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Theoretical prediction on thickness distribution of cement paste among neighboring aggregates in concrete

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Abstract. By virtue of chord-length density function from the field of statistical physics, this paper introduced a quantitative approach to estimate the distribution of cement paste thickness between aggregates in concrete. Dynamics mixing method based on molecular dynamics was employed to generate one model structure, then image analysis algorithm was used to obtain the distribution of thickness of cement paste in model structure for the purpose of verification. By comparison of probability density curves and cumulative probability curves of the cement paste thickness among neighboring aggregates, it is found that the theoretical results are consistent with the simulation. Furthermore, for the model mortar and concrete mixtures with practical volume fraction of Fuller-type aggregate, this analytical formula was employed to predict the influence of aggregate volume fraction and aggregate fineness. And evolution of its mean values were also investigated with the variation of volume fraction of aggregate as well as the fineness of aggregates in model mortars and concretes.

Keywords: concrete; cement paste; particle size distribution; aggregate; probability density function; cumulative probability function.

1. Introduction

The spacing among inclusions (such as aggregates and fiber) is an important parameter to learn about the coalescence of initial micro-crack under loading (Choi and Shah 1999, Scrivener *et al.* 2004, Ayyar and Chawla 2006), overlapping between neighboring interfacial transition zones (ITZs) (Chen *et al.* 2004, 2006, 2005a), connectivity of ITZs around inclusions (Bentz *et al.* 1995, Scrivener and Netami 1996), although overestimation of actual ITZ by sectional analysis often happened in the literature (Chen *et al.* 2007). For instance, the core effect of inclusions at different scale levels, crack propagation and fracture energy dissipation are closely related to the inclusions spacing (Carpinteri *et al*. 2004, van Mier and Lilliu 2004). Besides, multi-scale modeling technique gradually becomes a commonly-used approach to study microstructure of materials and further to build the quantitative relationship between microstructure and macro-properties of materials (Raabe and Dierk 1998). However, the size of model at each scale-level should be set in a valid range. For

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the micro-model that focuses on the ITZ microstructure, the size of model should be set based on the actual surface spacing between aggregates in concrete. However, due to the opacity and 3-dimensional spatial distribution of constitutes of concrete, a few researchers have considered calculating the surface spacing of inclusions in concrete. Diamond *et al.* (1982) are pioneers investigating the spacing between aggregates in concrete. To get a general idea on the order of magnitude on the smallest separation between adjacent sand grains in realistic concrete, they manually measured SEM image of the polished surface of concrete slices. The results indicated that the mean value of the smallest surface spacing between neighboring aggregate particles in concrete slices ranged from 75 mm to 100 mm. They also noted that fineness of aggregate in concrete affected the results of mean surface spacing among aggregates, but no analytical formula is given. van Breugel (1991) mentioned that from straightforward stereological consideration, the average thickness of paste layer between the aggregate particles varies between 50~200 μm in concrete with aggregate percentage ranging from 75% to 80%. But he did not give the detail formula. Later, Koenders (1997) developed a "Ribbon Model" to quantitatively evaluate the influence of fineness of aggregate and volume fraction of aggregate on the mean surface spacing between neighboring aggregate grains. Unfortunately, this model was incorrect. As indicated by Chen *et al*. (2003), it did not consider the volume fraction of cement paste that is required to fill the void between aggregates. Then, Chen *et al*. (2003) developed a regular dodecahedron model to evaluate the influence of aggregate fineness as well as of the aggregate volume fraction on the mean surface spacing between neighboring aggregate grains. However, this regular dodecahedron model was based on the assumption of monosize aggregate particle system. It was only suitable for the system in which the volume fraction of aggregate was not greater than 75%, but the volume fraction of aggregate in normal concrete varied from 60% to 80%. Afterwards, Chen *et al.* (2005b), employed "mean free path" formula (Eq. (1)), proposed by Fullman (1953), to estimate the mean surface spacing among aggregates. The merit of such model was no special requirement on size, shape or volume fraction of aggregate. However, it was not possible to obtain the detail on the distribution of the surface spacing among

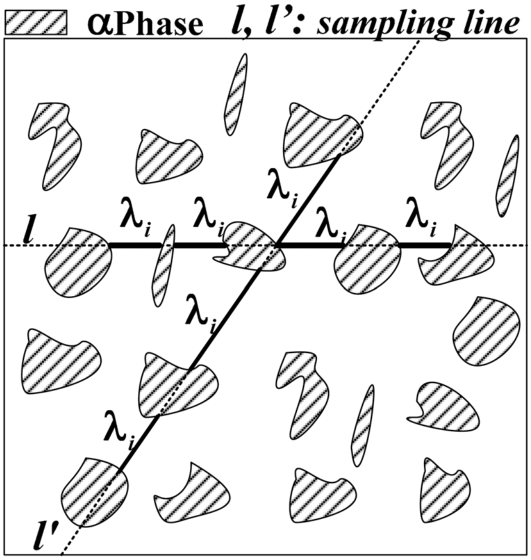


Fig. 1 Schematic diagram of mean free path of dispersed phase for two-phase composites

aggregate grains.

$$\lambda = 4(1-V_{agg})/S_{agg} \tag{1}$$

where, λ is the mean free path between particles (mm); it is defined as the mean edge-to-edge distance along a straight line between particles (in Fig. 1) (Underwood 1970); V_{agg} is volume fraction of aggregate in concrete; S_{agg} is the surface area of aggregate per unit volume of concrete (mm^{-1}).

It is worth mentioning that researchers (Yang *et al.* 2001) in the field of metal employed Dirichlet tessellation approach (Parse and Wert 1993) to obtain nearest-neighbor distance between particle centroids in 2D slice of sample. The mean nearest-neighbor distance minus the mean particle diameter may reflect the nearest-surface distance. This approach was also used in 3D case for concrete system (Hu *et al.* 2006, Stroeven *et al.* 2009). But it is still not possible to precisely obtain the detail on the influence of aggregate size distribution and aggregate volume fraction on the distribution of surface spacing among aggregate grains.

Therefore, if an approach is available to obtain the analytical solution on the distribution of the unobstructed surface spacing between aggregate grains (i.e. thickness of cement paste between aggregates), it will be very attractive. One of the chord-length density functions, proposed by Torquato (Torquato and Lu 1993), seems to provide a possible solution to such problem.

2. Description of theory

The chord-length density function, $p^{(i)}(x)$, is defined for statistically random isotropic media as follows

$p^{(i)}(x)dx$ = the probability of finding a chord of length between x and $x+dx$ in phase i of composites. (2)

where, chords are all of the line segments between intersections of an infinitely long line with the two phase interface (see λ_i in Fig. 1).

Since it is a probability density function (having dimensions of inverse length), $p^{(i)}(x) \geq 0$ for all x, and it normalizes to unity, i.e. $\int_0^\infty p^{(i)}dx = 1$. Thus, if the phase of interest is cement paste in concrete, x should be the intercept length between an infinitely long line and cement paste. At this moment, p(x) describes the probability density function of surface spacing among aggregate grains obtained by arbitrary sampling line, rather than probability density function of the nearest neighbor surface to surface spacing between aggregates (Chen *et al.* 2005c). In other words, $p(x)$ indicates probability density function of cement paste thickness obtain by arbitrary sampling line. Consequently, the first moment of $p(x)$ should be equal to the mean free path between aggregate particles given in Eq. (1).

According to Torquato's (Torquato and Lu 1993, Torquato 2004), for model cement based composites reinforced with multisize spherical aggregates in random equilibrium state, the probability density function of the aggregate surface spacing, $p(x)$, can be expressed as

$$p(x) = A\exp(-Ax) \tag{3}$$

where x is the cement paste thickness (mm), $A = 3V_{agg}\overline{R_N^2}/[4(1-V_{agg})\overline{R_N^3}]$, V_{agg} is the volume fraction of aggregate in concrete, $\overline{R_N^2}$ and $\overline{R_N^3}$ are the 2nd moment and the 3rd moment of the radius of aggregate, respectively.

Then, the cumulative probability function of the cement paste thickness, $P(x)$, is given by

$$P(x) = \int_0^x p(x)dx = 1 - \exp(-Ax) \tag{4}$$

And the mean thickness of the cement paste $\overline{t_p}$ is

$$\overline{t_p} = \int_0^\infty xp(x)dx = 1/A = [4(1-V_{agg})\overline{R_N^3}]/(3V_{agg}\overline{R_N^2}) \tag{5}$$

Noted that the total surface area of aggregate in per unit volume of concrete, S_{agg}, can be expressed as

$$S_{agg} = (3V_{agg}\overline{R_N^2})/\overline{R_N^3} \tag{6}$$

Therefore, Eq. (5) is the same as the aforementioned stereological formula (Eq. (1)) of the mean free path.

Based on Torquato's description (Torquato and Lu 1993, Torquato 2004), the only assumption of the model made from Eq. (3) to Eq. (6) is that all particles of concern should be impenetrable spheres.

3. Verification of theoretical solution

3.1 Generation of model structure

To verify the validity of the aforementioned theoretical formula, one dilute random structure is generated in cubic container with periodic boundaries (shown in Fig. 2). Afterwards, a dynamic mixing algorithm (Streoven 1999) is employed to compact this dilute structure. In this contribute, the volume fraction of solid in densified structure is equal to 65%, which falls in the practical volume fraction of aggregate (60%~80%) in actual concrete. The size distribution of aggregate is presented in Fig. 3. Other relative physical parameters of the target structures are listed in Table 1.

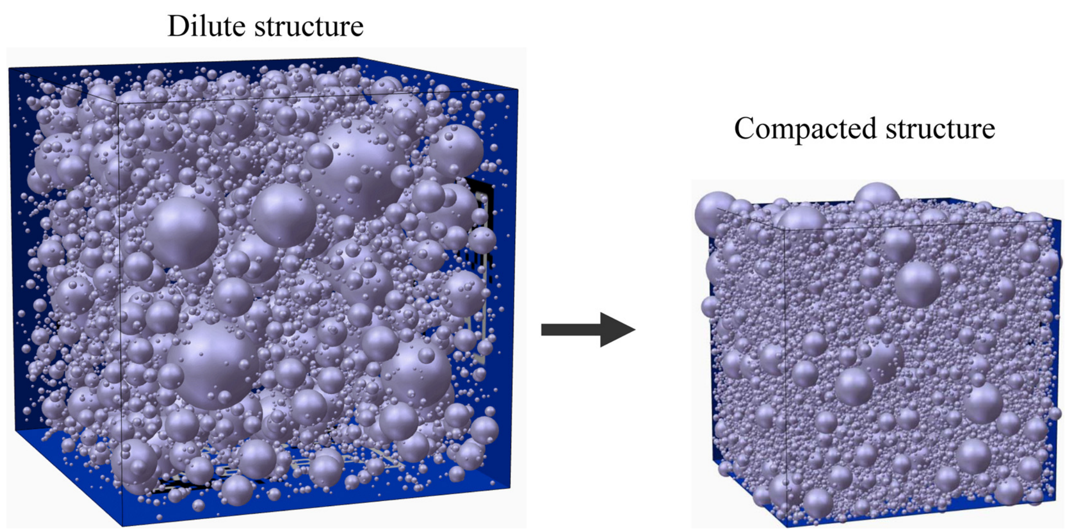


Fig. 2 Schematic diagram of spatial distribution of particles in cubic container with periodic boundary

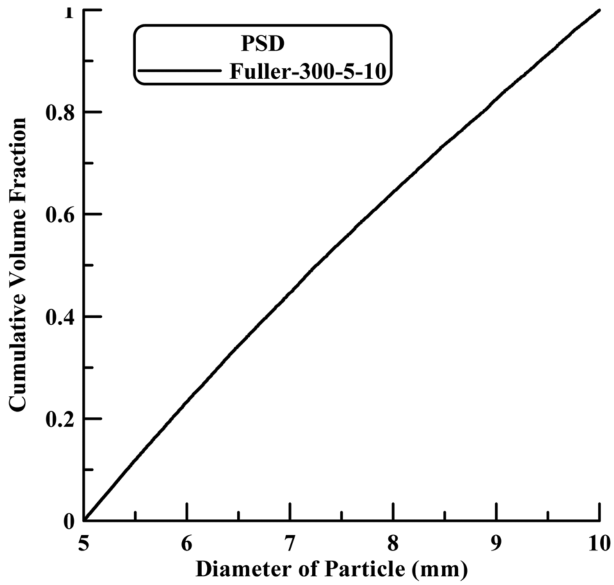


Fig. 3 Particle size distribution of aggregates in model structure

Table 1 Physical parameters of target structure

No.	Diameter/mm	Side length of cube/mm	V_{agg}	Number of particles
Fuller-300-5-10-65	5.0-10.0	233	65.0%	49903

3.2 Description of algorithm

Algorithm of serial section analysis is developed to acquire the statistical information on cement paste thickness between neighboring aggregate grains along a sampling line. The basic idea of serial section approach is to analysis slice by slice the 3D target structure. In each slice, the point of a feature will be identified as a certain type of subset (solid or void) and assigned a color. A systematic line sampling method is applied in the slice. Since the unobstructed spacing between particles is considered, only the length of line segment which located in region of void is recorded. This process yields information about cement paste thickness between circles along the scan line. The whole range of spacing is divided into a certain number of intervals by trial and error beforehand. Each length of such line segment will be assessed and put into the corresponding interval so as to obtain their probability distribution. The average thickness is estimated based on the number of all valid line segments as well as their lengths.

3.3 Verification

Apparently, reliability of result depends on the image resolution as well as the number of slices. Higher image resolution provides possibility to estimate smaller thickness. Larger number of slice may provide much more data for statistical purpose. But both of them will result in the increase of labor work. Since this section considers the accuracy of prediction by theoretical solution. It is necessary to investigate the influence of image resolution on the simulation result. Therefore, at

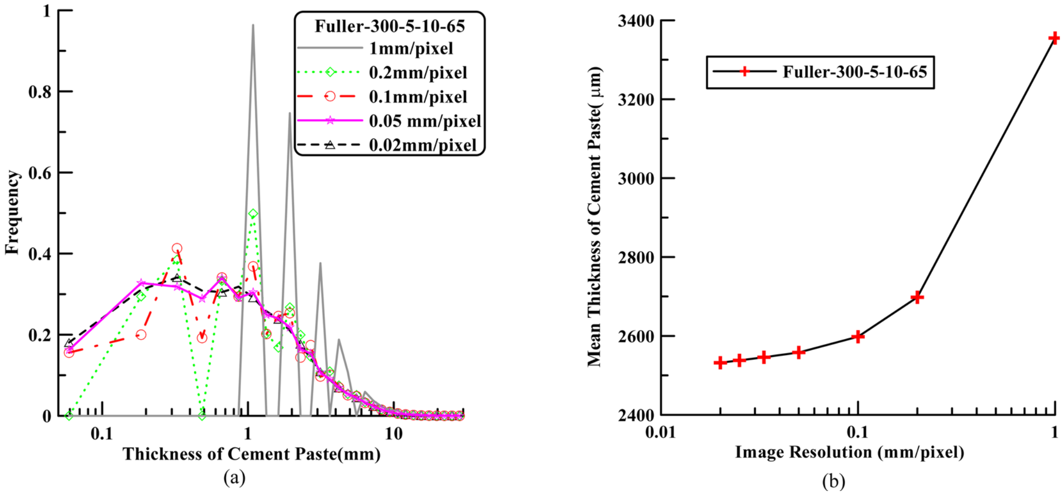


Fig. 4 Influence of image resolution on predicting precise of cement paste thickness

constant number of slices, seven different resolutions, (i.e.1 mm/pixel, 0.2 mm/pixel, 0.1 mm/pixel, 0.05 mm/pixel, 0.033 mm/pixel, 0.025 mm/pixel, 0.02 mm/pixel), are used on this model structure to investigate the influence of image resolution on predicting precision of cement paste thickness. The result is shown in Fig. 4. Fig. 4. (a) represents probability density curve; Fig. 4(b) displays the evolution of mean value of cement paste thickness.

Apparently, the prediction is more accurate with increasing image resolution. After image resolution reaches to 0.05 μm, there is no significant increase in the predicting precision with increasing resolution. Therefore, in this contribution, the image resolution of 0.02 mm/pixel and the slice thickness of 1 mm are imposed on the model structure given in Table 1.

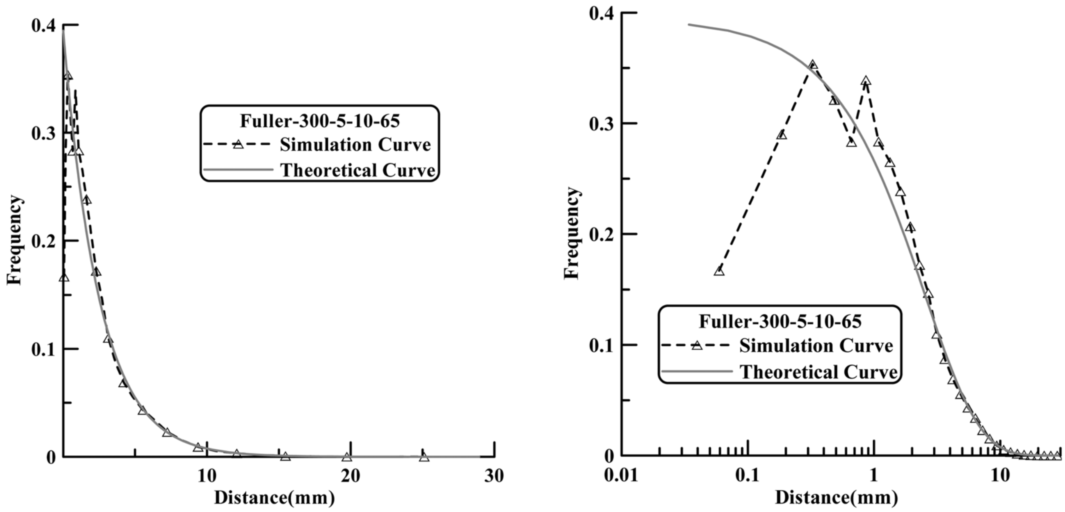
To obtain the distribution curve of cement paste thickness, it is necessary to specify the dividing rule of intervals, the latter should be fixed. Since the probability of occurrence is higher for smaller than for larger cement paste thickness, the partitioning rule given in Eq. (7) will be used for all model structures as well as in the theoretical derivation.

$$x_i = \left(2^{i\times\left(\frac{5.0}{M}\right)} - 1.0\right)\frac{x_{max}-x_{min}}{(2^{5.0}-1.0)} + x_{min}, \qquad 0 \le i \le M \tag{7}$$

where $\Delta x_i = x_{i+1} - x_i$, $x_i \in [x_{min}, x_{max}]$, $x_0 = x_{min}$, $x_M = x_{max}$, $i = 0, 1, \ldots, M$; M is the number of intervals ($M = 30$).

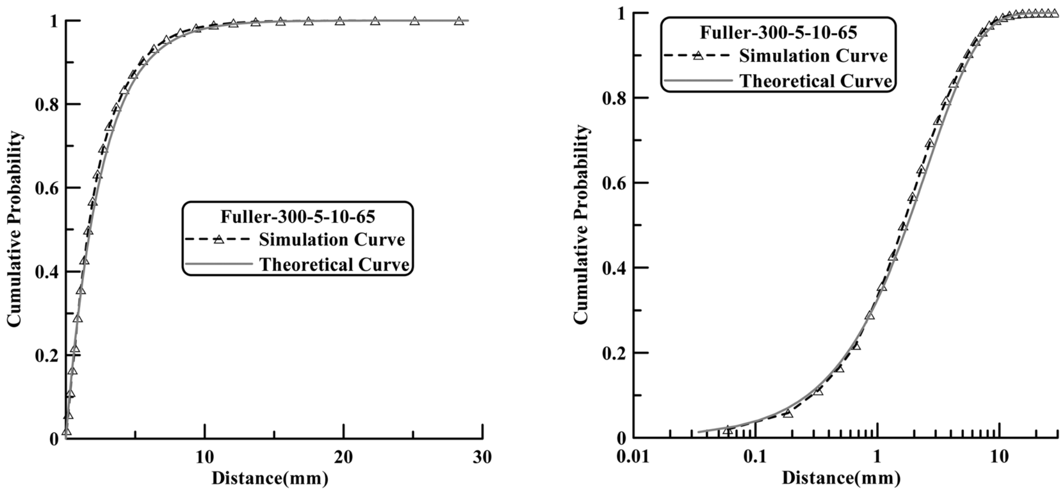
Comparison between simulation and theoretical result is shown in Fig. 5, Fig. 6 and Table 2. Fig. 5 displays the probability density curve of cement paste thickness. Fig. 6 gives the cumulative probability curve. Table 2 lists statistical mean value. The difference between Fig. 5(a) and Fig. 5(b) is that Fig. 5(a) has a linear scale, whereas a logarithmic scale ($\log_{10}$ basis) is used in Fig. 5(b). The purpose of Fig. 5(b) is to clearly show the variation of curves for smaller cement paste thickness, while the linear horizontal axis of Fig. 5(a) more clearly reveals the variations among larger cement paste thickness. The same purpose holds for Fig. 6.

Fig. 5(a) indicates that the theoretical solution give a pretty good prediction for the larger cement paste thickness. For the very smaller surface spacings (Fig. 5(b)), it does not predict well. The "very



(a) (b)

Fig. 5 Probability density curve of cement paste thickness



(a) (b)

Fig. 6 Cumulative probability curve of cement paste thickness

Table 2 Mean value of cement paste thickness

Simulated value (mm)	Theoretical value (mm)	Error*
2.532	2.534	-0.08%

Error = 100×(theoretical value-simulated value)/theoretical value

smaller cement paste thickness" is actually a relative concept, which is derived based on the comparison of cement paste thickness with bad prediction to the mean value in Table 2. Since the percentage of smaller cement paste thickness occupy only small part in cumulative probability curves of Fig. 6, it does not cause serious effect on accuracy of prediction in cumulative probability curve. This viewpoint can find support from the comparison of mean value of cement paste thickness (Table 2). Beside, one may notice that the degree of correspondence between theoretical and simulation results is better for the cumulative probability curves (Fig. 6) than for the probability density curves (Fig. 5). This is due to "frequency" being more sensitive than "cumulative probability" to the variation of structure (Freudenthal 1950).

As a whole, the theoretical solutions may provide accurate approximation on the distribution of cement paste thickness between aggregate particles in concrete. Therefore, they can be employed to predict the distribution of cement paste thickness in practical cementitious materials.

4. Application

Generally speaking, the aggregate gradation of real mortar/concrete varies significantly. And the particle of aggregate is not exactly sphere. To apply the model as shown in Eq. (3) to predict the distribution of cement paste thickness in actually concrete, the particle will be simplified as spherical particle. In addition, the number-based 2nd moment ($\overline{R_N^2}$), the number-based 3rd moment ($\overline{R_N^3}$) of the radius of aggregate required by Eq. (3) should be calculated.

Normally, the sieve analysis test is used to characterize the weight-based particle size distribution curve of aggregate. Then, the volume fraction of the particles per fraction can be determined by dividing the weight fraction by the specific density of the aggregate particle. The number of particles per fraction can be further determined by dividing the aggregate volume of a fraction by the volume of a single particle of that particular fraction. In the end, it is easy to obtain the number-based 2nd moment ($\overline{R_N^2}$), the number-based 3rd moment ($\overline{R_N^3}$) of the radius of aggregate required by Eq. (3), and further to obtain the distribution of cement paste thickness in actual mortar/concrete.

Since Fuller function (Eq. (8)) is a common-used formula to represent the particle size distribution of aggregates in actual concrete (Walraven 1980, Zheng 2000), as an example, the section will employ it to predict the distribution of cement paste thickness in model mortars and concretes with Fuller-type aggregate.

$$F_V(D) = \frac{D^{\frac{1}{2}} - D_{min}^{\frac{1}{2}}}{D_{max}^{\frac{1}{2}} - D_{min}^{\frac{1}{2}}} \tag{8}$$

where $F_V(D)$ is the volume based cumulative distribution function of aggregate, D is the diameter of aggregate grain (mm), D_{max} is the maximum diameter of aggregate grain (mm), and D_{min} is the minimum diameter of aggregate grain (mm).

Based on Eq. (4), the cumulative probability curves of the cement paste thickness in same type of model mortars and concretes are given in Fig. 7. The variation of mean value of cement paste thickness can be calculated according to Eq. (5) with the volume fraction and fineness of aggregate. The results are displayed in Fig. 8.

For the model mortars, Fig. 7(a) reveals that if 2.5% located in the lower bound and upper bound is ignored, major part of the distribution curve of cement paste thickness varies from 0.02~2 mm to 0.006~0.5 mm when the volume fraction of aggregate increase from 40% to 70%. Whereas, for the model concretes with coarser aggregate (Fig. 7(d)), the dominant portion of the distribution curve of

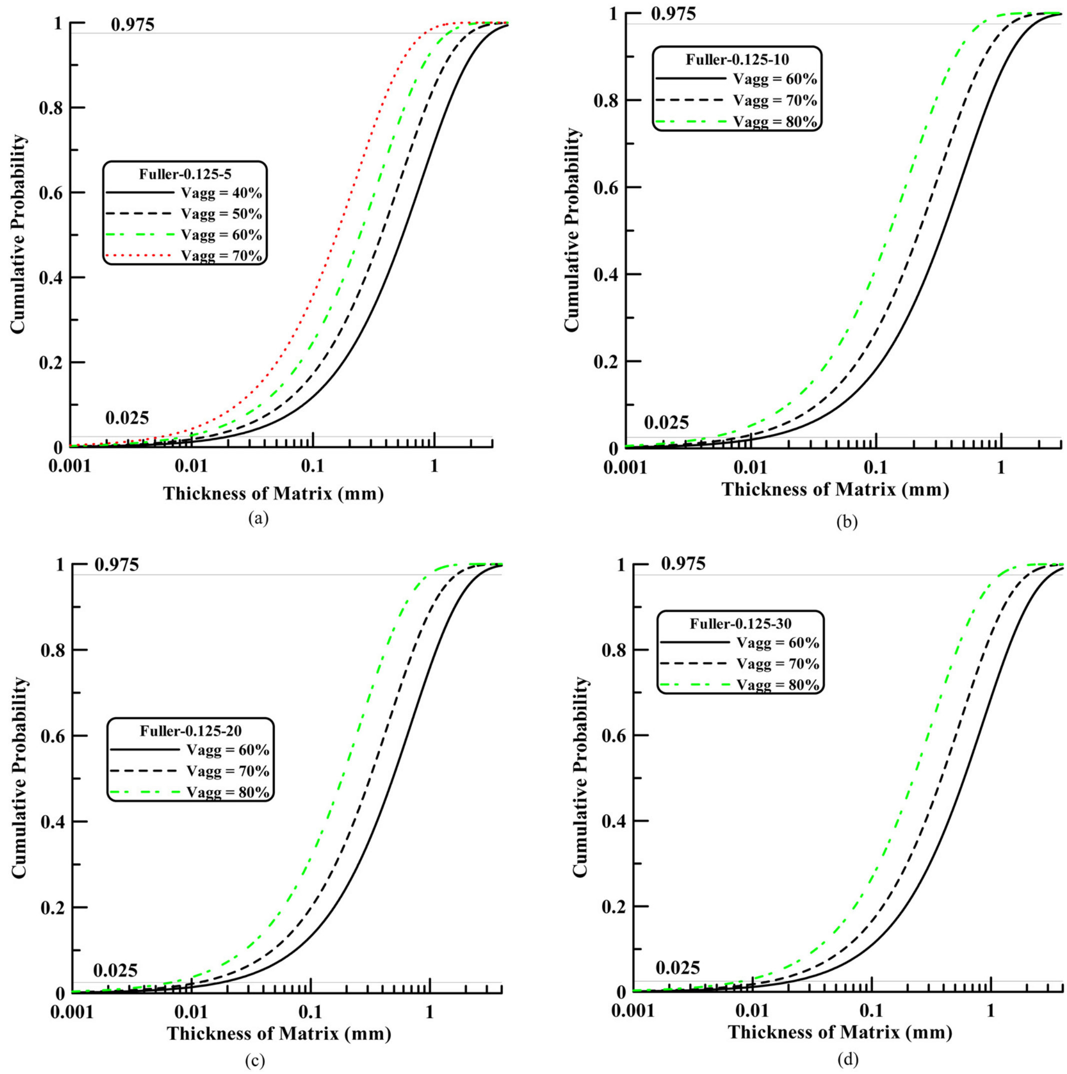


Fig. 7 Influence of volume fraction of aggregate on the cumulative probability curve of cement paste thickness in model mortars and concretes

cement paste thickness varies from 0.02~3 mm to 0.08~1 mm with the increasing volume fraction of aggregate. Major fraction of surface spacing occurs in the range of 0.01~1.5 mm. Further, Fig. 8 indicates that the mean value of cement paste thickness varies from ~190 μm to ~860 μm. At constant volume fraction of aggregate, the increase of aggregate fineness will lead to the decrease in mean value of cement paste thickness.

5. Comparison with other models

It is worth noting that many models for predictions of paste thickness of concrete have been reported in the literature, such as mean free path model (Fullman 1953, Chen *et al.* 2005b), regular dodecahedron model (Chen *et al.* 2003), ribbon model (Koenders 1997), nearest-neighbor surface distance model $\overline{\Delta_{3S}}$ (Delta_3S model, Underwood 1968, Hu *et al.* 2006, Stroeven *et al.* 2009), nearest neighbor surface-to surface spacing model (NNS2S spacing model, Chen *et al.* 2005c, Chen *et al.* 2005d), etc. So, it is necessary to make a comparison between these models and the chord-length model proposed in this paper.

As mentioned in the last paragraph of Section 2, mean value of cement paste thickness obtained based on chord-length model is exactly the same as that derived from mean free path model. The only difference between them is that chord-length model may obtain the distribution of cement paste thickness, but mean free path model can not. So, the results derived from regular dodecahedron model (Chen *et al.* 2003), Ribbon model (Koenders 1997), Delta_3S model $\overline{\Delta_{3S}}$ (Underwood 1968, Hu *et al.* 2006, Stroeven *et al.* 2009) and NNS2S spacing model (Chen *et al.* 2005c, Chen *et al.* 2005d) will be compared with that from chord-length model developed in this contribution.

For the sake of convenience, the Fuller distribution function (shown in Eq. (8)) will still be used for the comparison purpose. And the maximum and minimal diameter of particle is fixed as 20 mm and 0.125 mm, respectively. The results of mean cement paste thickness versus volume fraction of aggregate based on different models are given in Fig. 9. It can be found from Fig. 9 that none of curves based on the models in the literature is consistent with that from our model. The possible reason is analyzed as follows:

(1) In regular dodecahedron model, the whole concrete is assumed as a monosize dodecahedral composite particle packing system. The arbitrary dodecahedral composite particle consists of a monosize spherical aggregate particle and a cement paste layer. Such assumption definitely leads to the volume fraction of aggregate not greater than 74.05%. In addition, the thickness of cement paste

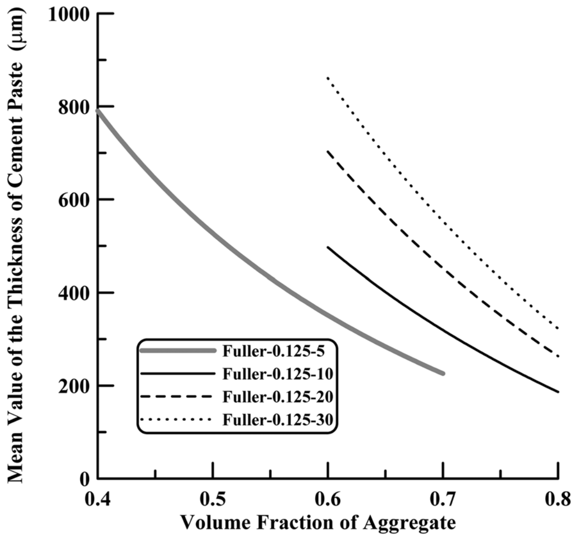


Fig. 8 Influence of volume fraction and fineness of aggregate on cement paste thickness in model mortars and concretes

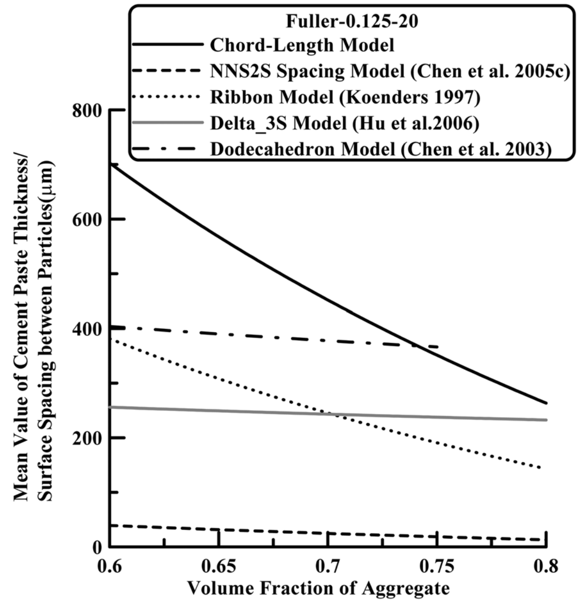


Fig. 9 Comparison of mean values of cement paste thickness based on different models

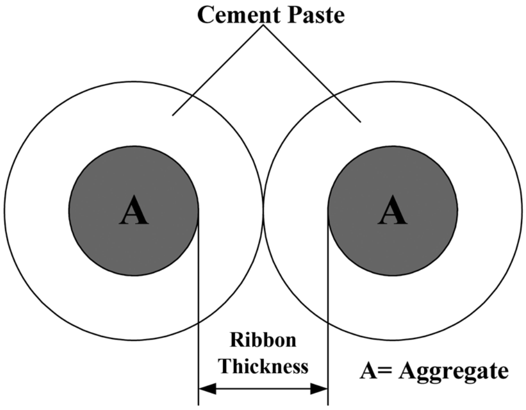


Fig. 10 Schematical representation of ribbon thickness between two aggregate particles (redraw from Koenders 1997)

derived from dodecahedron model is actually the nearest neighboring surface spacing between monosize spherical aggregates which strictly follow regular dodecahedron packing pattern. However, the chord-length model or mean free path model actually employs random sampling line to obtain the thickness of cement paste. That is the reason why the mean value of cement paste thickness from dodecahedron model is smaller than that from our model.

(2) Ribbon model (Koenders 1997) employed Eq. (9) and Fig. 10 to calculate the thickness of cement paste. In Fig. 10, the whole concrete is also assumed as a monosize spherical composite particle packing system. The spherical composite particle is composed of a monosize spherical aggregate core and a spherical cement paste shell. According to Fig. 10, the Ribbon model seems to get the nearest neighboring surfaces spacing between spherical aggregate particles. So, the value obtained from Ribbon Model must be smaller than that from our model. Moreover, it is noted in Fig. 9 that if all cement paste is used to cover the spherical aggregate particle, no extra paste is available to fill the void between these monosize spherical composite particles. Then, volume of aggregate plus volume of cement paste will be not equal to volume of concrete. Probably, the Ribbon Model does not correctly predict the thickness of cement paste in concrete.

$$R_t = \frac{2V_P}{S_{agg}} = \frac{2(1-V_{agg})}{S_{agg}} \tag{9}$$

where R_t is ribbon thickness (i.e. thickness of cement paste) in concrete, V_P is volume fraction of cement paste, V_{agg} is volume fraction of aggregate, S_{agg} is the total specific surface of the aggregates particles in the concrete mix.

(3) The Delta_3S model originated from the formula (as shown in Eq. (10a)) for calculation of average distance between nearest-neighbor pairs of point particles which are dilutedly dispersed in a test volume (Underwood 1970, Hu *et al.* 2006). Then, $\overline{\Delta_3}$ minus average diameter of aggregates (as shown in Eq. (10b)) reflects nearest surface spacing between aggregates. Strictly speaking, Eq. (10a) only pertains to dilutely dispersed point particles. Therefore, if the volume fraction of particles is high enough and the size of particle is not small enough, the reliability of Eq. (10b) probably needs to verify beforehand.

$$\overline{\Delta_3} = 0.554\frac{1}{\sqrt[3]{N_V}} = 0.554\sqrt[3]{\frac{\pi}{6V_{agg}}\overline{D_N^3}} = 0.446\sqrt[3]{\frac{\overline{D_N^3}}{V_{agg}}} \tag{10a}$$

where N_V is the total number of aggregate particle in unit volume of concrete, $\overline{D_N^3}$ is the number based 3rd moment of the diameter of aggregate.

$$\overline{\Delta_{3S}} = \overline{\Delta_3} - \overline{D_N} \tag{10b}$$

where $\overline{\Delta_{3S}}$ is average surface distance between nearest-neighbor particles of certain size distribution, $\overline{D_N}$ is number-based average diameter of aggregate.

(4) According to Chen *et al*. (2005c, 2005d), if the particle size distribution and volume fraction of aggregate is available, the NNS2S spacing model is actually used to predict the nearest neighboring surface-to-surface spacing between spherical aggregates in concrete. It is the reason why the value of mean value based on the NNS2S spacing model is much smaller than that from chord-length model developed in this paper.

In summary, combination of chord-length model with NNS2S spacing model may provide a potential tool for the study of microstructure and property of concrete.

6. Conclusions

An analytical formulation for the distribution of cement paste thickness between neighboring aggregate particles in arbitrary section plane of concrete is developed based on one of the chord-length density functions given by Torquato. A comparison between theoretical solutions and simulation results demonstrated that the analytical approach may satisfactorily predict the distribution of cement paste thickness between neighboring aggregate particles. Therefore, this theoretical formulation, together with the nearest neighboring surface-to-surface spacing model (Chen *et al.*2005c, Chen *et al.* 2005d) may provide a potential tool for the study of microstructure and property of concrete.

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