent and volume D_{50} , is shown:

$$\begin{aligned} & \rho_1 \pi D_1^3 / 6 + \rho_2 \pi D_2^3 / 6 + \dots + \rho_N \pi D_N^3 / 6 \\ & = \rho_{D_{50}} \pi D_{50}^3 / 6 \end{aligned} \quad (2)$$

If the equation (1) has written for equal diameter coordinates:

$$\rho = f(D_{50}, D_{\max}, D_{\min}, \rho_{\min}, \rho_{\max}) \quad (3)$$

The equal diameter getting from two above equation. In order to complete the modeling, the aggregates amount should be calculated with equal diameter and the base element model should be used. For this means, several change coefficients would be needed which their way of getting coefficients would be explained as follows.

3.2. Selection of base element shape

For distribution of aggregates could be considered a cubic element fill of isometric spheres on two arrangements: a): regular lap b): regular compact. Considering the amount of spheres and the sizes for cubes is the most important propound question. If spheres with different radius are used then the arrangement results with radius: 1, 0.75, 0.5 and 0.25 cm on (a) statue will be like figures (6) and table (1).

Consideration the smallest and repeated base element has been the important matter. The number of spheres on Z direction (vertical to page), will not effect the results. According to the chart above, aggregates volume percent is a fix number and equal to %56 on whole statues. If the (b) statue according to figure (7) is considered, the results achieved for arrangement of aggregates will be according to table (2). Also in this statue, the smallest repeated base element has been considered. If in this statue, instead of 6 spheres according to Figure (7), 8 spheres according to figure (7) had been used, it wouldn't effect the result. In this statue, the volume aggregates percent is a fixed number and equal to %52.3. In this statue, we have considered the smallest repeated base element. Regarding to mentioned results, the volumes of the samples respectively are $5.6 D^3$ and $6 D^3$.

3.3. Mathematical formulation

With regard to aggregates amount and variety of sizes, for concrete geometrical modeling and preparation of sample for behavioral modeling, the curve could be changed to a sample consisted of isometric spherical aggregates through help of several Coefficient For this means, it is possible to usage of proportions between volume and special surface of aggregates to equal spherical a volume and special surface aggregates.

If in a concrete mix design, cement content per unit volume c (kg/cm^3), aggregate content per unit volume a (kg/cm^3), for a given specimen, with volume V_m , the total mass of aggregates is $M = a.V_m$ and volume of aggregate is $V_v = V_m.f$ (f is a volume fraction of aggregates) and volume of paste is V_p . The number of aggregates of each characteristic size D_i can be computed by the following equation:

$$N_i^a = \frac{\Psi_i M}{\rho_a V_i} \quad i=1, \dots, N \quad (4)$$

where V_i is the volume of an aggregate, Ψ_i is the ratio between the mass of aggregates which have characteristic dimension D_i and the total mass of aggregates, ρ_a is the mass density of aggregates and N is the number of characteristic sizes chosen to describe the aggregate

distribution. When the mass density of aggregates, is unknown, it can be computed from water cement ratio w/c and mass density of cement ρ_c (w (kg/m^3) is the water content), mass density of water is $\rho_w = 1000kg/m^3$, and the mass density of cement ρ_c depends on the type of cement but for ordinary Portland cement is $3150 kg/m^3$.

$$\rho_a = \frac{a}{1 - \frac{C}{\rho_c} - \frac{w}{\rho_w}} \quad (5)$$

If the volume and specific surface area of aggregates on concrete for one definite sample respectively would V_v and S_c and the special surfaces of equal spheres Respectively would V_{cr} and S_{cr} , the below proportions could be considered:

$$\alpha = \frac{V_{cr}}{V_v} \quad \beta = \frac{S_{cr}}{S_c} \quad (6)$$

And with considering aggregates in spherical shape with a definite size D , volume fractions of aggregates namely proportion of spherical

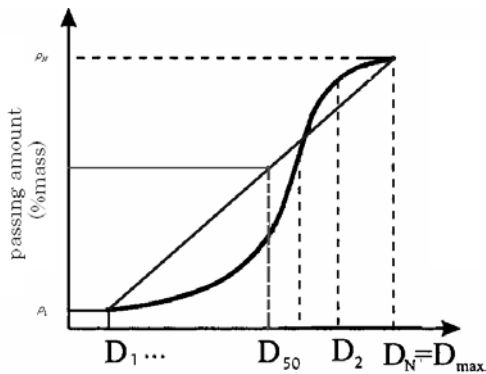


Fig. 5 the grading curve with linear approximated

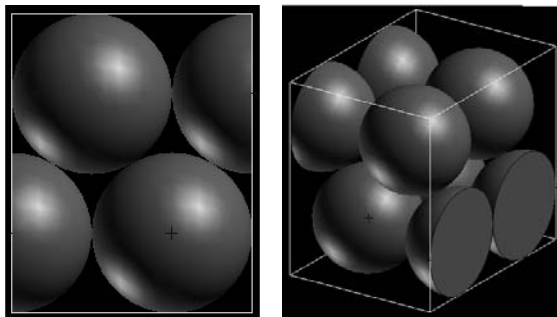


Fig. 6 arrangement : a): regular over lap

aggregates to whole volume : $f_1 = \frac{N(\pi D^3)/6}{V_m}$ and the surface area of particles: $A_{ag} = N\pi D^2$ and

matrix or cement paste volume are V_p . Then for spherical aggregates, the aggregates specific surface area namely proportion between surface area to volume equal to $S_{cr} = \frac{N\pi D^2}{V_m}$, after replacement, we have:

$$S_{cr} = \frac{6N(\pi D^3)/6}{V_m/D} = 6f_1/D \quad (7)$$

$$S_c = \frac{f \sum_{i=1}^n 6V_i/D_i}{V_m} \quad (8)$$

$$\beta = \frac{S_{cr}}{S_c} = \frac{6f_1/D}{S_c} \quad (9)$$

$$\alpha = \frac{V_{cr}}{V_v} = \frac{N\pi.D^3/6}{f.V_m} \quad (10)$$

3.4. Apply proposed theory

If in a mix design water, cement, gravel and sand quantities for constructing a concrete sample were: 155, 369, 992 and 760 kg/m^3 and the components volumes respectively were 0.155, 0.117, 0.370, 0.288 m^3 and some kind of grading curve have used; the resultant on following chart would be summarized. If the

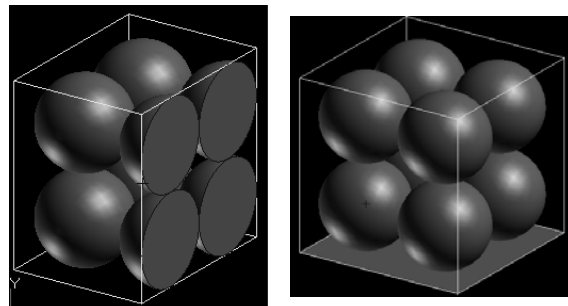
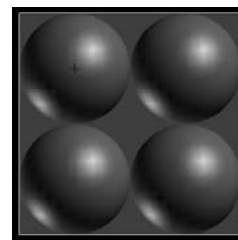


Fig. 7 arrangement b): regular compact, with 6 and 8 spheres

Table 1. result of arrangement (a)

Radius of Sphere (cm)(r)	dimension Cubic sample (cm)	Volume of Sample (cm ³)	Volume of Sphere (cm ³)	Volume of Matrix cm ³	volume fractions of aggregates
1	3*4*.73205	44.7846	25.12	19.664	0.56%
0.75	2.25*3*2.799	18.89	10.59	8.3	0.56%
0.5	1.2*2*1.866025	5.598	3.14	2.458	0.56%
0.25	0.75*1*0.932	0.69975	0.392	0.30775	0.56%

Table 2. result of arrangement (b)

Radius of Sphere (cm)(r)	dimension Cubic sample (cm)	Volume of Sample (cm ³)	Volume of Sphere (cm ³)	Volume of Matrix cm ³	volume fractions of aggregates
1	3*4*4	48	25.12	22.88	52.3%
0.75	2.25*3*3	20.25	10.5975	9.6525	52.3%
0.5	1.5*2*2	6	3.14	2.86	52.3%
0.25	0.75*1*1	0.75	0.3925	0.3575	52.3%

grading curve No (1), Fig (8-a) has used, the equation. (3) Would be written

As follows:

$$\rho = 2.4342 D + 7.2943 \quad (11)$$

By putting D_{50} on above equation, we

Have:

$$\rho_{50} = 2.4342 D_{50} + 7.2943 \quad (12)$$

If we write the equation (2) for D_{50} then:

$$\begin{aligned} &995\pi(.15^3)/6+97\pi(3^3)/6+9\pi(.6^3)/6+ \\ &8\pi(1.18^3)/6+83\pi(2.36^3)/6+7\pi(4.75^3)/6+ \\ &66\pi(9.5^3)/6+50\pi(19^3)/6+0\pi(381^3)/6= \\ &\rho_{D_{50}}\pi D_{50}^3/6 \end{aligned}$$

Through solving the mentioned equations, equal diameter, $D_{50}=19.5$ mm would result. The results of this curve, are presented in table No. (3). Respectively if the curves No 2-8 (Fig. 8,a,b,c,d,e,f,g,h) is used, the same results are reached.

After solving the equation and determining the properties, the results will be like table No. (4) for two kinds of arrangement(a,b), With regard to the mentioned chart , it has seen, although the

effective diameter in rows 3,7 and 8 rows equal and parallel to 15 mm but regarding the grading curve and Coefficient β , the fine aggregate amount in rows 8 and then 7 have surpassed. Therefore the special surface has surpassed and as a result the β coefficient is reduced.

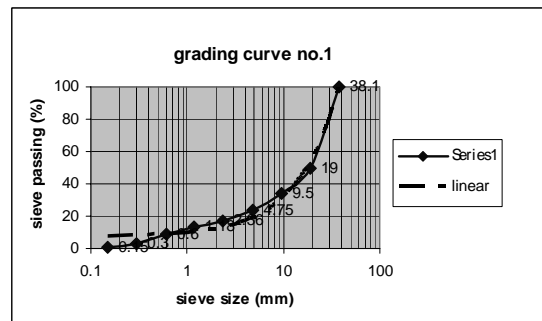


Fig. 8-a grading curve no.1

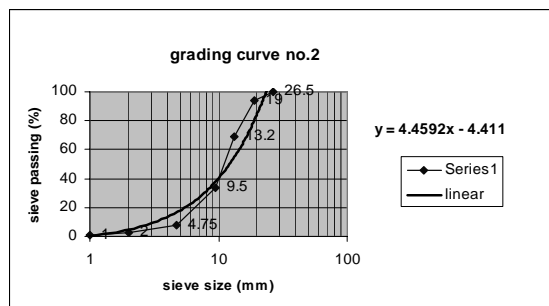


Fig. 8-b grading curve no.2

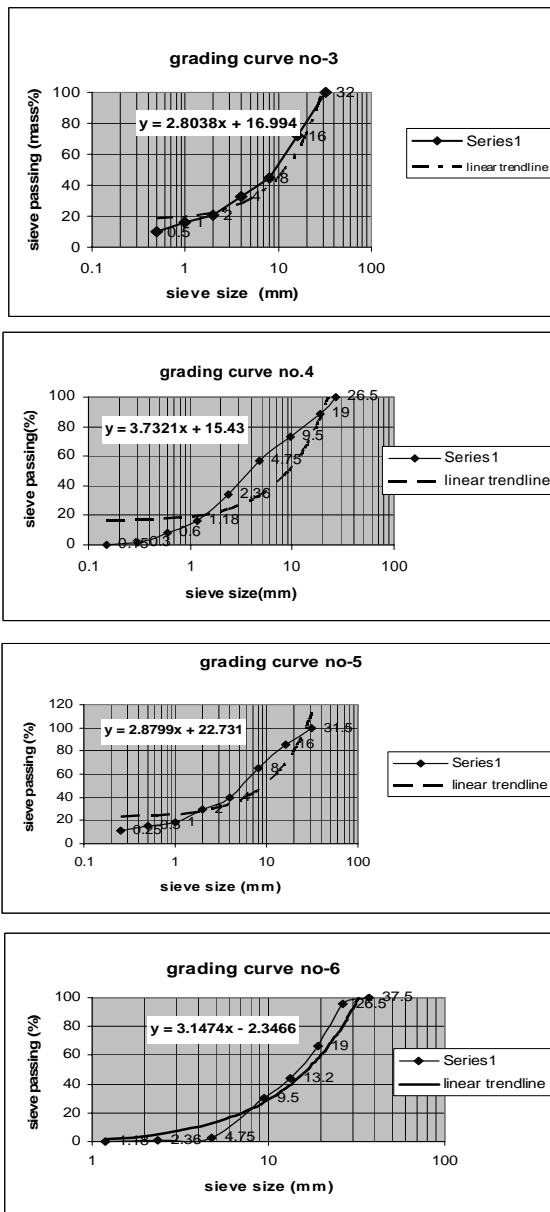


Fig. 8-c,d,e,f grading curve no. 3,4,5,6

Considering this effect and the limit of volume

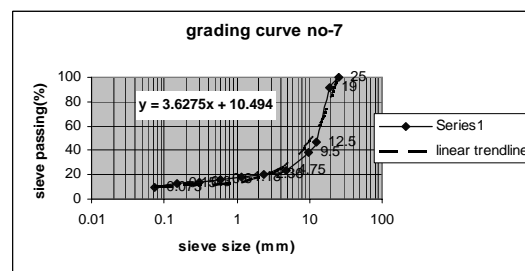
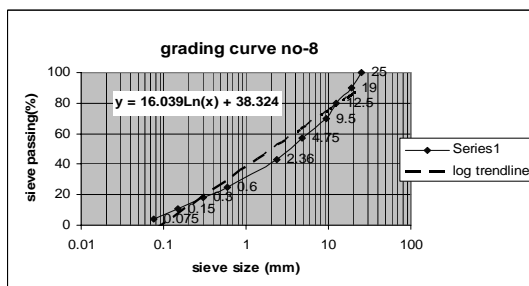


Fig. 8-, g, h. grading curve no. 7, 8

fractions of aggregates on two arrangement **a** and **b** (limit %52.3, %56) the effective diameter must be corrected. Therefore the reformed effective diameter would show in table No (5).

4. Conclusion

Based on the result, following conclusions are reached:

- The base element volume of the two arrangements a and b (max and min compact) respectively is $5.6 D^3$ and $6 D^3$.

- The proportion between $\frac{S_{cr1}}{S_{cr2}}$ in two arrangement a and b respectively is 0.86 and 0.8.

- By having a grading curve and mix design and with acquiring the effective Diameter, a base element with two arrangements can be selected.

- The variety of β coefficient demonstrates the consideration of this parameter with the exception of the effective diameter.

By considering that if the fine aggregate increase on grading curve then the special surface will increase we result that the diameters should be improved and the β will be an improved coefficient.

Then instead of relying on probability or the complicating portrayal methods, and by having a grading curve and a mixed plan of concrete sample, the effective diameter can be acquired by this simple mentioned way. After defining the geometrical model of the base element, it would use for determining the behavior on different loading statuses.

This is an issue that will be presented in the next article.

Table 3. result of mix design with grading curve no.1

Sample 20*20 M=14kg		$v_v = 0.00526$ $v_m = 0.008$ $m^3 v_p = 0.0028$					
Sieve size (mm)	Cumulative remained percent	Cumulative passing percent	remained percent	remained weight kg	coefficient ψ	Number of aggregate	Volume of aggregate m^3
38.1	0	100	0	0	0	0	0
19	50	50	50	7	0.5	810	0.00436
9.5	66	34	16	2.24	0.16	2074	0.00139
4.75	76	24	10	1.4	0.11	10370	0.000872
2.36	83	17	7	0.98	0.07	59188	0.000610
1.18	87	13	4	0.56	0.04	270574	0.000438
0.6	91	9	4	0.56	0.04	2058163	0.000348
0.3	97	3	2	0.84	0.06	10290815	0.000128
0.15	99.5	0.5	2.5	0.35	0.025	82326524	0.0000128
				=14			$\sum = 0.005$
				\sum			
19.5				14	1	1498	0.005

Table 4. Result grading curves no .1 until no.8

NO. curve	arrangement	(mm) D_{50}	(m^3) v_m $*10^{-6}$	$v_v (m^3)$ $*10^{-6}$	$v_p (m^3)$ $*10^{-6}$	S_{cr1} base element	S_{cr2} element	S_c	$=m^3 V_c$ V_{cr}	β	α
1	a	19.5	41.509	23.282	18.22	172	200	1939	0.005	0.103	1 \approx
	b	19.5	44.489	23.282	20.207	160					
2	a	14	15.36	8.62	6.74	240	278	664.5	0.005	0.418	1 \approx
	b	14	16.46	8.62	7.84	224					
3	a	15	18.89	10.60	9.65	224	260	1325	0.005	0.418	1 \approx
	b	15	20.25	10.60	8.29	209					
4	a	12	9.68	5.42	4.26	280	325	3374	0.005	0.096	1 \approx
	b	12	10.37	5.42	4.95	262					
5	a	11.5	8.52	4.77	3.75	292	339	2122	0.005	0.160	1 \approx
	b	11.5	9.13	4.77	4.36	273					
6	a	20	44.8	25.1	19.7	168	195	534	0.005	0.365	1 \approx
	b	20	48	25.1	22.9	157					
7	a	15	18.89	10.60	9.65	224	260	3010	0.005	0.086	1 \approx
	b	15	20.25	10.60	8.29	209					
8	a	15	18.89	10.60	9.65	224	260	8518	0.005	0.03	1 \approx
	b	15	20.25	10.60	8.29	209					

Table 5. Reformed diameter

Curve Number	1	2	3	4	5	6	7	8
Prime D_{50} Diameter(mm)	19.6	14	15	12	11.5	20	15	15
Removed Diameter	19	13	14	11	11	18	12.5	10

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